

Angular momentum and linear momentum: circular cylindrical coordinates

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1. Introduction

In the $|\mathbf{r}\rangle$ representation, we have the following relations,

$$\langle \mathbf{r} | \hat{\mathbf{p}} | \psi \rangle = \mathbf{p} \langle \mathbf{r} | \psi \rangle = \frac{\hbar}{i} \nabla \psi(\mathbf{r}),$$

for the linear momentum operator, and

$$\langle \mathbf{r} | \hat{\mathbf{L}} | \psi \rangle = \langle \mathbf{r} | \hat{\mathbf{r}} \times \hat{\mathbf{p}} | \psi \rangle = (\mathbf{r} \times \mathbf{p}) \langle \mathbf{r} | \psi \rangle = \frac{\hbar}{i} (\mathbf{r} \times \nabla) \psi(\mathbf{r}).$$

The Schrodinger equation can be rewritten as

$$\langle \mathbf{r} | \hat{H} | \psi \rangle = \langle \mathbf{r} | \frac{1}{2\mu} \hat{\mathbf{p}}^2 + V(\hat{\mathbf{r}}) | \psi \rangle = \left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(\mathbf{r}) \right] \langle \mathbf{r} | \psi \rangle = E \langle \mathbf{r} | \psi \rangle$$

So that the wave function and the differential operators in quantum mechanics can be expressed by differential operators in the $|\mathbf{r}\rangle$ representation. Is it possible to calculate equations including differential operators? The answer is yes. The Mathematica has an excellent function for that. One can make use of the pure function of Mathematica. We learned this technique from a famous textbook, *Mathematica for Physics* book, 2nd edition by R.L. Zimmerman and F.I. Olness (Addison-Wesley, 2002). Such differential operators can be realized in the Mathematica (combination of # and &). For example, the operator of the linear momentum \mathbf{p} , we use the following notations,

$$p_x := \frac{\hbar}{i} D[\#, x] \&, \quad p_x[n] := Nest[p_x, \#, n] \& ,$$

in the Mathematica. In this case, we have

$$p_x[\psi[x]] = \frac{\hbar}{i} \frac{\partial}{\partial x} \psi[x], \quad p_x[n][\psi[x]] = \left(\frac{\hbar}{i} \right)^n \frac{\partial^n}{\partial x^n} \psi[x].$$

The syntax $D[\#, x] \&$ represents a pure function that will take a single argument (in our case, wave function) $\psi[x]$. The argument is inserted in slot number one represented by the symbol $\#$. The symbol $\&$ is short hand notation for the Function function.

Using our original programs based on these techniques of Mathematica, we will discuss the angular momentum and linear momentum, and so in the cylindrical co-ordinates.

2. Cylindrical coordinates

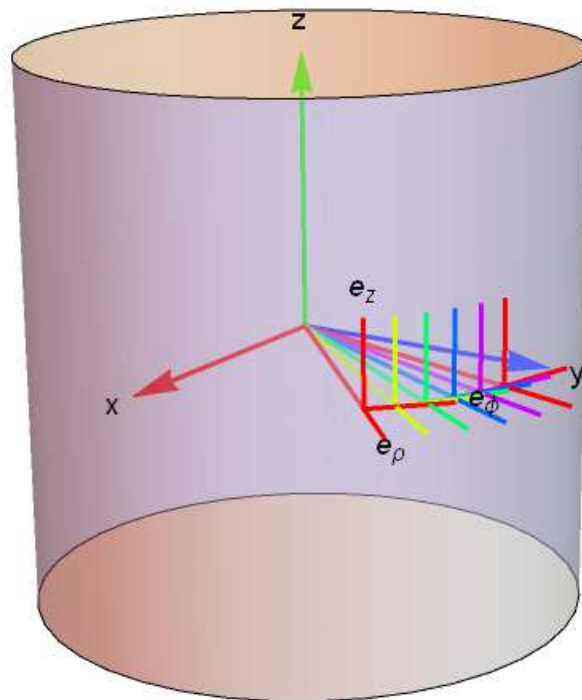


Fig. Cylindrical coordinates. The angle between the unit vectors \mathbf{e}_ρ and \mathbf{e}_z is ϕ .

The vector \mathbf{r} is represented by

$$\mathbf{r} = \rho \mathbf{e}_\rho + z \mathbf{e}_z = \mathbf{e}_x \rho \cos \phi + \mathbf{e}_y \rho \sin \phi + \mathbf{e}_z z.$$

The unit vectors:

$$\mathbf{e}_\rho = \frac{\partial \mathbf{r}}{\partial \rho} = \mathbf{e}_x \cos \phi + \mathbf{e}_y \sin \phi$$

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

$$\mathbf{e}_z = \frac{\partial \mathbf{r}}{\partial z} = \mathbf{e}_z$$

which are dependent on ϕ . Using the matrix form, we get

$$\begin{pmatrix} \mathbf{e}_\rho \\ \mathbf{e}_\phi \\ \mathbf{e}_z \end{pmatrix} = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{e}_x \\ \mathbf{e}_y \\ \mathbf{e}_z \end{pmatrix}$$

and

$$\begin{pmatrix} \mathbf{e}_x \\ \mathbf{e}_y \\ \mathbf{e}_z \end{pmatrix} = \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{e}_\rho \\ \mathbf{e}_\phi \\ \mathbf{e}_z \end{pmatrix}$$

