Vector Analysis for quantum mechanics

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Here we show Mathematica programs for the calculations of Laplacian, gradient, divergence, and rotation in the spherical co-ordinates and the cylindrical co-ordinates, as well as the Cartesian co-ordinates. These programs are very useful for the discussions on a variety of topics, such as the central field problem on the electron motion near a hydrogen atom.

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1. Gradient ∇

$\nabla\varphi$ (φ; scalar) Nabra, gradient, del

The gradient φ is defined as

$$\nabla\varphi = \hat{x}\frac{\partial\varphi}{\partial x} + \hat{y}\frac{\partial\varphi}{\partial y} + \hat{z}\frac{\partial\varphi}{\partial z} = (\frac{\partial\varphi}{\partial x}, \frac{\partial\varphi}{\partial y}, \frac{\partial\varphi}{\partial z}) ; \quad \text{gradient of the scalar } \varphi$$

((**Example**))

$$f = f(r)$$

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

$$\begin{aligned}
\nabla f(r) &= \hat{x}\frac{\partial f}{\partial x} + \hat{y}\frac{\partial f}{\partial y} + \hat{z}\frac{\partial f}{\partial z} \\
&= \hat{x}\frac{df}{dr}\frac{\partial r}{\partial x} + \hat{y}\frac{df}{dr}\frac{\partial r}{\partial y} + \hat{z}\frac{df}{dr}\frac{\partial r}{\partial z} \\
&= \frac{1}{r}\frac{df}{dr}(x\hat{x} + y\hat{y} + z\hat{z}) \\
&= \frac{\boldsymbol{r}}{r}\frac{df}{dr} = \hat{\boldsymbol{r}}\frac{df}{dr}
\end{aligned}$$

where

$$\frac{\partial r}{\partial x} = \frac{x}{r}, \qquad \frac{\partial r}{\partial y} = \frac{y}{r}, \qquad \frac{\partial r}{\partial z} = \frac{z}{r} .$$

2. Divergence

Now we define the divergence of the vector as

$$\nabla \cdot \boldsymbol{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}.$$

(A) $\nabla \cdot \boldsymbol{F}$ is a real scalar.

(B) **Definition of solenoid**

$\nabla \cdot \boldsymbol{B} = 0$. $\leftrightarrow$ $\boldsymbol{B}$ is said to be soloenoid.

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3. $\nabla \times \boldsymbol{F}$

We define the rotation of the vector as

$$\boldsymbol{W} = \nabla \times \boldsymbol{F} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_x & F_y & F_z \end{vmatrix}.$$

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4. Successive application of ∇

(i) $\nabla \cdot (\nabla \varphi)$

This is defined by a Laplacian,

$$\nabla \cdot \nabla \varphi = \nabla^2 \varphi = \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2}.$$

The equation $\nabla^2 \varphi = 0$ is called as the *Laplace equation*.

(ii) $\nabla \varphi$ is irrotational.

$$\nabla \times (\nabla \varphi) = 0,$$

since

$$\nabla \times (\nabla \varphi) = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ \frac{\partial \varphi}{\partial x} & \frac{\partial \varphi}{\partial y} & \frac{\partial \varphi}{\partial z} \end{vmatrix} = 0.$$

Thus $\nabla\varphi$ is irrotational.

(iii) $(\nabla\times\boldsymbol{F})$ is solenoid.

$$\nabla\cdot(\nabla\times\boldsymbol{F}) = \begin{vmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial x} & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_x & F_y & F_z \end{vmatrix} = 0 .$$

(iv) Formula

$$\nabla\times(\nabla\times\boldsymbol{F}) = \nabla(\nabla\cdot\boldsymbol{F}) - \nabla^2\boldsymbol{F} .$$

((Proof))
We use the formula given by

$$\boldsymbol{A}\times(\boldsymbol{B}\times\boldsymbol{C}) = \boldsymbol{B}(\boldsymbol{A}\cdot\boldsymbol{C}) - (\boldsymbol{A}\cdot\boldsymbol{B})\boldsymbol{C} .$$

with $\boldsymbol{A} = \nabla$, $\boldsymbol{B} = \nabla$, and $\boldsymbol{C} = \boldsymbol{F}$. Then we find

$$\nabla\times(\nabla\times\boldsymbol{F}) = \nabla(\nabla\cdot\boldsymbol{F}) - \nabla^2\boldsymbol{F} .$$

((Example)) Calculations

If $\boldsymbol{A} = (x^2 y, -2xz, 2yz)$, find $\nabla\times\boldsymbol{A}$, $\nabla\times(\nabla\times\boldsymbol{A})$, and $\nabla\times(\nabla\times(\nabla\times\boldsymbol{A}))$.

