Differential operators in Cartesian coordinates

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Here we discuss the differential operators for the Cartesian coordinates with the use of Mathematica. To this end. we use the problems of Goswami (quantum mechanics) and Binney and Skipper (quantum mechanics).

1. Cartesian coordinates (Mathematica))

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

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

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

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

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

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

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

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

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

$$LP \rightarrow L_x + iL_y$$

$$LM \rightarrow L_x - iL_y$$

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

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

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

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

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

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

$$p_r \rightarrow \frac{1}{2}(\frac{\mathbf{r}}{r} \cdot \mathbf{p} + \mathbf{p} \cdot \frac{\mathbf{r}}{r})$$

$$\mathbf{r} \rightarrow x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z$$

$$R \rightarrow \sqrt{x^2 + y^2 + z^2}\ .$$

((**Mathematica**)) Differential operators in Cartesian coordinates

```
Clear["Global`"];
ux = {1, 0, 0};
uy = {0, 1, 0};
uz = {0, 0, 1};
r = {x, y, z};
R = √(r.r) ;
L := (-ⅈ ℏ (Cross[r, Grad[#, {x, y, z}, "Cartesian"]]) &) // Simplify;
p = (-ⅈ ℏ Grad[#, {x, y, z}, "Cartesian"] &) // Simplify;
Lx := (ux.L[#]) &;
Ly := (uy.L[#]) &;
Lz := (uz.L[#]) &;
px := (ux.p[#]) &;
py := (uy.p[#]) &;
pz := (uz.p[#]) &;
Lap := Laplacian[#, { x, y, z}, "Cartesian"] &;
Gra := Grad[#, { x, y, z}, "Cartesian"] &;
Cur := Curl[#, {x, y, z}, "Cartesian"] &;
Diva := Div[#, {x, y, z}, "Cartesian"] &;
prq := (-ⅈ ℏ) 1/2 (r/R.Gra[#] + Diva[r/R #]) &;
Lsq := (Nest[Lx, #, 2] + Nest[Ly, #, 2] + Nest[Lz, #, 2]) &;
```

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2. Commutation relation (I)

Show that

$$\left[\hat{L}_i, \hat{x}_j\right] = i\hbar \sum_{k,} \varepsilon_{ijk} \hat{x}_k \qquad \text{(formula)}$$

((**Proof**))

$$\begin{aligned}
\left[\hat{L}_i, \hat{x}_j\right] &= \sum_{k,l} \varepsilon_{ikl} \left[\hat{x}_k \hat{p}_l, \hat{x}_j\right] \\
&= \sum_{k,l} \varepsilon_{ikl} (\hat{x}_k \hat{p}_l \hat{x}_j - \hat{x}_j \hat{x}_k \hat{p}_l) \\
&= \sum_{k,l} \varepsilon_{ikl} (\hat{x}_k \hat{p}_l \hat{x}_j - \hat{x}_k \hat{x}_j \hat{p}_l) \\
&= \sum_{k,l} \varepsilon_{ikl} \hat{x}_k [\hat{p}_l, \hat{x}_j] \\
&= -i\hbar \sum_{k,l} \varepsilon_{ikl} \hat{x}_k \delta_{lj} \\
&= i\hbar \sum_{k,l} \varepsilon_{ilk} \hat{x}_k \delta_{lj}
\end{aligned}$$

where ε_{ijk} is the Levi-Civita coefficient; $\varepsilon_{ikj} = -\varepsilon_{ilk}$. Thus, we have

$$\left[\hat{L}_i, \hat{x}_j\right] = i\hbar \sum_{k,} \varepsilon_{ijk} \hat{x}_k$$

Using this relation, we get

$$\left[\hat{L}_x, \hat{x}\right] = 0, \qquad \left[\hat{L}_x, \hat{y}\right] = i\hbar \hat{z}, \qquad \left[\hat{L}_x, \hat{z}\right] = -i\hbar \hat{y}$$

$$\left[\hat{L}_y, \hat{x}\right] = -i\hbar \hat{z}, \qquad \left[\hat{L}_y, \hat{y}\right] = 0, \qquad \left[\hat{L}_y, \hat{z}\right] = i\hbar \hat{x}$$

$$\left[\hat{L}_z, \hat{x}\right] = i\hbar \hat{z}, \qquad \left[\hat{L}_z, \hat{y}\right] = -i\hbar \hat{x}, \qquad \left[\hat{L}_z, \hat{z}\right] = 0$$

((**Mathematica**))