Or

$$\mathbf{e}_x = \mathbf{e}_\rho \cos \phi - \mathbf{e}_\phi \sin \phi,$$

$$\mathbf{e}_y = \mathbf{e}_\rho \sin \phi + \mathbf{e}_\phi \cos \phi$$

$$\mathbf{e}_z = \mathbf{e}_z$$

We also have

$$\mathbf{e}_r = \frac{1}{r} \mathbf{r} = \frac{1}{r} (\rho \mathbf{e}_\rho + z \mathbf{e}_z)$$

$$d\mathbf{r} = \mathbf{e}_\rho d\rho + \mathbf{e}_\phi \rho d\phi + \mathbf{e}_z dz = \mathbf{e}_\rho h_\rho d\rho + \mathbf{e}_\phi h_\phi d\phi + \mathbf{e}_z h_z dz$$

with $h_\rho = 1, h_\phi = \rho, h_z = 1$

2. Differential operators; \mathbf{p} and \mathbf{L}

The orbital angular momentum \mathbf{L} is given by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \frac{\hbar}{i} \mathbf{r} \times \nabla,$$

With the linear momentum as

$$\mathbf{p} = \frac{\hbar}{i} \nabla = \frac{\hbar}{i} \text{Grad}.$$

We note that

$$L_x = \mathbf{e}_x \cdot \mathbf{L}, \quad L_y = \mathbf{e}_y \cdot \mathbf{L}, \quad L_z = \mathbf{e}_z \cdot \mathbf{L}$$

The raising operator:

$$L_+ = L_x + iL_y$$

The lowering operator:

$$L_- = L_x - iL_y$$

The radial linear momentum is defined by

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

Note that

$$p_x = \mathbf{e}_x \cdot \mathbf{p} = \frac{\hbar}{i} \mathbf{e}_x \cdot \nabla, \quad p_y = \mathbf{e}_y \cdot \mathbf{p} = \frac{\hbar}{i} \mathbf{e}_y \cdot \nabla, \quad p_z = \mathbf{e}_z \cdot \mathbf{p} = \frac{\hbar}{i} \mathbf{e}_z \cdot \nabla.$$

and

$$p_\rho = \mathbf{e}_\rho \cdot \mathbf{p} = \frac{\hbar}{i} \mathbf{e}_\rho \cdot \nabla, \quad p_\phi = \mathbf{e}_\phi \cdot \mathbf{p} = \frac{\hbar}{i} \mathbf{e}_\phi \cdot \nabla, \quad p_z = \mathbf{e}_z \cdot \mathbf{p} = \frac{\hbar}{i} \mathbf{e}_z \cdot \nabla$$

3. Mathematica program for differential operators in cylindrical coordinates

The following Mathematica program (combination of #, &, pure function) is made by us for calculating differential operators in the cylindrical coordinates.

$$L \rightarrow \frac{\hbar}{i} \mathbf{r} \times \nabla, \quad p \rightarrow \frac{\hbar}{i} \nabla$$

Vector analysis

Angular momentum in the cylindrical coordinates

```

Clear["Global`"];
r1 =  $\sqrt{z^2 + \rho^2}$ ;
ux = {Cos[ $\phi$ ], -Sin[ $\phi$ ], 0};
uy = {Sin[ $\phi$ ], Cos[ $\phi$ ], 0};
uz = {0, 0, 1};
r = { $\rho$ ,  $\theta$ , z};
ur =  $\frac{1}{r1}$  { $\rho$ ,  $\theta$ , z};
Gra := Grad[#, { $\rho$ ,  $\phi$ , z}, "Cylindrical"] &;
Lap := Laplacian[#, { $\rho$ ,  $\phi$ , z}, "Cylindrical"] &;
Curla := Curl[#, { $\rho$ ,  $\phi$ , z}, "Cylindrical"] &;
Diva := Div[#, { $\rho$ ,  $\phi$ , z}, "Cylindrical"] &;
L := (- $i \hbar$  Cross[r, Gra[#]]) &;
Lx := (ux.L[#] &) // Simplify;
Ly := (uy.L[#] &) // Simplify;
Lz := (uz.L[#] &) // Simplify;
LP := (Lx[#] +  $i$  Ly[#]) &;
LM := (Lx[#] -  $i$  Ly[#]) &;
prq :=  $\left( \frac{-i \hbar}{2} \text{ur} \cdot \text{Gra}[\#] + \frac{-i \hbar}{2} \text{Diva}[\# \text{ur}] \right)$  &;
Leq := (Nest[Lx, #, 2] + Nest[Ly, #, 2] + Nest[Lz, #, 2]) &;
p := (- $i \hbar$  Gra[#]) &;
px := (ux.p[#]) &;
py := (uy.p[#]) &;
pz := (uz.p[#]) &;
p $\rho$  := ({1, 0, 0} . p[#]) &;