We use the Mathematica.

```
Clear["Gobal`"];

Needs["VectorAnalysis`"]

SetCoordinates[Cartesian[x, y, z]];

A1 = {x^2 y, -2 x z , 2 y z};

Curl[A1]

{2 x + 2 z, 0, -x^2 - 2 z}

Curl[Curl[A1]]

{0, 2 + 2 x, 0}

Curl[Curl[Curl[A1]]]

{0, 0, 2}
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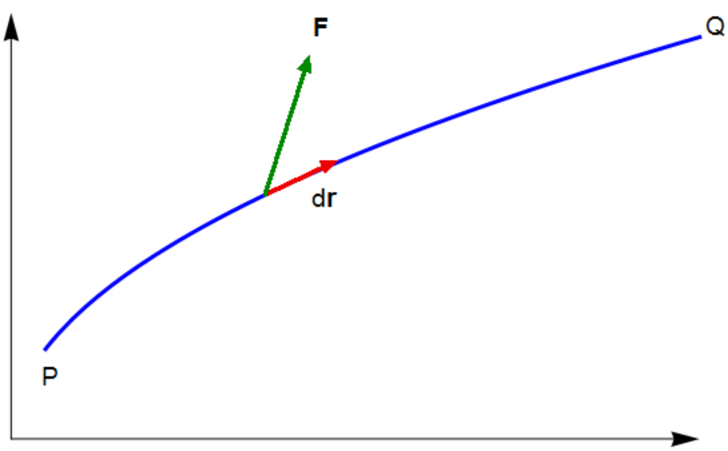
5. Line and surface integral

We consider about the line integral

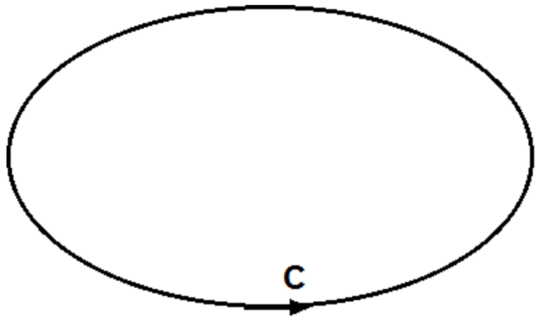


$$I = \int_{PQ} \mathbf{A} \cdot d\mathbf{r} \,,$$

where $|d\mathbf{r}| = ds$ and the tangential component is assumed to be As'

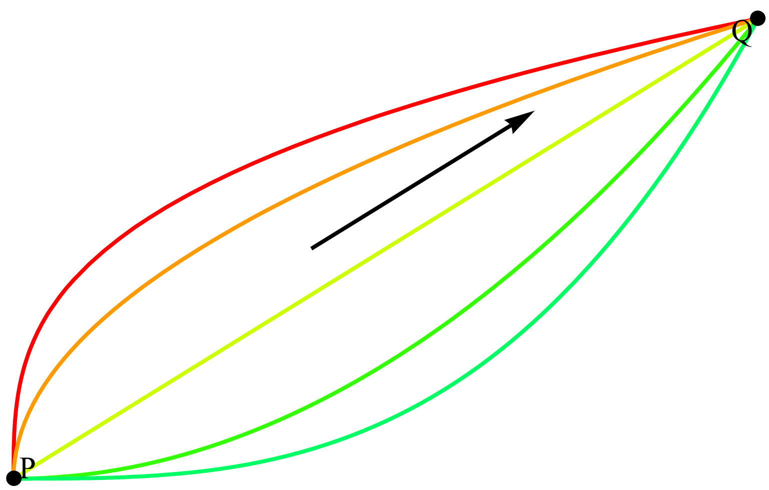
$$I = \int_{PQ} A_s ds \,.$$

If the contour is closed, we can write down as



$$\oint \boldsymbol{A} \cdot d\boldsymbol{r} \, .$$

In general the line integral depends on the choice of path. If $\boldsymbol{F} = \nabla \varphi$ (φ; scalar)



$$I = \int_{PQ} \boldsymbol{F} \cdot d\boldsymbol{r} = \int_{PQ} \nabla \varphi \cdot d\boldsymbol{r} = \varphi(Q) - \varphi(P) \, .$$

This value does not depend on the path of integral.

6. Surface Integral

$\hat{n}$ normal vector to the surface

$$d\boldsymbol{a} = \boldsymbol{n} da \, . \qquad \text{(}da\text{; area element)}$$

Then the surface integral is defined by

$$\int_S \boldsymbol{F} \cdot d\boldsymbol{a} = \int_S \boldsymbol{F} \cdot \boldsymbol{n} da \, .$$

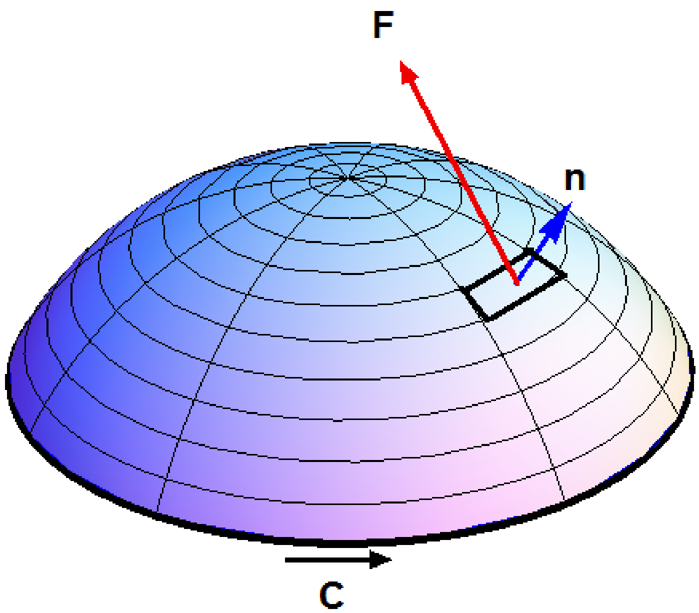
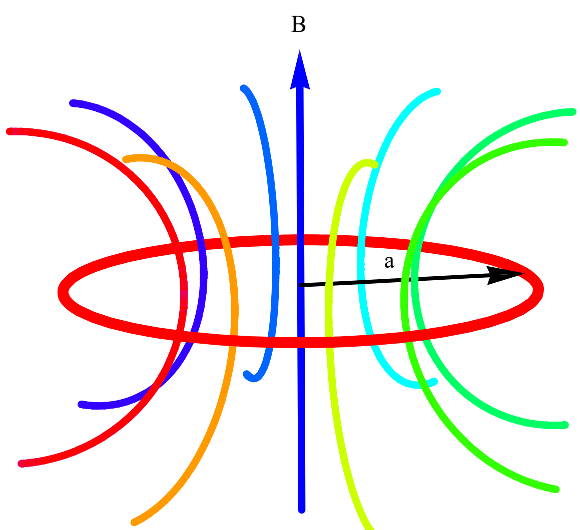


Fig. Right-hand rule for the positive normal.

If $\boldsymbol{F}$ corresponds to the magnetic field; $\boldsymbol{F} = \boldsymbol{B}$,

$\Phi = \int_S \boldsymbol{B} \cdot d\boldsymbol{a}$ is a magnetic flux through the area element S.



7. Gauss's theorem

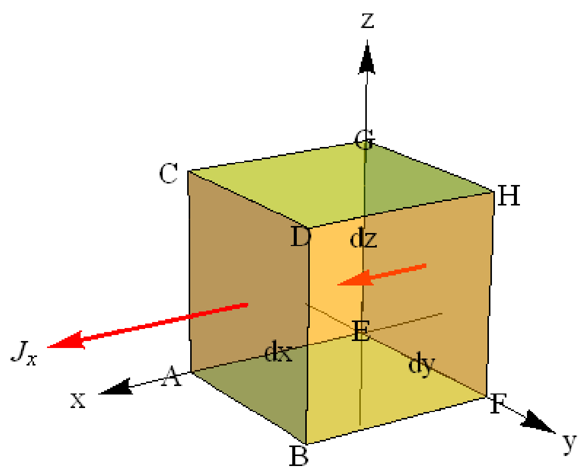
Here we define the volume integral as

$$\int_V \phi d\tau ,$$

where ϕ is a scalar.

(i) Gauss's theorem

$$\int_V \nabla \cdot \boldsymbol{F} d\tau = \int_S \boldsymbol{F} \cdot d\boldsymbol{a} .$$



First we consider the physical interpretation of $\nabla \cdot \boldsymbol{F}$. Suppose that $\boldsymbol{F}$ = $\boldsymbol{J}$ (current density). The current coming out through ABCD is

$$J_x |_{x=dx} \, dydz = (J_x |_{x=0} + \frac{\partial J_x}{\partial x} dx) dydz .$$

The current coming in through EFGH is equal to

$$J_x |_{x=0} \, dydz .$$

Thus the net current through EFGH is equal to

$$\frac{\partial J_x}{\partial x} dxdydz .$$

Thus the net current along the x direction through this small region is

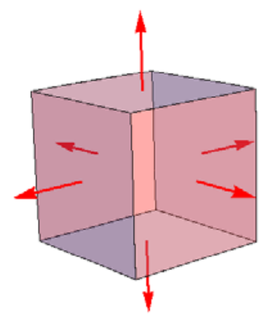
$$\frac{\partial J_x}{\partial x} dxdydz .$$

Similarly for the y and z components, we have the net current along the y-direction and z-direction through the small region as

$$\frac{\partial J_y}{\partial y} dxdydz , \qquad \frac{\partial J_z}{\partial z} dxdydz ,$$

respectively. Therefore the net current coming out through the volume element $d\tau = dxdydz$ can be expressed by

$$\sum_{\substack{Six\\surface}} \boldsymbol{J} \cdot d\boldsymbol{a} = (\nabla \cdot \boldsymbol{J}) d\tau .$$

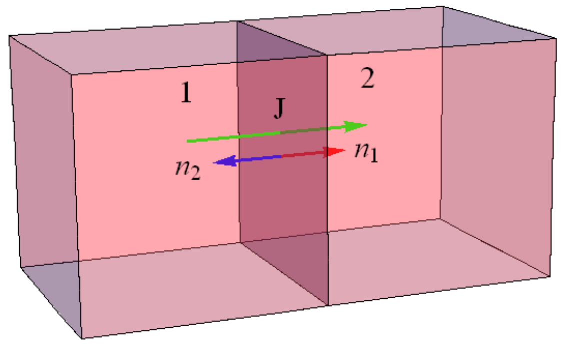


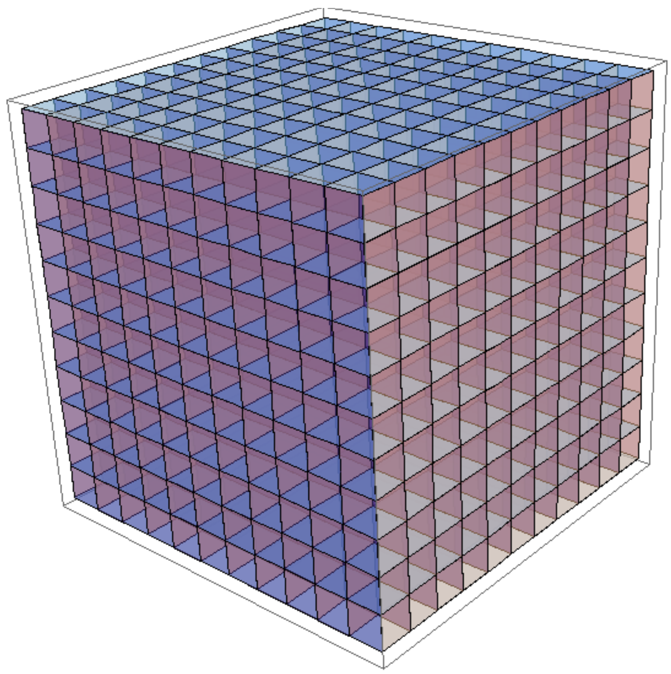
Summing over all parallel-pipes, we find that $\boldsymbol{J} \cdot d\boldsymbol{a}$ terms cancel out for all interior faces. Only the contributions of the exterior surface survive.

$$\sum_{\substack{exterior\\surface}} \boldsymbol{J} \cdot d\boldsymbol{a} = \sum_{volume} (\nabla \cdot \boldsymbol{J}) d\tau ,$$

or

$$\int_A \boldsymbol{J} \cdot d\boldsymbol{a} = \int_V \nabla \cdot \boldsymbol{J} d\tau . \qquad \text{(Gauss' theorem)}$$





(ii) **Gauss' theorem**

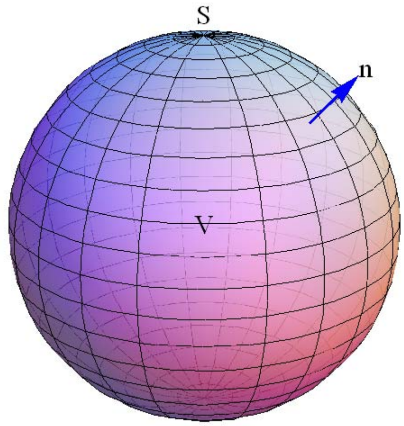