We show that the differential operators satisfy

$$\left[L_x, x\right] = 0, \qquad \left[L_x, y\right] = i\hbar z, \qquad \left[L_x, z\right] = -i\hbar y$$

Using Mathematica.

```
eq1 = Lx[x ψ[x, y, z]] - x Lx[ψ[x, y, z]] // Simplify

0

eq2 = Lx[y ψ[x, y, z]] - y Lx [ψ[x, y, z]] -
   ⅈ ℏ z ψ[x, y, z] // FullSimplify

 0

eq3 =
 Lx[z ψ[x, y, z]] - z Lx[ψ[x, y, z]] +
   ⅈ y ℏ ψ[x, y, z] // Simplify
```

3 Commutation relation (II)

$$\left[\hat{\boldsymbol{L}}^2, \hat{x}_k\right] = -i\hbar \sum_{i,j} \varepsilon_{ijk} (\hat{L}_i \hat{x}_j + \hat{x}_j \hat{L}_i) \qquad \text{(formula)}$$

((**Proof**))

$$\hat{\boldsymbol{L}}^2 = \hat{L}_x{}^2 + \hat{L}_y{}^2 + \hat{L}_z{}^2$$

$$\begin{aligned}\left[\hat{L}_i{}^2, \hat{x}_j\right] &= \hat{L}_i \hat{L}_i \hat{x}_j - \hat{x}_j \hat{L}_i \hat{L}_i \\ &= \hat{L}_i (\hat{L}_i \hat{x}_j - \hat{x}_j \hat{L}_i) + (\hat{L}_i \hat{x}_j \hat{L}_i - \hat{x}_j \hat{L}_i \hat{L}_i) \\ &= \hat{L}_i \left[\hat{L}_i, \hat{x}_j\right] + \left[\hat{L}_i, \hat{x}_j\right] \hat{L}_i \\ &= i\hbar \sum_k \varepsilon_{ijk} (\hat{L}_i \hat{x}_k + \hat{x}_k \hat{L}_i)\end{aligned}$$

or

$$\left[\hat{L}_1{}^2, \hat{x}_j\right] = i\hbar \sum_k \varepsilon_{1jk} (\hat{L}_1 \hat{x}_k + \hat{x}_k \hat{L}_1)$$

$$\left[\hat{L}_2{}^2, \hat{x}_j\right] = i\hbar \sum_k \varepsilon_{2jk} (\hat{L}_2 \hat{x}_k + \hat{x}_k \hat{L}_2)$$

$$\left[\hat{L}_3{}^2, \hat{x}_j\right] = i\hbar \sum_k \varepsilon_{3jk} (\hat{L}_3 \hat{x}_k + \hat{x}_k \hat{L}_3)$$

Then we get

$$\begin{aligned}\left[\hat{\boldsymbol{L}}^2, \hat{x}_k\right] &= \left[\hat{L}_1{}^2, \hat{x}_k\right] + \left[\hat{L}_2{}^2, \hat{x}_k\right] + \left[\hat{L}_3{}^2, \hat{x}_k\right] \\ &= i\hbar\sum_j \varepsilon_{1kj}(\hat{L}_1\hat{x}_j + \hat{x}_j\hat{L}_1) + i\hbar\sum_k \varepsilon_{2kj}(\hat{L}_2\hat{x}_j + \hat{x}_j\hat{L}_2) \\ &\quad + i\hbar\sum_j \varepsilon_{3kj}(\hat{L}_3\hat{x}_j + \hat{x}_j\hat{L}_3) \\ &= i\hbar\sum_{i,j} \varepsilon_{ikj}(\hat{L}_i\hat{x}_j + \hat{x}_j\hat{L}_i) \\ &= -i\hbar\sum_{i,j} \varepsilon_{ijk}(\hat{L}_i\hat{x}_j + \hat{x}_j\hat{L}_i)\end{aligned}$$

or

$$\left[\hat{\boldsymbol{L}}^2, \hat{x}_k\right] = -i\hbar\sum_{i,j} \varepsilon_{ijk}(\hat{L}_i\hat{x}_j + \hat{x}_j\hat{L}_i)$$

We have the following relations with differential operators.

$$\begin{aligned}\left[\boldsymbol{L}^2, x\right] &= -i\hbar\varepsilon_{231}(L_2x_3 + x_3L_2) - i\hbar\varepsilon_{321}(L_3x_2 + x_2L_3) \\ &= -i\hbar(L_y z + zL_y) + i\hbar(L_z y + yL_z)\end{aligned}$$

$$\left[\boldsymbol{L}^2, y\right] = -i\hbar(L_z x + xL_z) + i\hbar(L_x z + zL_x)$$

$$\left[\boldsymbol{L}^2, z\right] = -i\hbar(L_x y + yL_x) + i\hbar(L_y x + xL_y)$$