```

4. Expressions of Laplacian ∇^2 , Gradient, Divergence, and Curl (Rotation) in the cylindrical co-ordinates

$$\begin{aligned}\nabla^2\psi(\rho,\phi,z) &= \frac{\partial^2}{\partial\rho^2}\psi(\rho,\phi,z) + \frac{1}{\rho}\frac{\partial}{\partial\rho}\psi(\rho,\phi,z) \\ &\quad + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\psi(\rho,\phi,z) + \frac{\partial^2}{\partial z^2}\psi(\rho,\phi,z) \\ &= \frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial}{\partial\rho}\psi(\rho,\phi,z)\right] + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\psi(\rho,\phi,z) + \frac{\partial^2}{\partial z^2}\psi(\rho,\phi,z)\end{aligned}$$

$$\nabla\psi(\rho,\phi,z) = \mathbf{e}_\rho\frac{\partial}{\partial\rho}\psi(\rho,\phi,z) + \mathbf{e}_\phi\frac{1}{\rho}\frac{\partial}{\partial\phi}\psi(\rho,\phi,z) + \mathbf{e}_z\frac{\partial}{\partial z}\psi(\rho,\phi,z)$$

$$\begin{aligned}\nabla\cdot\mathbf{V}(\rho,\phi,z) &= \frac{\partial}{\partial\rho}V_\rho(\rho,\phi,z) + \frac{1}{\rho}V_\rho(\rho,\phi,z) + \frac{1}{\rho}\frac{\partial}{\partial\phi}V_\phi(\rho,\phi,z) + \frac{\partial}{\partial z}V_z(\rho,\phi,z) \\ &= \frac{1}{\rho}\frac{\partial}{\partial\rho}[\rho V_\rho(\rho,\phi,z)] + \frac{1}{\rho}\frac{\partial}{\partial\phi}V_\phi(\rho,\phi,z) + \frac{\partial}{\partial z}V_z(\rho,\phi,z)\end{aligned}$$

$$\begin{aligned}\nabla\times\mathbf{V}(\rho,\phi,z) &= \frac{1}{\rho}\mathbf{e}_\rho\left[\frac{\partial}{\partial\phi}V_z(\rho,\phi,z) - \frac{\partial}{\partial z}\rho V_\phi(\rho,\phi,z)\right] \\ &\quad - \frac{1}{\rho}(\rho\mathbf{e}_\phi)\left[\frac{\partial}{\partial\rho}V_z(\rho,\phi,z) - \frac{\partial}{\partial z}V_\rho(\rho,\phi,z)\right] \\ &\quad + \frac{1}{\rho}\mathbf{e}_z\left[\frac{\partial}{\partial\rho}\rho V_\phi(\rho,\phi,z) - \frac{\partial}{\partial\phi}V_\rho(\rho,\phi,z)\right]\end{aligned}$$

or

$$\nabla\times\mathbf{V}(\rho,\phi,z) = \frac{1}{\rho}\begin{vmatrix} \mathbf{e}_\rho & \rho\mathbf{e}_\phi & \mathbf{e}_z \\ \frac{\partial}{\partial\rho} & \frac{\partial}{\partial\phi} & \frac{\partial}{\partial z} \\ V_\rho(\rho,\phi,z) & \rho V_\phi(\rho,\phi,z) & V_z(\rho,\phi,z) \end{vmatrix}$$

((Mathematica))

Laplacian, grad, div, and rot (curl)

Lap $[\psi[\rho, \phi, z]]$ // Simplify

$$\psi^{(0,0,2)}[\rho, \phi, z] + \frac{\psi^{(0,2,0)}[\rho, \phi, z]}{\rho^2} + \left| \frac{\psi^{(1,0,0)}[\rho, \phi, z]}{\rho} + \psi^{(2,0,0)}[\rho, \phi, z] \right.$$

Gra $[\psi[\rho, \phi, z]]$ // Simplify

$$\left\{ \psi^{(1,0,0)}[\rho, \phi, z], \frac{\psi^{(0,1,0)}[\rho, \phi, z]}{\rho}, \psi^{(0,0,1)}[\rho, \phi, z] \right\}$$

Diva $[\{V\rho[\rho, \phi, z], V\phi[\rho, \phi, z], Vz[\rho, \phi, z]\}]$

$$Vz^{(0,0,1)}[\rho, \phi, z] + \frac{V\rho[\rho, \phi, z] + V\phi^{(0,1,0)}[\rho, \phi, z]}{\rho} + V\rho^{(1,0,0)}[\rho, \phi, z]$$

Curla $[\{V\rho[\rho, \phi, z], V\phi[\rho, \phi, z], Vz[\rho, \phi, z]\}]$ // Simplify

$$\left\{ -V\phi^{(0,0,1)}[\rho, \phi, z] + \frac{Vz^{(0,1,0)}[\rho, \phi, z]}{\rho}, V\rho^{(0,0,1)}[\rho, \phi, z] - Vz^{(1,0,0)}[\rho, \phi, z], \frac{V\phi[\rho, \phi, z] - V\rho^{(0,1,0)}[\rho, \phi, z] + \rho V\phi^{(1,0,0)}[\rho, \phi, z]}{\rho} \right\}$$

5. Expressions of the orbital angular momentum in the cylindrical coordinates

We discuss the differential operators in the cylindrical coordinates,

$$L_x, L_y, L_z, L_x \pm iL_y, L^2 = L_x^2 + L_y^2 + L_z^2$$

in the cylindrical coordinates. The results are as follows.