Let $\boldsymbol{F}$ be a continuous and differentiable vector throughtout a region V of the space. Then

$$\int_S \boldsymbol{F}\cdot d\boldsymbol{a} = \int_S \boldsymbol{F}\cdot \boldsymbol{n} da = \int_V \nabla\cdot \boldsymbol{F} d\tau ,$$

where the surface integral is taken over the entire surface that encloses V.

((**Example-1**))

In the maxwell's equation, we have



$$\nabla \cdot \boldsymbol{E} = \frac{\rho}{\varepsilon_0},$$

where ρ is the charge density. From the Gauss's law, we have

$$\int_V \nabla \cdot \boldsymbol{E} d\tau = \int_V \frac{\rho}{\varepsilon_0} d\tau = \int_S \boldsymbol{E} \cdot d\boldsymbol{a} .$$

We assume that the volume V is formed of sphere with radius r. From the symmetry, $\boldsymbol{E}$ is perpendicular to the sphere surfaces,

$$\boldsymbol{E} = E_r \boldsymbol{e}_r .$$

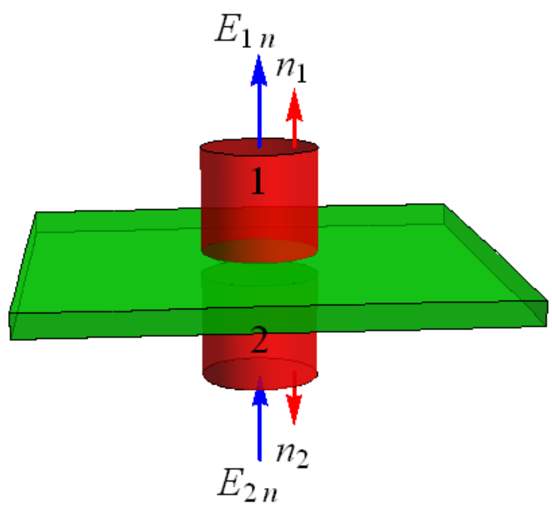
Thus we have

$$\int_V \frac{\rho}{\varepsilon_0} d\tau = \int_S E_r \boldsymbol{e}_r \cdot d\boldsymbol{a} .$$

Since $Q = \int_V \rho d\tau$, we get

$$E_r = \frac{Q}{4\pi\varepsilon_0 r^2} . \qquad \text{(Coulomb's law)}$$

((**Example-2**))



$$\nabla \cdot \boldsymbol{E} = 0,$$

if $\rho = 0$.

From the Gauss's law, we have

$$\int_V \nabla \cdot \boldsymbol{E} d\tau = \int_V \frac{\rho}{\varepsilon_0} d\tau = 0 = \int_S \boldsymbol{E} \cdot d\boldsymbol{a}.$$

E_{1n} and E_{2n} are the normal components of $\boldsymbol{E}_1$ and $\boldsymbol{E}_2$. Then we have

$$(E_{1n} - E_{2n})\Delta a = 0.$$

Therefore we have the boundary condition for $\boldsymbol{E}$ as

$$E_{1n} = E_{2n}.$$

8. Green's theorem

$$\int_V (\psi\nabla^2\phi - \phi\nabla^2\psi) d\tau = \int_S (\psi\nabla\phi - \phi\nabla\psi) \cdot d\mathbf{a}.$$

((**Proof**)) In the Gauss's theorem, we put

$$\mathbf{A} = \psi\nabla\phi.$$

Then we have

$$I_1 = \int_V \nabla \cdot \boldsymbol{A} d\tau = \int_V \nabla \cdot (\psi \nabla \phi) d\tau = \int_S (\psi \nabla \phi) \cdot d\boldsymbol{a} .$$

Noting that

$$\nabla \cdot (\psi \nabla \phi) = \psi \nabla^2 \phi + \nabla \psi \cdot \nabla \phi ,$$

we have

$$I_1 = \int_V (\psi \nabla^2 \phi + \nabla \psi \cdot \nabla \phi) d\tau = \int_S (\psi \nabla \phi) \cdot d\mathbf{a} .$$

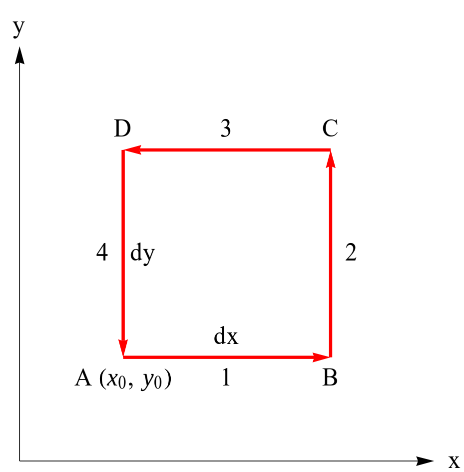
By replacing $\psi \leftrightarrow \phi$, we also have

$$I_1 = \int_V (\phi \nabla^2 \psi + \nabla \phi \cdot \nabla \psi) d\tau = \int_S (\phi \nabla \psi) \cdot d\mathbf{a} .$$

Thus we find the Green's theorem

$$I_1 - I_2 = \int_V (\psi \nabla^2 \phi - \phi \nabla^2 \psi) d\tau = \int_S (\psi \nabla \phi - \phi \nabla \psi) \cdot d\mathbf{a} .$$

9. Stokes' theorem



$$\begin{aligned}\oint \boldsymbol{F}\cdot d\boldsymbol{l} &= (circulation)_{1234}\\ &= \int_1 F_x dx + \int_2 F_y dy - \int_3 F_x dx - \int_4 F_y dy\\ &= \int_1 \{F_x(x,y_0) - F_x(x,y_0+dy)\}dx + \int_2 \{F_y(x_0+dx,y) - F_y(x_0,y)\}dy\end{aligned}$$

Note that

$$F_x(x,y_0+dy) - F_x(x,y_0) = \left(\frac{\partial F_x}{\partial y}\right)_{x_0,y_0} dy$$

$$F_y(x_0+dx,y) - F_y(x_0,y) = \left(\frac{\partial F_y}{\partial x}\right)_{x_0,y_0} dx$$

Then we have

$$(circulation)_{1234} = (\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y})dxdy = (\nabla\times\boldsymbol{F})_z\, dxdy\ .$$

We can write down this as

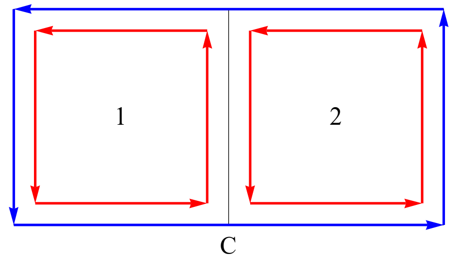
$$\sum_{\substack{Four\\ sides}} \boldsymbol{F}\cdot d\boldsymbol{l} = (\nabla\times\boldsymbol{F})\cdot\boldsymbol{e}_z dxdy = (\nabla\times\boldsymbol{F})\cdot d\boldsymbol{a}_1\ ,$$

where

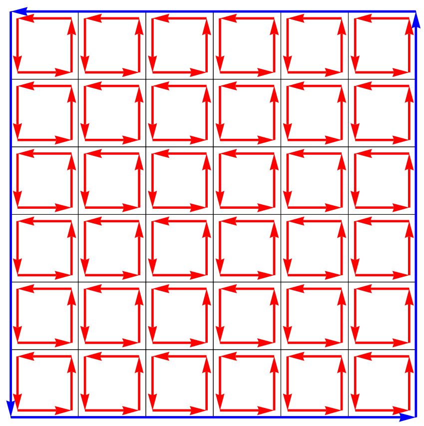
$$d\boldsymbol{a}_1 = \boldsymbol{e}_z dxdy\ .$$

Imagine that paths 1 and 2 are expanded out until they coalesce with path C (or path 3). Since the line integrals of $\boldsymbol{F}$ along the potions that 1 and 2 have in common will cancel each other,