((**Mathematica**))

```
eq1 = Lsq[x ψ[x, y, z]] - x Lsq[ ψ[x, y, z]] +
   i ℏ (Ly[z ψ[x, y, z]] + z Ly[ ψ[x, y, z]]) -
   i ℏ (Lz[y ψ[x, y, z]] + y Lz[ψ[x, y, z]]) // FullSimplify

0

eq2 = Lsq[y ψ[x, y, z]] - y Lsq[ ψ[x, y, z]] +
   i ℏ (Lz[x ψ[x, y, z]] + x Lz[ ψ[x, y, z]]) -
   i ℏ (Lx[z ψ[x, y, z]] + z Lx[ψ[x, y, z]]) // FullSimplify

0

eq3 = Lsq[z ψ[x, y, z]] - z Lsq[ ψ[x, y, z]] +
   i ℏ (Lx[y ψ[x, y, z]] + y Lx[ ψ[x, y, z]]) -
   i ℏ (Ly[x ψ[x, y, z]] + x Ly[ψ[x, y, z]]) //
  FullSimplify

0
```

4. Commutation relation (III)

$$[\hat{\boldsymbol{L}}^2, [\hat{\boldsymbol{L}}^2, \hat{x}_k]] = 2\hbar^2(\hat{\boldsymbol{L}}^2\hat{x}_k + \hat{x}_k\hat{\boldsymbol{L}}^2) \qquad \text{(formula)}$$

((**Proof**))

$$[\hat{\boldsymbol{L}}^2, [\hat{\boldsymbol{L}}^2, \hat{x}_k]] = -i\hbar\sum_{i,j}\varepsilon_{ijk}[\hat{\boldsymbol{L}}^2, (\hat{L}_i\hat{x}_j + \hat{x}_j\hat{L}_i)]$$

with

$$\begin{aligned}
[\hat{\boldsymbol{L}}^2, \hat{L}_i\hat{x}_j] &= \hat{\boldsymbol{L}}^2\hat{L}_i\hat{x}_j - \hat{L}_i\hat{x}_j\hat{\boldsymbol{L}}^2 \\
&= \hat{L}_i\hat{\boldsymbol{L}}^2\hat{x}_j - \hat{L}_i\hat{x}_j\hat{\boldsymbol{L}}^2 \\
&= \hat{L}_i[\hat{\boldsymbol{L}}^2, \hat{x}_j] \\
&= (-i\hbar)\hat{L}_i\sum_{l,m}\varepsilon_{lmj}(\hat{L}_l\hat{x}_m + \hat{x}_m\hat{L}_l) \\
&= (-i\hbar)\sum_{l,m}\varepsilon_{lmj}(\hat{L}_i\hat{L}_l\hat{x}_m + \hat{L}_i\hat{x}_m\hat{L}_l)
\end{aligned}$$

and

$$
\begin{aligned}
[\hat{\boldsymbol{L}}^2, \hat{x}_j \hat{L}_i] &= \hat{\boldsymbol{L}}^2 \hat{x}_j \hat{L}_i - \hat{x}_j \hat{L}_i \hat{\boldsymbol{L}}^2 \\
&= \hat{\boldsymbol{L}}^2 \hat{x}_j \hat{L}_i - \hat{x}_j \hat{\boldsymbol{L}}^2 \hat{L}_i \\
&= [\hat{\boldsymbol{L}}^2, \hat{x}_j] \hat{L}_i \\
&= (-i\hbar) \sum_{l,m} \varepsilon_{lmj} (\hat{L}_l \hat{x}_m \hat{L}_i + \hat{x}_m \hat{L}_l \hat{L}_i)
\end{aligned}
$$