(a)

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$$

(b)

$$L_x = i\hbar \left(z \sin \phi \frac{\partial}{\partial \rho} + \frac{z}{\rho} \cos \phi \frac{\partial}{\partial \phi} - \rho \sin \phi \frac{\partial}{\partial z} \right)$$

(c)

$$L_y = i\hbar \left(-z \cos \phi \frac{\partial}{\partial \rho} + \frac{z}{\rho} \sin \phi \frac{\partial}{\partial \phi} + \rho \cos \phi \frac{\partial}{\partial z} \right)$$

The ladder operators for angular momentum,

$$\begin{aligned} L_+ &= L_x + iL_y \\ &= i\hbar \left(z \sin \phi \frac{\partial}{\partial \rho} + \frac{z}{\rho} \cos \phi \frac{\partial}{\partial \phi} - \rho \sin \phi \frac{\partial}{\partial z} \right) \\ &\quad + i\hbar \left(-iz \cos \phi \frac{\partial}{\partial \rho} + \frac{z}{\rho} i \sin \phi \frac{\partial}{\partial \phi} + i\rho \cos \phi \frac{\partial}{\partial z} \right) \\ &= i\hbar e^{i\phi} \left(-iz \frac{\partial}{\partial \rho} + i\rho \frac{\partial}{\partial z} + \frac{z}{\rho} \frac{\partial}{\partial \phi} \right) \end{aligned}$$

$$\begin{aligned} L_- &= L_x - iL_y \\ &= i\hbar \left(z \sin \phi \frac{\partial}{\partial \rho} + \frac{z}{\rho} \cos \phi \frac{\partial}{\partial \phi} - \rho \sin \phi \frac{\partial}{\partial z} \right) \\ &\quad + i\hbar \left(iz \cos \phi \frac{\partial}{\partial \rho} - \frac{z}{\rho} i \sin \phi \frac{\partial}{\partial \phi} - i\rho \cos \phi \frac{\partial}{\partial z} \right) \\ &= i\hbar e^{-i\phi} \left(iz \frac{\partial}{\partial \rho} - i\rho \frac{\partial}{\partial z} + \frac{z}{\rho} \frac{\partial}{\partial \phi} \right) \end{aligned}$$

((Mathematica))

Angular momentum in the cylindrical coordinate

L , L_x , L_y , L_z , L_x+iL_y , L_x-iL_y

$L[\psi[\rho, \phi, z]] // \text{Simplify}$

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

$L_x[\psi[\rho, \phi, z]] // \text{FullSimplify}$

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

$L_y[\psi[\rho, \phi, z]] // \text{FullSimplify}$

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

$L_x[\psi[\rho, \phi, z]] + i L_y[\psi[\rho, \phi, z]] // \text{FullSimplify}$

$$\frac{e^{i\phi} \hbar \left(\rho^2 \psi^{(\theta,\theta,1)}[\rho, \phi, z] - i z \psi^{(\theta,1,\theta)}[\rho, \phi, z] - z \rho \psi^{(1,\theta,\theta)}[\rho, \phi, z] \right)}{\rho}$$

$L_x[\psi[\rho, \phi, z]] - i L_y[\psi[\rho, \phi, z]] // \text{FullSimplify}$

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

$L_z[\psi[\rho, \phi, z]] // \text{Simplify}$

$$-i \hbar \psi^{(\theta,1,\theta)}[\rho, \phi, z]$$

6. Commutation relations of angular momentum

Next, we discuss the commutation relations for the angular momentum using Mathematica.

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

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

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

((Mathematica))

```
Lx[Ly[ψ[ρ, φ, z]]] - Ly[Lx[ψ[ρ, φ, z]]] -  
i ħ Lz[ψ[ρ, φ, z]] // Simplify
```

0

```
Ly[Lz[ψ[ρ, φ, z]]] - Lz[Ly[ψ[ρ, φ, z]]] -  
i ħ Lx[ψ[ρ, φ, z]] // Simplify
```

0

```
Lz[Lx[ψ[ρ, φ, z]]] - Lx[Lz[ψ[ρ, φ, z]]] -  
i ħ Ly[ψ[ρ, φ, z]] // Simplify // Simplify
```

0

Leq[Lx[ψ[ρ, φ, z]]] - Lx[Leq[ψ[ρ, φ, z]]] // Simplify
 0

Leq[Ly[ψ[ρ, φ, z]]] - Ly[Leq[ψ[ρ, φ, z]]] // Simplify
 0

Leq[Lz[ψ[ρ, φ, z]]] - Lz[Leq[ψ[ρ, φ, z]]] // Simplify
 0

Lz[LP[ψ[ρ, φ, z]]] - LP[Lz[ψ[ρ, φ, z]]] - ħ LP[ψ[ρ, φ, z]] // Simplify
 0

Lz[LM[ψ[ρ, φ, z]]] - LM[Lz[ψ[ρ, φ, z]]] + ħ LM[ψ[ρ, φ, z]] // Simplify
 0

7. Expression of $L^2 = L_x^2 + L_y^2 + L_z^2$ in the circular cylindrical coordinates.

The square of the magnitude of total angular momentum is obtained as

$$\begin{aligned} L^2 &= L_x^2 + L_y^2 + L_z^2 \\ &= -\frac{\hbar^2}{\rho^2} \left\{ -2z\rho^2 \frac{\partial}{\partial z} + \rho^4 \frac{\partial^2}{\partial z^2} + (z^2 + \rho^2) \frac{\partial^2}{\partial \phi^2} \right. \\ &\quad \left. + z^2 \rho \frac{\partial}{\partial \rho} - \rho^3 \frac{\partial}{\partial \rho} + 2z\rho^3 \frac{\partial}{\partial \rho} \frac{\partial}{\partial z} + z^2 \rho^2 \frac{\partial^2}{\partial \rho^2} \right\} \end{aligned}$$

((Mathematica))

L^2 in the cylindrical coordinate

$$\text{eq1} = \text{Lx}[\text{Lx}[\psi[\rho, \phi, z]]] + \text{Ly}[\text{Ly}[\psi[\rho, \phi, z]]] + \text{Lz}[\text{Lz}[\psi[\rho, \phi, z]]] // \text{Simplify}$$