$$\begin{aligned}&\oint_C \boldsymbol{F}\cdot d\boldsymbol{l}\\ &= \oint_1 \boldsymbol{F}\cdot d\boldsymbol{l} + \oint_2 \boldsymbol{F}\cdot d\boldsymbol{l}\\ &= (\nabla\times\boldsymbol{F})\cdot d\boldsymbol{a}_1 + (\nabla\times\boldsymbol{F})\cdot d\boldsymbol{a}_2 = \int_{1,2}(\nabla\times\boldsymbol{F})\cdot d\boldsymbol{a}\end{aligned}\ .$$



Now let the surface S be divided up into a large number N of elements.

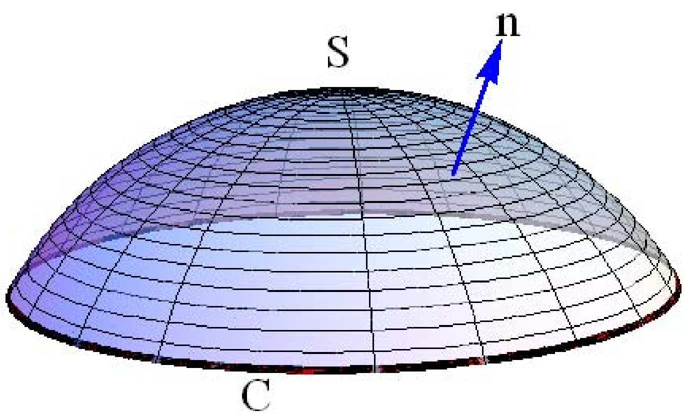


The above idea is extended to arrive at

$$\oint_C \boldsymbol{F} \cdot d\boldsymbol{l} = \int_S (\nabla \times \boldsymbol{F}) \cdot d\boldsymbol{a} .$$

((Stoke's theorem))
Let S be a surface of any shape bounded by a closed curve C. If F is a vector, then

$$\oint_C \boldsymbol{F} \cdot d\boldsymbol{l} = \int_S (\nabla \times \boldsymbol{F}) \cdot d\boldsymbol{a} = \int_S (\nabla \times \boldsymbol{F}) \cdot \boldsymbol{n} da .$$



10 Curvilinear co-ordinates

10.1 General definition

We consider that new co-ordinate (q_1, q_2, q_3) are related to (x, y, z) through

$$x = x(q_1, q_2, q_3) \qquad\qquad q_1 = q_1(x, y, z)$$
$$y = y(q_1, q_2, q_3) \qquad \text{or} \qquad q_2 = q_2(x, y, z)$$
$$z = z(q_1, q_2, q_3) \qquad\qquad q_3 = q_3(x, y, z)$$

Since

$$d\mathbf{r} = \frac{\partial \mathbf{r}}{\partial q_1} dq_1 + \frac{\partial \mathbf{r}}{\partial q_2} dq_2 + \frac{\partial \mathbf{r}}{\partial q_3} dq_3 = \sum_j \frac{\partial \mathbf{r}}{\partial q_j} dq_j \ ,$$

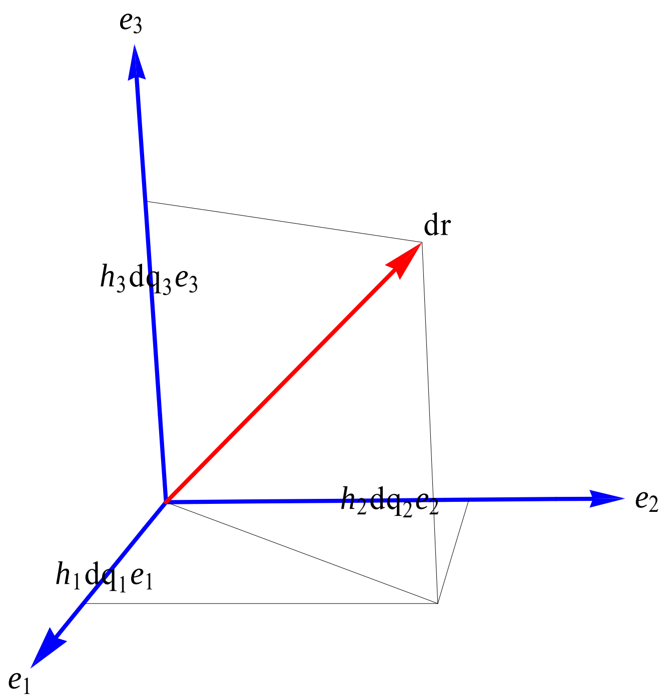
we have

$$ds^2 = d\mathbf{r} \cdot d\mathbf{r} = \sum_{i,j} \left(\frac{\partial \mathbf{r}}{\partial q_i} \cdot \frac{\partial \mathbf{r}}{\partial q_j}\right) dq_i dq_j = \sum_{i,j} g_{ij} dq_i dq_j \ ,$$

where

$$g_{ij} = \frac{\partial \mathbf{r}}{\partial q_i} \cdot \frac{\partial \mathbf{r}}{\partial q_j} = \frac{\partial x}{\partial q_i} \cdot \frac{\partial x}{\partial q_j} + \frac{\partial y}{\partial q_i} \cdot \frac{\partial y}{\partial q_j} + \frac{\partial z}{\partial q_i} \cdot \frac{\partial z}{\partial q_j} \ \text{(second rank tensor).}$$

We now consider the general coordinate system. The relation between the constants h_1, h_2, and h_3 and the tensor g_{ij} will be discussed later.



$$
\begin{aligned}
d\boldsymbol{r} &= ds_1\boldsymbol{e}_1 + ds_2\boldsymbol{e}_2 + ds_3\boldsymbol{e}_3 \\
&= h_1 dq_1\boldsymbol{e}_1 + h_2 dq_2\boldsymbol{e}_2 + h_3 dq_3\boldsymbol{e}_3 \\
&= \sum_i h_i dq_i \boldsymbol{e}_i
\end{aligned}
$$

$$
ds^2 = d\boldsymbol{r}\cdot d\boldsymbol{r} = \sum_{i,j} h_i h_j dq_i dq_j (\boldsymbol{e}_i \cdot \boldsymbol{e}_i),
$$

or we have

$$
g_{ij} = h_i h_j (\boldsymbol{e}_i \cdot \boldsymbol{e}_i),
$$

or

$$
g_{ii} = h_i^2 .
$$

Then

$$
\frac{g_{ij}}{\sqrt{g_{ii} g_{jj}}} = (\boldsymbol{e}_i \cdot \boldsymbol{e}_i) .
$$

Now we limit ourselves to orthogonal co-ordinate system.

g_{ij} for $i \neq j$.

In order to simplify the notation, we use $g_{ii} = h_i^2$, so that

$$ds^2 = \sum_i (h_i dq_i)^2$$

$$\begin{aligned} d\boldsymbol{r} &= ds_1\boldsymbol{e}_1 + ds_2\boldsymbol{e}_2 + ds_3\boldsymbol{e}_3 \\ &= h_1 dq_1\boldsymbol{e}_1 + h_2 dq_2\boldsymbol{e}_2 + h_3 dq_3\boldsymbol{e}_3 \\ &= \sum_i h_i dq_i \boldsymbol{e}_i \end{aligned}$$

Where $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, and $\boldsymbol{e}_3$ are unit vectors which are perpendicular to each other.

$$\boldsymbol{e}_1 = \frac{1}{h_1}\frac{\partial \boldsymbol{r}}{\partial q_1} = \frac{\partial \boldsymbol{r}}{\partial s_1}$$