Using the above relations, we get

$$
\begin{aligned}
[\hat{\boldsymbol{L}}^2, \left[\hat{\boldsymbol{L}}^2, \hat{x}_k\right] &= (-i\hbar)^2 \sum_{i,j,l,m} \varepsilon_{ijk} \varepsilon_{lmj} (\hat{L}_i \hat{L}_l \hat{x}_m + \hat{L}_i \hat{x}_m \hat{L}_l + \hat{L}_l \hat{x}_m \hat{L}_i + \hat{x}_m \hat{L}_l \hat{L}_i) \\
&= \hbar^2 \sum_{i,j,l,m} \varepsilon_{ikj} \varepsilon_{lmj} (\hat{L}_i \hat{L}_l \hat{x}_m + \hat{L}_i \hat{x}_m \hat{L}_l + \hat{L}_l \hat{x}_m \hat{L}_i + \hat{x}_m \hat{L}_l \hat{L}_i)
\end{aligned}
$$

with

$$
\varepsilon_{ijk} \varepsilon_{lmj} = -\varepsilon_{jik} \varepsilon_{jlm}
$$

Using the formula for the Levi-Civita

$$
\sum_j \varepsilon_{jik} \varepsilon_{jlm} = \delta_{il} \delta_{km} - \delta_{im} \delta_{kl}
$$

we have

$$
\begin{aligned}
[\hat{\boldsymbol{L}}^2, \left[\hat{\boldsymbol{L}}^2, \hat{x}_k\right] &= \hbar^2 \sum_{i,l,m} (\delta_{il} \delta_{km} - \delta_{im} \delta_{kl}) (\hat{L}_i \hat{L}_l \hat{x}_m + \hat{L}_i \hat{x}_m \hat{L}_l + \hat{L}_l \hat{x}_m \hat{L}_i + \hat{x}_m \hat{L}_l \hat{L}_i) \\
&= \hbar^2 \sum_i [(\hat{L}_i \hat{L}_i \hat{x}_k + \hat{x}_k \hat{L}_i \hat{L}_i + \hat{L}_i \hat{x}_k \hat{L}_i + \hat{L}_i \hat{x}_k \hat{L}_i) - (\hat{L}_i \hat{L}_k \hat{x}_i + \hat{L}_i \hat{x}_i \hat{L}_k + \hat{L}_k \hat{x}_i \hat{L}_i + \hat{x}_i \hat{L}_k \hat{L}_i)] \\
&= \hbar^2 (\hat{\boldsymbol{L}}^2 \hat{x}_k + \hat{x}_k \hat{\boldsymbol{L}}^2) + \hbar^2 \sum_{i,i} (\hat{L}_i \hat{x}_k \hat{L}_i + \hat{L}_i \hat{x}_k \hat{L}_i) - \hbar^2 \sum_i (\hat{L}_i \hat{L}_k \hat{x}_i + \hat{L}_i \hat{x}_i \hat{L}_k + \hat{L}_k \hat{x}_i \hat{L}_i + \hat{x}_i \hat{L}_k \hat{L}_i)] \\
&= 2\hbar^2 (\hat{\boldsymbol{L}}^2 \hat{x}_k + \hat{x}_k \hat{\boldsymbol{L}}^2) - i\hbar^3 \sum_{i,l} \varepsilon_{ikl} [\hat{L}_i, \hat{x}_l] - \hbar^2 \sum_i (\hat{L}_i \hat{L}_k \hat{x}_i + \hat{L}_i \hat{x}_i \hat{L}_k + \hat{L}_k \hat{x}_i \hat{L}_i + \hat{x}_i \hat{L}_k \hat{L}_i)] \\
&= 2\hbar^2 (\hat{\boldsymbol{L}}^2 \hat{x}_k + \hat{x}_k \hat{\boldsymbol{L}}^2)
\end{aligned}
$$

(a)

$$\left[\hat{L}_i,\hat{x}_k\right]=i\hbar\sum_l \varepsilon_{ikl}\hat{x}_l\,,\qquad\qquad \left[\hat{L}_k,\hat{x}_i\right]=i\hbar\sum_l \varepsilon_{kil}\hat{x}_l$$

or

$$\hat{L}_i\hat{x}_k-\hat{x}_k\hat{L}_i=i\hbar\sum_l \varepsilon_{ikl}\hat{x}_l$$

(b)

$$\begin{aligned}\hat{L}_i\hat{x}_k\hat{L}_i+\hat{L}_i\hat{x}_k\hat{L}_i&=\hat{L}_i[\hat{L}_i\hat{x}_k-i\hbar\sum_l \varepsilon_{ikl}\hat{x}_l]+[\hat{x}_k\hat{L}_i+i\hbar\sum_l \varepsilon_{ikl}\hat{x}_l]\hat{L}_i\\&=\hat{L}_i\hat{L}_i\hat{x}_k+\hat{x}_k\hat{L}_i\hat{L}_i+\hbar^2\sum_{l,m}\varepsilon_{ikl}\varepsilon_{ilm}\hat{x}_m\end{aligned}$$