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

$$\text{eq2} = \text{Leq}[\psi[\rho, \phi, z]] // \text{Simplify}$$

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

$$\text{eq12} = \text{eq1} - \text{eq2} // \text{Simplify}$$

0

8. Radial linear momentum

The radial linear momentum is defined by

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

Using the Mathematica, the corresponding differential operator is obtained as

$$p_r = \frac{\hbar}{i} \frac{1}{\sqrt{\rho^2 + z^2}} \left(1 + z \frac{\partial}{\partial z} + \rho \frac{\partial}{\partial \rho} \right)$$

Note that

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

((Mathematica))

Radial momentum (quantum)

`prq[ψ[ρ, φ, z]] // Simplify`

$$\frac{i \hbar \left(\psi[\rho, \phi, z] + z \psi^{(0,0,1)}[\rho, \phi, z] + \rho \psi^{(1,0,0)}[\rho, \phi, z] \right)}{\sqrt{z^2 + \rho^2}}$$

Commutation relation for radial momentum and magnitude of r

`prq[r1 ψ[ρ, φ, z]] - r1 prq[ψ[ρ, φ, z]] // Simplify`

$$-i \hbar \psi[\rho, \phi, z]$$

9. Expression of \mathbf{p}^2

We show that the differential operator \mathbf{p}^2 is expressed by

$$\mathbf{p}^2 = p_r^2 + \frac{\mathbf{L}^2}{z^2 + \rho^2}$$

using Mathematica. The expression is so complicated that we expect. However, the expression is mathematically correct.

$$\mathbf{p}^2 = -\frac{\hbar^2}{\rho^2} \left(\rho^2 \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial \phi^2} + \rho \frac{\partial}{\partial \rho} + \rho^2 \frac{\partial^2}{\partial \rho^2} \right),$$

$$p_r^2 = -\frac{\hbar^2}{z^2 + \rho^2} \left(2z \frac{\partial}{\partial z} + z^2 \frac{\partial^2}{\partial z^2} + 2\rho \frac{\partial}{\partial \rho} + 2\rho z \frac{\partial^2}{\partial \rho \partial z} + \rho^2 \frac{\partial^2}{\partial \rho^2} \right),$$

Thus, we have

$$\mathbf{p}^2 - p_r^2 = -\frac{\hbar^2}{\rho^2} \left(\rho^2 \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial \phi^2} + \rho \frac{\partial}{\partial \rho} + \rho^2 \frac{\partial^2}{\partial \rho^2} \right) \\ + \frac{\hbar^2}{z^2 + \rho^2} \left(2z \frac{\partial}{\partial z} + z^2 \frac{\partial^2}{\partial z^2} + 2\rho \frac{\partial}{\partial \rho} + 2\rho z \frac{\partial^2}{\partial \rho \partial z} + \rho^2 \frac{\partial^2}{\partial \rho^2} \right)$$

So that we get

$$(\mathbf{p}^2 - p_r^2)(\rho^2 + z^2) = \mathbf{L}^2 \\ = -\frac{\hbar^2}{\rho^2} \left[-2z\rho^2 \frac{\partial}{\partial z} + \rho^4 \frac{\partial^2}{\partial z^2} + (z^2 + \rho^2) \frac{\partial^2}{\partial \phi^2} \right. \\ \left. + z^2 \rho \frac{\partial}{\partial \rho} - \rho^3 \frac{\partial}{\partial \rho} + 2z\rho^3 \frac{\partial}{\partial \rho} \frac{\partial}{\partial z} + z^2 \rho^2 \frac{\partial^2}{\partial \rho^2} \right]$$

or

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

((Mathematica))

p^2 in the cylindrical coordinate

eq1 = px[px[ψ[ρ, φ, z]]] + py[py[ψ[ρ, φ, z]]] +
pz[pz[ψ[ρ, φ, z]]] // Simplify

$$-\frac{1}{\rho^2} \hbar^2 \left(\rho^2 \psi^{(0,0,2)}[\rho, \phi, z] + \psi^{(0,2,0)}[\rho, \phi, z] + \right. \\ \left. \rho \left(\psi^{(1,0,0)}[\rho, \phi, z] + \rho \psi^{(2,0,0)}[\rho, \phi, z] \right) \right)$$

pr^2 in the cylindrical coordinate

eq2 = prq[prq[ψ[ρ, φ, z]]] // Simplify

$$-\frac{1}{z^2 + \rho^2} \hbar^2 \left(2 z \psi^{(0,0,1)}[\rho, \phi, z] + \right. \\ \left. z^2 \psi^{(0,0,2)}[\rho, \phi, z] + \rho \left(2 \psi^{(1,0,0)}[\rho, \phi, z] + \right. \right. \\ \left. \left. 2 z \psi^{(1,0,1)}[\rho, \phi, z] + \rho \psi^{(2,0,0)}[\rho, \phi, z] \right) \right)$$

eq12 = (eq1 - eq2) (z² + ρ²) // Simplify

$$-\frac{1}{\rho^2} \hbar^2 \left(-2 z \rho^2 \psi^{(0,0,1)} [\rho, \phi, z] + \rho^4 \psi^{(0,0,2)} [\rho, \phi, z] + \right. \\ \left. z^2 \psi^{(0,2,0)} [\rho, \phi, z] + \rho^2 \psi^{(0,2,0)} [\rho, \phi, z] + \right. \\ \left. z^2 \rho \psi^{(1,0,0)} [\rho, \phi, z] - \rho^3 \psi^{(1,0,0)} [\rho, \phi, z] - \right. \\ \left. 2 z \rho^3 \psi^{(1,0,1)} [\rho, \phi, z] + z^2 \rho^2 \psi^{(2,0,0)} [\rho, \phi, z] \right)$$