$$\boldsymbol{e}_2 = \frac{1}{h_2}\frac{\partial \boldsymbol{r}}{\partial q_2} = \frac{\partial \boldsymbol{r}}{\partial s_2}$$
$$\boldsymbol{e}_3 = \frac{1}{h_3}\frac{\partial \boldsymbol{r}}{\partial q_3} = \frac{\partial \boldsymbol{r}}{\partial s_3}$$

where

$$h_i^2 = g_{ii} = \frac{\partial \boldsymbol{r}}{\partial q_i} \cdot \frac{\partial \boldsymbol{r}}{\partial q_j},$$

or

$$h_i = \sqrt{g_{ii}} = \sqrt{\frac{\partial \boldsymbol{r}}{\partial q_i} \cdot \frac{\partial \boldsymbol{r}}{\partial q_i}} = \sqrt{\left(\frac{\partial x}{\partial q_i}\right)^2 + \left(\frac{\partial y}{\partial q_i}\right)^2 + \left(\frac{\partial z}{\partial q_i}\right)^2}\ .\ \text{(second rank tensor).}$$

The volume element for an orthogonal curvilinear coordinate system is given by

$$dV = h_1 dq_1 \mathbf{e}_1 \cdot \{(h_2 dq_2 \mathbf{e}_2) \times (h_3 dq_3 \mathbf{e}_3)\} = h_1 h_2 h_3 dq_1 dq_2 dq_3\ .$$

10.2 Spherical coordinate

(i) Unit vectors

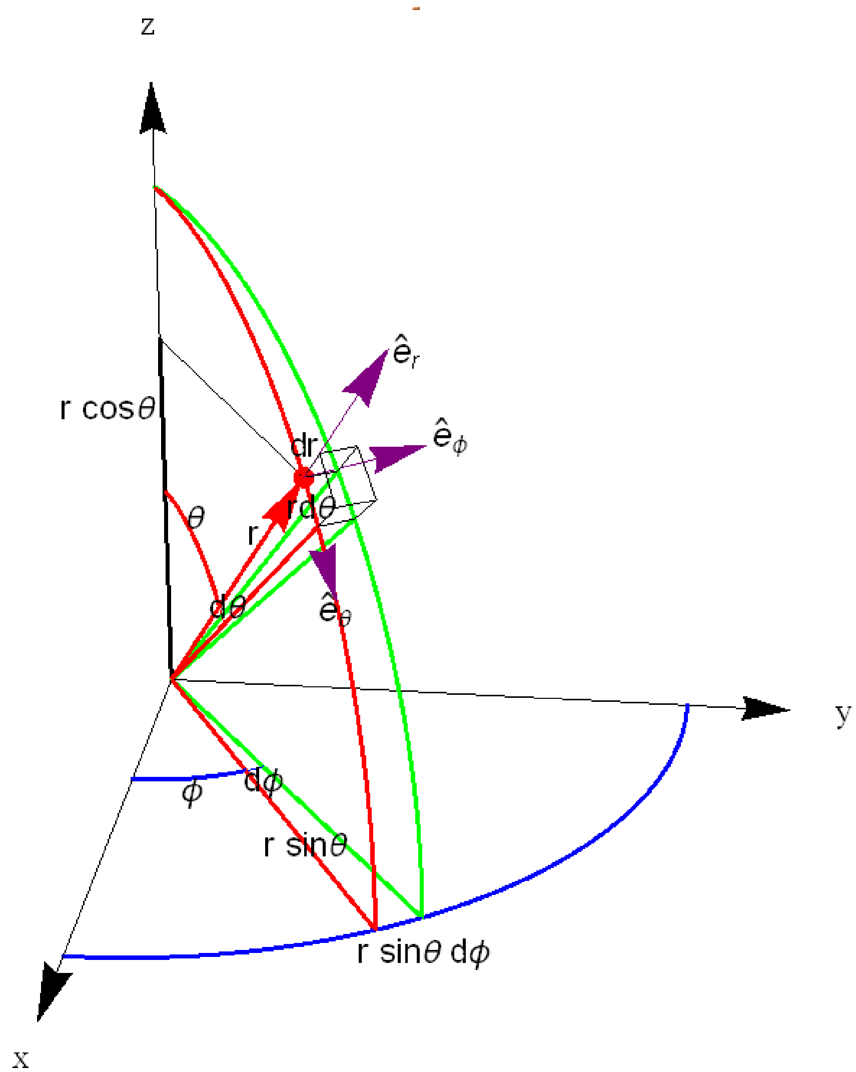
The position of a point P with Cartesian coordinates x, y, and z may be expressed in terms of r, θ, and ϕ of the spherical coordinates;

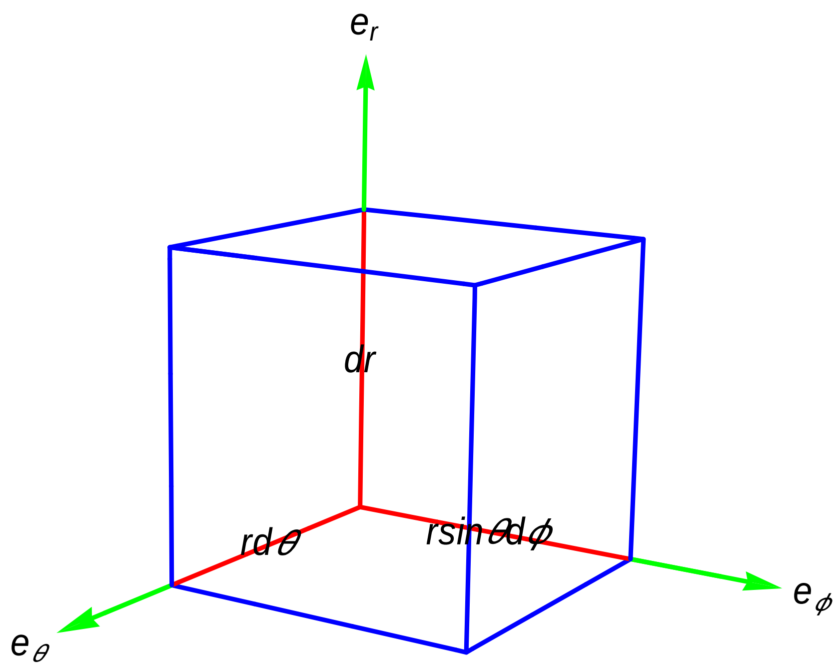
$$x = r\sin\theta\cos\phi, \qquad y = r\sin\theta\sin\phi, \qquad z = r\cos\theta,$$

or

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

$$d\boldsymbol{r} = \sum_{j=1}^{3}\boldsymbol{e}_j ds_j = \sum_{j=1}^{3}\boldsymbol{e}_j h_j dq_j .$$





$$h_r = \sqrt{\left(\frac{\partial x}{\partial r}\right)^2 + \left(\frac{\partial y}{\partial r}\right)^2 + \left(\frac{\partial z}{\partial r}\right)^2} = 1$$

$$h_\theta = \sqrt{\left(\frac{\partial x}{\partial \theta}\right)^2 + \left(\frac{\partial y}{\partial \theta}\right)^2 + \left(\frac{\partial z}{\partial \theta}\right)^2} = r$$

$$h_\phi = \sqrt{\left(\frac{\partial x}{\partial \phi}\right)^2 + \left(\frac{\partial y}{\partial \phi}\right)^2 + \left(\frac{\partial z}{\partial \phi}\right)^2} = r\sin\theta$$

or

$$d\boldsymbol{r} = h_r\boldsymbol{e}_r dr + h_\theta \boldsymbol{e}_\theta d\theta + h_\phi \boldsymbol{e}_\phi d\phi =_r \boldsymbol{e}_r dr + r\boldsymbol{e}_\theta d\theta + r\sin\theta \boldsymbol{e}_\phi d\phi ,$$

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

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

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

This can be described using a matrix A as

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

or by using the inverse matrix A^{-1} as

$$\begin{pmatrix} \boldsymbol{e}_x \\ \boldsymbol{e}_y \\ \boldsymbol{e}_z \end{pmatrix} = \boldsymbol{A}^{-1} \begin{pmatrix} \boldsymbol{e}_r \\ \boldsymbol{e}_\theta \\ \boldsymbol{e}_\phi \end{pmatrix} = \boldsymbol{A}^{T} \begin{pmatrix} \boldsymbol{e}_r \\ \boldsymbol{e}_\theta \\ \boldsymbol{e}_\phi \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \cos\theta\cos\phi & -\sin\phi \\ \sin\theta\sin\phi & \cos\theta\sin\phi & \cos\phi \\ \cos\theta & -\sin\theta & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{e}_r \\ \boldsymbol{e}_\theta \\ \boldsymbol{e}_\phi \end{pmatrix}.$$

or

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

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

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

in the spherical coordinate systems.

(ii) Solid angle

An object's solid angle in steradians is equal to the area of the segment of a unit sphere, centered at the angle's vertex, that the object covers. A solid angle in steradians equals the area of a segment of a unit sphere in the same way a planar angle in radians equals the length of an arc of a unit circle.

The area element dA:

$$dA = (rd\theta)(r\sin\theta d\phi) = r^2\sin\theta d\theta d\phi = r^2 d\Omega.$$