(d)

$$\begin{aligned}\sum_i(\hat{L}_i\hat{x}_k\hat{L}_i+\hat{L}_i\hat{x}_k\hat{L}_i)&=\sum_i\{\hat{L}_i\hat{L}_i\hat{x}_k+\hat{x}_k\hat{L}_i\hat{L}_i-i\hbar\sum_{i,l}\varepsilon_{ikl}[\hat{L}_i,\hat{x}_l]\}\\&=\hat{\boldsymbol{L}}^2\hat{x}_k+\hat{x}_k\hat{\boldsymbol{L}}^2+\hbar^2\sum_{i,l,m}\varepsilon_{ikl}\varepsilon_{ilm}\hat{x}_m\end{aligned}$$

(d)

$$\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{r}}=\sum_i \hat{L}_i\hat{x}_i=0\,,\qquad \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{L}}\cdot=\sum_i \hat{x}_i\hat{L}_i=0$$

So we need to show that

$$-i\hbar^3\sum_{i,l}\varepsilon_{ikl}[\hat{L}_i,\hat{x}_l]-\hbar^2\sum_i(\hat{L}_i\hat{L}_k\hat{x}_i+\hat{L}_i\hat{x}_i\hat{L}_k+\hat{L}_k\hat{x}_i\hat{L}_i+\hat{x}_i\hat{L}_k\hat{L}_i)]=0$$

where

$$\sum_{i,l}\varepsilon_{ikl}[\hat{L}_i,\hat{x}_l]=-2i\hbar x_k\,,\qquad -i\hbar^3\sum_{i,l}\varepsilon_{ikl}[\hat{L}_i,\hat{x}_l]=-i\hbar^3(-2i\hbar x_k)=-2\hbar^4 x_k$$

$$-\hbar^2\sum_i(\hat{L}_i\hat{L}_k\hat{x}_i+\hat{x}_i\hat{L}_k\hat{L}_i)=2\hbar^4 x_k$$

$$-\hbar^2\sum_i \hat{L}_i\hat{x}_i\hat{L}_k=0\qquad\qquad -\hbar^2\sum_i \hat{L}_k\hat{x}_i\hat{L}_i=0$$

((**Proof**))

$$\hat{L}_i\hat{L}_k\hat{x}_i + \hat{x}_i\hat{L}_k\hat{L}_i = \hat{L}_i(\hat{x}_i\hat{L}_k + i\hbar\sum_l \varepsilon_{kil}\hat{x}_l) + (\hat{L}_k\hat{x}_i - i\hbar\sum_l \varepsilon_{kil}\hat{x}_l)\hat{L}_i$$

$$\begin{aligned}\sum_i(\hat{L}_i\hat{L}_k\hat{x}_i + \hat{x}_i\hat{L}_k\hat{L}_i) &= \sum_i[\hat{L}_i(\hat{x}_i\hat{L}_k + i\hbar\sum_l \varepsilon_{kil}\hat{x}_l) + (\hat{L}_k\hat{x}_i - i\hbar\sum_l \varepsilon_{kil}\hat{x}_l)\hat{L}_i] \\ &= \sum_i(\hat{L}_i\hat{x}_i\hat{L}_k + \hat{L}_k\hat{x}_i\hat{L}_i) + i\hbar\sum_{i,l}\varepsilon_{kil}[\hat{L}_i,\hat{x}_l] \\ &= i\hbar\sum_{i,l}\varepsilon_{kil}[\hat{L}_i,\hat{x}_l] \\ &= -2\hbar^2\hat{x}_k\end{aligned}$$

((**Mathematica**))

We have the following relations with differential operators.

$$[\boldsymbol{L}^2,[\boldsymbol{L}^2,x]] = 2\hbar^2(\boldsymbol{L}^2x + x\boldsymbol{L}^2)$$

```
eq1 = Lsq[Lsq[x ψ[x, y, z]]] - Lsq[x Lsq[ψ[x, y, z]]] -
    Lsq[x Lsq[ ψ[x, y, z]]] + x Lsq[ Lsq[ψ[x, y, z]]] //
   FullSimplify
```