L² in the cylindrical coordinates

eq3 = Leq[ψ[ρ, φ, z]] // Simplify

$$-\frac{1}{\rho^2} \hbar^2 \left(-2 z \rho^2 \psi^{(0,0,1)} [\rho, \phi, z] + \rho^4 \psi^{(0,0,2)} [\rho, \phi, z] + \right. \\ \left. z^2 \psi^{(0,2,0)} [\rho, \phi, z] + \rho^2 \psi^{(0,2,0)} [\rho, \phi, z] + \right. \\ \left. z^2 \rho \psi^{(1,0,0)} [\rho, \phi, z] - \rho^3 \psi^{(1,0,0)} [\rho, \phi, z] - \right. \\ \left. 2 z \rho^3 \psi^{(1,0,1)} [\rho, \phi, z] + z^2 \rho^2 \psi^{(2,0,0)} [\rho, \phi, z] \right)$$

eq4 = eq12 - eq3 // Simplify

0

10. Example-1 (Goswami, Quantum Mechanics p.265 problem-4)

Prove the following equivalence:

$$p_r r^2 p_r = r p_r^2 r$$

with

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

((Proof))

We use the commutation relation $[p_r, r] = -i\hbar$.

$$\begin{aligned}
p_r r^2 p_r &= (p_r r)(r p_r) \\
&= (r p_r - i\hbar)(p_r r + i\hbar) \\
&= (r p_r p_r r) + i\hbar(r p_r - p_r r) + \hbar^2 \\
&= r p_r^2 r
\end{aligned}$$

((Mathematica))

```
prq[r1 ψ[ρ, φ, z]] - r1 prq[ψ[ρ, φ, z]] //
Simplify
```

```
-i ħ ψ[ρ, φ, z]
```

```
prq[r1^2 prq[ψ[ρ, φ, z]]] -
r1 prq[prq[r1 ψ[ρ, φ, z]]] // Simplify
```

```
0
```

11. Example-2: Goswami Quantum Mechanics, P.265 Problem 5

((Problem-5)) Find the expression for ∇^2 in the cylindrical coordinates. Then show that

$$\rho^2 \mathbf{p}^2 = (\rho p_\rho)^2 + L_z^2 + \rho^2 p_z^2$$

where

$$p_\rho = \mathbf{e}_\rho \cdot \mathbf{p} = \frac{\hbar}{i} \frac{\partial}{\partial \rho}, \quad L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}.$$

Using Mathematica we get

$$\rho^2 \mathbf{p}^2 = -\hbar^2 \left(\rho^2 \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial \phi^2} + \rho^2 \frac{\partial^2}{\partial \rho^2} + \rho \frac{\partial}{\partial \rho} \right)$$

$$(\rho p_\rho)^2 = \rho p_\rho \rho p_\rho = -\hbar^2 \left(\rho \frac{\partial}{\partial \rho} + \rho^2 \frac{\partial^2}{\partial \rho^2} \right)$$

$$L_z^2 = -\hbar^2 \frac{\partial^2}{\partial \phi^2}$$

$$\rho^2 p_z^2 = -\hbar^2 \rho^2 \frac{\partial^2}{\partial z^2}$$

$$\begin{aligned} \rho^2 \mathbf{p}^2 &= (\rho p_\rho)^2 + L_z^2 + \rho^2 p_z^2 \\ &= -\hbar^2 \left(\rho^2 \frac{\partial^2}{\partial \rho^2} + \rho \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial \phi^2} + \rho^2 \frac{\partial^2}{\partial z^2} \right) \end{aligned}$$

((Mathematica))

eq1 =

```
 $\rho^2$  (Nest[px,  $\psi[\rho, \phi, z]$ , 2] + Nest[py,  $\psi[\rho, \phi, z]$ , 2] +  
Nest[pz,  $\psi[\rho, \phi, z]$ , 2]) // Simplify
```

```
 $-\hbar^2$  ( $\rho^2 \psi^{(0,0,2)}$  [ $\rho, \phi, z$ ] +  $\psi^{(0,2,0)}$  [ $\rho, \phi, z$ ] +  
 $\rho$  ( $\psi^{(1,0,0)}$  [ $\rho, \phi, z$ ] +  $\rho \psi^{(2,0,0)}$  [ $\rho, \phi, z$ ]))
```

eq2 = ρ p ρ [ρ p ρ [$\psi[\rho, \phi, z]$]] // FullSimplify

```
 $-\rho \hbar^2$  ( $\psi^{(1,0,0)}$  [ $\rho, \phi, z$ ] +  $\rho \psi^{(2,0,0)}$  [ $\rho, \phi, z$ ])
```

eq3 = Lz[Lz[$\psi[\rho, \phi, z]$]] // FullSimplify

```
 $-\hbar^2 \psi^{(0,2,0)}$  [ $\rho, \phi, z$ ]
```

eq4 = ρ^2 pz[pz[$\psi[\rho, \phi, z]$]] // FullSimplify

```
 $-\rho^2 \hbar^2 \psi^{(0,0,2)}$  [ $\rho, \phi, z$ ]
```