where the solid $d\Omega$ is given by

$$\sin\theta d\theta d\phi = d\Omega.$$

The volume element:

$$dV = drdA = r^2 dr d\Omega.$$

(iii) $\nabla\psi$

From the definition of $\nabla\psi$, we have

$$\nabla\psi = \sum_{j=1}^{3} \boldsymbol{e}_j \frac{\partial\psi}{\partial s_j} = \sum_{j=1}^{3} \boldsymbol{e}_j \frac{\partial\psi}{h_j \partial q_j},$$

or,

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

where ψ is a scalar function of r, θ, and ϕ.

(iv) $\nabla\cdot\boldsymbol{A}$

When a vector $\boldsymbol{A}$ is defined by

$$\boldsymbol{A} = A_r\boldsymbol{e}_r + A_\theta\boldsymbol{e}_\theta + A_\phi\boldsymbol{e}_\phi .$$

The divergence is given by

$$\nabla\cdot\boldsymbol{A} = \frac{1}{h_r h_\theta h_\phi}[\frac{\partial}{\partial r}(h_\theta h_\phi A_r) + \frac{\partial}{\partial\theta}(h_\phi h_r A_\theta) + \frac{\partial}{\partial\phi}(h_r h_\theta A_\phi)]$$
$$= \frac{1}{r^2\sin\theta}[\frac{\partial}{\partial r}(r^2\sin\theta A_r) + \frac{\partial}{\partial\theta}(r\sin\theta A_\theta) + \frac{\partial}{\partial\phi}(rA_\phi)]$$

or

$$\nabla\cdot\boldsymbol{A} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 A_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_\theta) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}A_\phi .$$

(v) $\nabla\times\boldsymbol{A}$

$\nabla\times\boldsymbol{A}$ is given by

$$\nabla\times\boldsymbol{A} = \frac{1}{h_r h_\theta h_\phi}\begin{vmatrix} h_r\boldsymbol{e}_r & h_\theta\boldsymbol{e}_\theta & h_\phi\boldsymbol{e}_\phi \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial\theta} & \frac{\partial}{\partial\phi} \\ h_r A_r & h_\theta A_\theta & h_\phi A_\phi \end{vmatrix} = \frac{1}{r^2\sin\theta}\begin{vmatrix} \boldsymbol{e}_r & r\boldsymbol{e}_\theta & r\sin\theta\boldsymbol{e}_\phi \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial\theta} & \frac{\partial}{\partial\phi} \\ A_r & rA_\theta & r\sin\theta A_\phi \end{vmatrix}$$

(vi) Laplacian

$$\nabla^2\psi = \frac{1}{h_r h_\theta h_\phi}[\frac{\partial}{\partial r}(\frac{h_\theta h_\phi}{h_r}\frac{\partial \psi}{\partial r}) + \frac{\partial}{\partial \theta}(\frac{h_\phi h_r}{h_\theta}\frac{\partial \psi}{\partial \theta}) + \frac{\partial}{\partial \phi}(\frac{h_r h_\theta}{h_\phi}\frac{\partial \psi}{\partial \phi})]$$

$$= \frac{1}{r^2 \sin\theta}[\frac{\partial}{\partial r}(r^2 \sin\theta \frac{\partial \psi}{\partial r}) + \frac{\partial}{\partial \theta}(\sin\theta \frac{\partial \psi}{\partial \theta}) + \frac{\partial}{\partial \phi}(\frac{1}{\sin\theta}\frac{\partial \psi}{\partial \phi})]$$

$$= \frac{1}{r^2 \sin\theta}[\sin\theta \frac{\partial}{\partial r}(r^2 \frac{\partial \psi}{\partial r}) + \frac{\partial}{\partial \theta}(\sin\theta \frac{\partial \psi}{\partial \theta}) + \frac{1}{\sin\theta}\frac{\partial^2 \psi}{\partial \phi^2}]$$

or

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

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

We can rewrite the first term of the right hand side as

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial \psi}{\partial r}) = \frac{1}{r}\frac{\partial}{\partial r^2}(r\psi),$$

which can be useful in shortening calculations.

Note that we also use the expression for the operator

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

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

11. **Mathematica-1**

We derive the above formula using the Mathematica.

We use the Spherical co-rdinate.
We need a Vector Analysis Package. We also need SetCordinatinates.In this system the vector is expressed in terms of (Ar, Aθ, Aϕ)