$$4\hbar^4\left(x\,\psi[x,y,z] + 3\,x\,z\,\psi^{(0,0,1)}[x,y,z] - x^3\,\psi^{(0,0,2)}[x,y,z] - x\,y^2\,\psi^{(0,0,2)}[x,y,z] + 3\,x\,y\,\psi^{(0,1,0)}[x,y,z] + 2\,x\,y\,z\,\psi^{(0,1,1)}[x,y,z] - x^3\,\psi^{(0,2,0)}[x,y,z] - x\,z^2\,\psi^{(0,2,0)}[x,y,z] + 2\,x^2\,\psi^{(1,0,0)}[x,y,z] - y^2\,\psi^{(1,0,0)}[x,y,z] - z^2\,\psi^{(1,0,0)}[x,y,z] + 2\,x^2\,z\,\psi^{(1,0,1)}[x,y,z] + 2\,x^2\,y\,\psi^{(1,1,0)}[x,y,z] - x\,(y^2+z^2)\,\psi^{(2,0,0)}[x,y,z]\right)$$

```
eq2 = 2 ℏ^2 (x Lsq[ψ[x, y, z]] + Lsq[x ψ[x, y, z]]) //
  FullSimplify
```

$$4\hbar^4 \left(x\,\psi[x,y,z]+3\,x\,z\,\psi^{(0,0,1)}[x,y,z]-x^3\,\psi^{(0,0,2)}[x,y,z]-x\,y^2\,\psi^{(0,0,2)}[x,y,z]+3\,x\,y\,\psi^{(0,1,0)}[x,y,z]+2\,x\,y\,z\,\psi^{(0,1,1)}[x,y,z]-x^3\,\psi^{(0,2,0)}[x,y,z]-x\,z^2\,\psi^{(0,2,0)}[x,y,z]+2\,x^2\,\psi^{(1,0,0)}[x,y,z]-y^2\,\psi^{(1,0,0)}[x,y,z]-z^2\,\psi^{(1,0,0)}[x,y,z]+2\,x^2\,z\,\psi^{(1,0,1)}[x,y,z]+2\,x^2\,y\,\psi^{(1,1,0)}[x,y,z]-x\left(y^2+z^2\right)\psi^{(2,0,0)}[x,y,z]\right)$$

```
eq1 - eq2 // Simplify
```

0

5. Commutators

We calculate the differential operators in the Cartesian coordinates

$$[L_z, r^2] = 0\,,$$

$$[L_z, \mathbf{p}^2] = 0\,,$$

$$[\mathbf{L}^2, \mathbf{p}^2] = 0$$

Using Mathematica.

((**Mathematica**))

```
eq1 =
 Lz[(x^2 + y^2 + z^2) ψ[x, y, z]] -
   (x^2 + y^2 + z^2) Lz[ψ[x, y, z]] // Simplify

0

eq2 = Lz[Peq[ψ[x, y, z]]] - Peq[ Lz[ ψ[x, y, z]]] //
  Simplify

 0

 eq3 =
  Leq[Peq[ψ[x, y, z]]] - Peq[ Leq[ ψ[x, y, z]]] //
   Simplify

 0
```

REFERENCES

A. Goswami, Quantum Mechanics, 2nd edition (Wm. C. Brown Publishers, 1997).
J. Binney and D. Skinner, The Physics of Quantum Mechanics (Oxford, 2014).

APPENDIX

```
Clear["Global`"];
ux = {1, 0, 0};
uy = {0, 1, 0};
uz = {0, 0, 1};
r = {x, y, z};
R = √(r.r) ;
L := (-ⅈ ℏ ( Cross[r, Grad[#, {x, y, z}, "Cartesian"]]) &) // Simplify;
p = (-ⅈ ℏ Grad[#, {x, y, z}, "Cartesian"] &) // Simplify;
Lx := (ux.L[#]) &;
Ly := (uy.L[#]) &;
Lz := (uz.L[#]) &;
px := (ux.p[#]) &;
py := (uy.p[#]) &;
pz := (uz.p[#]) &;
Lap := Laplacian[#, { x, y, z}, "Cartesian"] &;
Gra := Grad[#, { x, y, z}, "Cartesian"] &;
Cur := Curl[#, {x, y, z}, "Cartesian"] &;
Diva := Div[#, {x, y, z}, "Cartesian"] &;
prq := (-ⅈ ℏ) 1/2 (r/R.Gra[#] + Diva[r/R #]) &;
```

```
Lsq := (Nest[Lx, #, 2] + Nest[Ly, #, 2] + Nest[Lz, #, 2]) &;
```