eq1 - (eq2 + eq3 + eq4) // Simplify

0

12. Example-3

Show that

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

With

$$x = \mathbf{e}_x \cdot \mathbf{r}$$

$$x1 = ux.r$$

$$\rho \text{Cos}[\phi]$$

$$\text{eq1} =$$

$$\text{Leq}[\text{Leq}[x1 \psi[\rho, \phi, z]]] - \text{Leq}[x1 \text{Leq}[\psi[\rho, \phi, z]]] - \\ \text{Leq}[x1 \text{Leq}[\psi[\rho, \phi, z]]] + x1 \text{Leq}[\text{Leq}[\psi[\rho, \phi, z]]] // \\ \text{FullSimplify}$$

$$\frac{1}{\rho} 4 \hbar^4 \left(\rho^2 \text{Cos}[\phi] \psi[\rho, \phi, z] + \right. \\ \left. (z^2 + \rho^2) \text{Sin}[\phi] \psi^{(0,1,0)}[\rho, \phi, z] - \right. \\ \left. \text{Cos}[\phi] \left(-3 z \rho^2 \psi^{(0,0,1)}[\rho, \phi, z] + \right. \right. \\ \left. z^2 \psi^{(0,2,0)}[\rho, \phi, z] + \rho \left(2 z^2 \psi^{(1,0,0)}[\rho, \phi, z] + \right. \right. \\ \left. \rho \left(\psi^{(0,2,0)}[\rho, \phi, z] + \rho \left(\rho \psi^{(0,0,2)}[\rho, \phi, z] - \right. \right. \right. \\ \left. \left. \left. \psi^{(1,0,0)}[\rho, \phi, z] - 2 z \psi^{(1,0,1)}[\rho, \phi, z] \right) + \right. \right. \\ \left. \left. \left. z^2 \psi^{(2,0,0)}[\rho, \phi, z] \right) \right) \right) \right)$$

$$\text{eq2} = 2 \hbar^2 (x1 \text{Leq}[\psi[\rho, \phi, z]] + \text{Leq}[x1 \psi[\rho, \phi, z]]) // \\ \text{FullSimplify}$$

$$\frac{1}{\rho} 4 \hbar^4 \left(\rho^2 \text{Cos}[\phi] \psi[\rho, \phi, z] + \right. \\ \left. (z^2 + \rho^2) \text{Sin}[\phi] \psi^{(0,1,0)}[\rho, \phi, z] - \right. \\ \left. \text{Cos}[\phi] \left(-3 z \rho^2 \psi^{(0,0,1)}[\rho, \phi, z] + \right. \right. \\ \left. z^2 \psi^{(0,2,0)}[\rho, \phi, z] + \rho \left(2 z^2 \psi^{(1,0,0)}[\rho, \phi, z] + \right. \right. \\ \left. \rho \left(\psi^{(0,2,0)}[\rho, \phi, z] + \rho \left(\rho \psi^{(0,0,2)}[\rho, \phi, z] - \right. \right. \right. \\ \left. \left. \left. \psi^{(1,0,0)}[\rho, \phi, z] - 2 z \psi^{(1,0,1)}[\rho, \phi, z] \right) + \right. \right. \\ \left. \left. \left. z^2 \psi^{(2,0,0)}[\rho, \phi, z] \right) \right) \right) \right)$$

$$\text{eq12} = \text{eq1} - \text{eq2} // \text{Simplify}$$

$$0$$

13. Example-4: Problem (9-23) Townsend, A Modern Approach to Quantum Mechanics

((9-23)) The Hamiltonian for a three-dimensional (3D) system with cylindrical symmetry is given by

$$\hat{H} = \frac{1}{2\mu} \hat{\mathbf{p}}^2 + V(\hat{\rho})$$

where $|\hat{\rho}| = \sqrt{\hat{x}^2 + \hat{y}^2}$.

- Use symmetry arguments to establish that both \hat{p}_z , the generator of translations in the z direction, and \hat{L}_z , the generator of rotations about the z axis, commute with \hat{H} .
- Use the fact that \hat{H} , \hat{p}_z , and \hat{L}_z have eigenstates in common to express the position-space eigenfunctions of the Hamiltonian in terms of those of \hat{p}_z and \hat{L}_z .
- What is the radial equation? Note: The Laplacian in cylindrical coordinates is given by

$$\nabla^2 \psi(\rho, \phi, z) = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left[\rho \frac{\partial}{\partial \rho} \psi(\rho, \phi, z) \right] + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \psi(\rho, \phi, z) + \frac{\partial^2}{\partial z^2} \psi(\rho, \phi, z)$$

((Solution))

The Hamiltonian:

$$\hat{H} = \frac{1}{2\mu} \hat{\mathbf{p}}^2 + V(\hat{\rho})$$

The commutation relation:

$$\left[\hat{H}, \hat{p}_z \right] = 0, \quad \left[\hat{H}, \hat{L}_z \right] = 0$$

Then, we have a simultaneous eigenket;

$$H |E, m, k_z\rangle = E |E, m, k_z\rangle, \quad \hat{L}_z |E, m, k_z\rangle = m\hbar |E, m, k_z\rangle$$

$$\hat{p}_z |E, m, k_z\rangle = \hbar k_z |E, m, k_z\rangle$$

The wave function can be expressed as

$$\psi(\rho, \phi, k_z) = e^{im\phi} e^{ik_z z} \chi(\rho)$$

$\chi(\rho)$ satisfies the following differential equation,

$$-\frac{\hbar^2}{2\mu\rho}[\chi'(\rho) + \rho\chi''(\rho)] + \left[\frac{\hbar^2}{2\mu}\left(k_z^2 + \frac{m^2}{\rho^2}\right) + V(\rho)\right]\chi(\rho) = E\chi(\rho)$$

or

$$-\frac{\hbar^2}{2\mu\rho} \frac{d}{d\rho}(\rho\chi'(\rho)) + \left[\frac{\hbar^2}{2\mu}\left(k_z^2 + \frac{m^2}{\rho^2}\right) + V(\rho)\right]\chi(\rho) = E\chi(\rho)$$