```
Clear["Gobal`"]; Gra := Grad[#, {r, θ, ϕ}, "Spherical"] &;
Diva := Div[#, {r, θ, ϕ}, "Spherical"] &;
Curla := Curl[#, {r, θ, ϕ}, "Spherical"] &;
Lap := Laplacian[#,  {r, θ, ϕ}, "Spherical"] &;
```

```
eq1 = Lap[ψ[r, θ, ϕ]] // Simplify
```

$$\frac{1}{r^2}\left(\mathrm{Csc}[\theta]^2\,\psi^{(0,0,2)}[r,\theta,\phi]+\mathrm{Cot}[\theta]\,\psi^{(0,1,0)}[r,\theta,\phi]+\psi^{(0,2,0)}[r,\theta,\phi]+2\,r\,\psi^{(1,0,0)}[r,\theta,\phi]+r^2\,\psi^{(2,0,0)}[r,\theta,\phi]\right)$$

```
eq2 = Gra[ψ[r, θ, ϕ]]
```

$$\left\{\psi^{(1,0,0)}[r,\theta,\phi],\ \frac{\psi^{(0,1,0)}[r,\theta,\phi]}{r},\ \frac{\mathrm{Csc}[\theta]\,\psi^{(0,0,1)}[r,\theta,\phi]}{r}\right\}$$