Goswami Quantum mechanics

Problem A-1

```
s11 = Lsq[x ψ[x, y, z]] - x Lsq[ ψ[x, y, z]] // Simplify
```

$$2\hbar^2\left(x\,\psi[x,y,z]+x\,z\,\psi^{(0,0,1)}[x,y,z]+x\,y\,\psi^{(0,1,0)}[x,y,z]-y^2\,\psi^{(1,0,0)}[x,y,z]-z^2\,\psi^{(1,0,0)}[x,y,z]\right)$$

```
s12 = Lsq[y ψ[x, y, z]] - y Lsq[ ψ[x, y, z]] // Simplify
```

$$2\hbar^2\left(y\,\psi[x,y,z]+y\,z\,\psi^{(0,0,1)}[x,y,z]-x^2\,\psi^{(0,1,0)}[x,y,z]-z^2\,\psi^{(0,1,0)}[x,y,z]+x\,y\,\psi^{(1,0,0)}[x,y,z]\right)$$

```
s13 = Lsq[z ψ[x, y, z]] - z Lsq[ ψ[x, y, z]] // Simplify
```

$$2\hbar^2\left(z\,\psi[x,y,z]-\left(x^2+y^2\right)\psi^{(0,0,1)}[x,y,z]+z\left(y\,\psi^{(0,1,0)}[x,y,z]+x\,\psi^{(1,0,0)}[x,y,z]\right)\right)$$

```
Lsq := (Nest[Lx, #, 2] + Nest[Ly, #, 2] + Nest[Lz, #, 2]) &;
```

Goswami Quantum mechanics

Problem A-1

```
s11 = Lsq[x ψ[x, y, z]] - x Lsq[ψ[x, y, z]] // Simplify
```

$$2\hbar^2 \left(x\,\psi[x,y,z] + x\,z\,\psi^{(0,0,1)}[x,y,z] + x\,y\,\psi^{(0,1,0)}[x,y,z] - y^2\,\psi^{(1,0,0)}[x,y,z] - z^2\,\psi^{(1,0,0)}[x,y,z]\right)$$

```
s12 = Lsq[y ψ[x, y, z]] - y Lsq[ψ[x, y, z]] // Simplify
```

$$2\hbar^2 \left(y\,\psi[x,y,z] + y\,z\,\psi^{(0,0,1)}[x,y,z] - x^2\,\psi^{(0,1,0)}[x,y,z] - z^2\,\psi^{(0,1,0)}[x,y,z] + x\,y\,\psi^{(1,0,0)}[x,y,z]\right)$$

```
s13 = Lsq[z ψ[x, y, z]] - z Lsq[ψ[x, y, z]] // Simplify
```

$$2\hbar^2 \left(z\,\psi[x,y,z] - \left(x^2+y^2\right)\psi^{(0,0,1)}[x,y,z] + z\left(y\,\psi^{(0,1,0)}[x,y,z] + x\,\psi^{(1,0,0)}[x,y,z]\right)\right)$$

Goswami Quantum mechanics

Problem A - 2

```
s21 = Lx[ψ[x, y, z]] - (y pz[ψ[x, y, z]] - z py[ψ[x, y, z]]) // Simplify
```

0

```
s22 = Ly[ψ[x, y, z]] - (z px[ψ[x, y, z]] - x pz[ψ[x, y, z]]) // Simplify
```

0

```
s23 = Lz[ψ[x, y, z]] - (x py[ψ[x, y, z]] - y px[ψ[x, y, z]]) // Simplify
```

0

Goswami Quantum mechanics

Problem A-3

```
s31 = Lsq[x ψ[x, y, z]] - x Lsq[ ψ[x, y, z]] // Simplify
```

$$2\hbar^2 \left(x\,\psi[x,y,z] + x\,z\,\psi^{(0,0,1)}[x,y,z] + x\,y\,\psi^{(0,1,0)}[x,y,z] - y^2\,\psi^{(1,0,0)}[x,y,z] - z^2\,\psi^{(1,0,0)}[x,y,z]\right)$$

```
s32 =
 -ⅈ ℏ (Ly[z ψ[x, y, z]] + z Ly[ ψ[x, y, z]]) +
   ⅈ ℏ (Lz[y ψ[x, y, z]] + y Lz [ψ[x, y, z]]) // Simplify
```

$$2\hbar^2 \left(x\,\psi[x,y,z] + x\,z\,\psi^{(0,0,1)}[x,y,z] + x\,y\,\psi^{(0,1,0)}[x,y,z] - y^2\,\psi^{(1,0,0)}[x,y,z] - z^2\,\psi^{(1,0,0)}[x,y,z]\right)$$

```
s32 - s31 // Simplify
```