((Mathematica))

Hamiltonian

$$H1 := \left(\frac{1}{2\mu} \text{Peq}[\#] + V1[\rho] \# \right) \&;$$

Schrodinger equation

$$\text{eq11} = H1[\psi[\rho, \phi, z]] - E1 \psi[\rho, \phi, z] // \text{Simplify}$$

$$\begin{aligned} & (-E1 + V1[\rho]) \psi[\rho, \phi, z] - \frac{1}{2\mu\rho^2} \\ & \hbar^2 \left(\rho^2 \psi^{(\theta, \theta, 2)}[\rho, \phi, z] + \psi^{(\theta, 2, \theta)}[\rho, \phi, z] + \right. \\ & \left. \rho \left(\psi^{(1, \theta, \theta)}[\rho, \phi, z] + \rho \psi^{(2, \theta, \theta)}[\rho, \phi, z] \right) \right) \end{aligned}$$

Commutation relation between H and L_z

$$\text{eq12} = H1[Lz[\psi[\rho, \phi, z]]] - Lz[H1[\psi[\rho, \phi, z]]] // \text{Simplify}$$

0

eq21 = Lz [H1 [\psi [\rho, \phi, z]]] // Simplify

$$-i \hbar V1[\rho] \psi^{(\theta,1,\theta)}[\rho, \phi, z] + \frac{1}{2\mu\rho^2} \\ i \hbar^3 \left(\rho^2 \psi^{(\theta,1,2)}[\rho, \phi, z] + \psi^{(\theta,3,\theta)}[\rho, \phi, z] + \right. \\ \left. \rho \left(\psi^{(1,1,\theta)}[\rho, \phi, z] + \rho \psi^{(2,1,\theta)}[\rho, \phi, z] \right) \right)$$

Commutation relation between H and pz

eq22 = H1 [pz [\psi [\rho, \phi, z]]] - pz [H1 [\psi [\rho, \phi, z]]] // Simplify

0

Simultaneous eigenket of pz and Lz

eq31 = H1 [Lz [\psi [\rho, \phi, z]]] - Lz [H1 [\psi [\rho, \phi, z]]] // Simplify

0

eq41 = LZ[ψ[ρ, φ, z]] == m ħ ψ[ρ, φ, z] // Simplify

$$-i \hbar \psi^{(\theta, 1, \theta)}[\rho, \phi, z] = m \hbar \psi[\rho, \phi, z]$$

eq42 = DSolve[eq41, ψ[ρ, φ, z], φ]

$$\left\{ \left\{ \psi[\rho, \phi, z] \rightarrow e^{i m \phi} c_1 \right\} \right\}$$

eq51 = pz[ψ[ρ, φ, z]] == ħ kz ψ[ρ, φ, z] // Simplify

$$-i \hbar \psi^{(\theta, \theta, 1)}[\rho, \phi, z] = k z \hbar \psi[\rho, \phi, z]$$

eq52 = DSolve[eq51, ψ[ρ, φ, z], z] // Simplify

$$\left\{ \left\{ \psi[\rho, \phi, z] \rightarrow e^{i k z} c_1 \right\} \right\}$$

ψ[ρ, φ, z] /. eq52

$$\left\{ e^{i k z} c_1 \right\}$$

eq41 = Lz[ψ[ρ, φ, z]] == m ħ ψ[ρ, φ, z] // Simplify

$$-i \hbar \psi^{(\theta, 1, \theta)}[\rho, \phi, z] = m \hbar \psi[\rho, \phi, z]$$

eq42 = DSolve[eq41, ψ[ρ, φ, z], φ]

$$\left\{ \left\{ \psi[\rho, \phi, z] \rightarrow e^{i m \phi} c_1 \right\} \right\}$$

eq51 = pz[ψ[ρ, φ, z]] == ħ kz ψ[ρ, φ, z] // Simplify

$$-i \hbar \psi^{(\theta, \theta, 1)}[\rho, \phi, z] = k z \hbar \psi[\rho, \phi, z]$$

eq52 = DSolve[eq51, ψ[ρ, φ, z], z] // Simplify

$$\left\{ \left\{ \psi[\rho, \phi, z] \rightarrow e^{i k z} c_1 \right\} \right\}$$

ψ[ρ, φ, z] /. eq52

$$\left\{ e^{i k z} c_1 \right\}$$

The form of the wave function

rule2 = {ψ → (χ[#1] Exp[i m #2] Exp[i kz #3] &)};

eq61 = eq11 /. rule2 // FullSimplify

$$\frac{1}{2 \mu \rho^2} e^{i(kz + m\phi)} \left((-2 E_1 \mu \rho^2 + (m^2 + kz^2 \rho^2) \hbar^2 + 2 \mu \rho^2 V_1[\rho]) \chi[\rho] - \rho \hbar^2 (\chi'[\rho] + \rho \chi''[\rho]) \right)$$

14. Summary

The differential operator in the Mathematica can be made with the Function function. Using the above Mathematica program, one may solve more complicated problems in quantum mechanics (circular cylindrical coordinates).

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