0

Goswami Quantum mechanics

Problem A - 4

```
s41 = Lsq[Lsq[x ψ[x, y, z]]] - Lsq[x Lsq[ψ[x, y, z]]] - Lsq[x Lsq[ ψ[x, y, z]]] +
  x Lsq[ Lsq[ψ[x, y, z]]] // FullSimplify
```

$$4\hbar^4\left(x\,\psi[x,y,z]+3xz\,\psi^{(0,0,1)}[x,y,z]-x^3\,\psi^{(0,0,2)}[x,y,z]-xy^2\,\psi^{(0,0,2)}[x,y,z]+3xy\,\psi^{(0,1,0)}[x,y,z]+2xyz\,\psi^{(0,1,1)}[x,y,z]-x^3\,\psi^{(0,2,0)}[x,y,z]-xz^2\,\psi^{(0,2,0)}[x,y,z]+2x^2\,\psi^{(1,0,0)}[x,y,z]-y^2\,\psi^{(1,0,0)}[x,y,z]-z^2\,\psi^{(1,0,0)}[x,y,z]+2x^2z\,\psi^{(1,0,1)}[x,y,z]+2x^2y\,\psi^{(1,1,0)}[x,y,z]-x\left(y^2+z^2\right)\psi^{(2,0,0)}[x,y,z]\right)$$

```
s42 = 2 ℏ^2 (x Lsq[ ψ[x, y, z]] + Lsq[x ψ[x, y, z]]) // FullSimplify
```

$$4\hbar^4\left(x\,\psi[x,y,z]+3xz\,\psi^{(0,0,1)}[x,y,z]-x^3\,\psi^{(0,0,2)}[x,y,z]-xy^2\,\psi^{(0,0,2)}[x,y,z]+3xy\,\psi^{(0,1,0)}[x,y,z]+2xyz\,\psi^{(0,1,1)}[x,y,z]-x^3\,\psi^{(0,2,0)}[x,y,z]-xz^2\,\psi^{(0,2,0)}[x,y,z]+2x^2\,\psi^{(1,0,0)}[x,y,z]-y^2\,\psi^{(1,0,0)}[x,y,z]-z^2\,\psi^{(1,0,0)}[x,y,z]+2x^2z\,\psi^{(1,0,1)}[x,y,z]+2x^2y\,\psi^{(1,1,0)}[x,y,z]-x\left(y^2+z^2\right)\psi^{(2,0,0)}[x,y,z]\right)$$

```
s42 - s41 // Simplify
```

]= 0

Show that s51+s52+s53+s54+s55==0

```
s51 =
 -ⅈ ℏ^3 (-Ly[z ψ[x, y, z]] + z Ly[ ψ[x, y, z]] + Lz[y ψ[x, y, z]] -
     y Lz[ ψ[x, y, z]]) // Simplify
```

$-2 x \hbar^4 \psi[x, y, z]$

```
s52 = -ℏ^2 (Lx[Lx[x ψ[x, y, z]]] + Ly[Lx[y ψ[x, y, z]]] + Lz[Lx[z ψ[x, y, z]]]) //
  FullSimplify
```

$\hbar^4 \left(2 x \psi[x, y, z] + x z \psi^{(0,0,1)}[x, y, z] + x y \psi^{(0,1,0)}[x, y, z] - \left(y^2 + z^2\right) \psi^{(1,0,0)}[x, y, z]\right)$

```
s53 = -ℏ^2 (Lx[x Lx[ψ[x, y, z]]] + Ly[y Lx [ψ[x, y, z]]] + Lz[z Lx[ ψ[x, y, z]]]) //
  FullSimplify
```

0

```
s54 = -ℏ^2 (Lx[x Lx[ψ[x, y, z]]] + Lx[y Ly [ψ[x, y, z]]] + Lx[z Lz[ ψ[x, y, z]]]) //
  FullSimplify
```

0


```
s54 = -ℏ^2 (Lx[x Lx[ψ[x, y, z]]] + Lx[y Ly [ψ[x, y, z]]] + Lx[z Lz[ ψ[x, y, z]]]) //
  FullSimplify
```

0


```
s55 = -ℏ^2 (x Lx[ Lx[ψ[x, y, z]]] + y Lx[ Ly [ψ[x, y, z]]] + z Lx[Lz[ ψ[x, y, z]]]) //
  FullSimplify
```

$\hbar^4 \left(-x \left(z \psi^{(0,0,1)}[x, y, z] + y \psi^{(0,1,0)}[x, y, z]\right) + \left(y^2 + z^2\right) \psi^{(1,0,0)}[x, y, z]\right)$

```
s51 + s52 + s53 + s54 + s55 // FullSimplify
```

0

```
s52 + s55 // Simplify
```

$2 x \hbar^4 \psi[x, y, z]$

```
Lx[x ψ[x, y, z]] - x Lx[ ψ[x, y, z]] // Simplify
```

0