```
A = {Ar[r, θ, ϕ], Aθ[r, θ, ϕ], Aϕ[r, θ, ϕ]};
```

```
eq3 = Curla[A] // Simplify
```

$$\left\{\frac{1}{r}\left(A\phi[r,\theta,\phi]\,\mathrm{Cot}[\theta]-\mathrm{Csc}[\theta]\,A\theta^{(0,0,1)}[r,\theta,\phi]+A\phi^{(0,1,0)}[r,\theta,\phi]\right),\ -\frac{1}{r}\left(A\phi[r,\theta,\phi]-\mathrm{Csc}[\theta]\,Ar^{(0,0,1)}[r,\theta,\phi]+r\,A\phi^{(1,0,0)}[r,\theta,\phi]\right),\ \frac{1}{r}\left(A\theta[r,\theta,\phi]-Ar^{(0,1,0)}[r,\theta,\phi]+r\,A\theta^{(1,0,0)}[r,\theta,\phi]\right)\right\}$$

```
eq3 = Diva[A] // Simplify
```

$$\frac{1}{r}\left(2\,Ar[r,\theta,\phi]+A\theta[r,\theta,\phi]\,\mathrm{Cot}[\theta]+\mathrm{Csc}[\theta]\,A\phi^{(0,0,1)}[r,\theta,\phi]+A\theta^{(0,1,0)}[r,\theta,\phi]+r\,Ar^{(1,0,0)}[r,\theta,\phi]\right)$$

12. Quantum mechanical orbital angular momentum

The orbital angular momentum in the quantum mechanics is defined by

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = -i\hbar(\boldsymbol{r} \times \nabla),$$

using the expression

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

in the spherical coordinate. Then we have

$$\boldsymbol{L} = -i\hbar(\boldsymbol{r} \times \nabla) = -i\hbar \boldsymbol{e}_r r \times (\boldsymbol{e}_r \frac{\partial}{\partial r} + \boldsymbol{e}_\theta \frac{1}{r}\frac{\partial}{\partial \theta} + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi})$$

$$= i\hbar(-\boldsymbol{e}_\phi \frac{\partial}{\partial \theta} + \boldsymbol{e}_\theta \frac{1}{\sin\theta}\frac{\partial}{\partial \phi})$$

.

The angular momentum L_x, L_y, and L_z (Cartesian components) can be described by

$$\boldsymbol{L} = i\hbar[-(-\sin\phi \boldsymbol{e}_x + \cos\phi \boldsymbol{e}_y)\frac{\partial}{\partial \theta} + (\cos\theta\cos\phi \boldsymbol{e}_x + \cos\theta\sin\phi \boldsymbol{e}_y - \sin\theta \boldsymbol{e}_z)\frac{1}{\sin\theta}\frac{\partial}{\partial \phi}].$$

or

$$L_x = i\hbar(\sin\phi \frac{\partial}{\partial \theta} + \cot\theta\cos\phi \frac{\partial}{\partial \phi}),$$

$$L_y = i\hbar(-\cos\phi \frac{\partial}{\partial \theta} + \cot\theta\sin\phi \frac{\partial}{\partial \phi}),$$

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

We define L_+ and L_- as

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

and

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

We note that the operator ∇ can be expressed using the operator $\boldsymbol{L}$ as

$$\nabla = \boldsymbol{e}_r \frac{\partial}{\partial r} - \frac{i}{\hbar}\frac{\boldsymbol{r}\times\boldsymbol{L}}{r^2}.$$

The proof of this equation is given as follows.

$$\frac{(\boldsymbol{r}\times\boldsymbol{L})}{i\hbar} = r\boldsymbol{e}_r \times(-\boldsymbol{e}_\phi \frac{\partial}{\partial\theta} + \boldsymbol{e}_\theta \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}) = r(\boldsymbol{e}_\theta \frac{\partial}{\partial\theta} + \boldsymbol{e}_\phi \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}),$$

or

$$\frac{(\boldsymbol{r}\times\boldsymbol{L})}{i\hbar r^2} = \frac{1}{r}\boldsymbol{e}_\theta \frac{\partial}{\partial\theta} + \boldsymbol{e}_r \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} = \nabla - \boldsymbol{e}_r \frac{\partial}{\partial r},$$

or

$$\nabla = \boldsymbol{e}_r \frac{\partial}{\partial r} - \frac{i(\boldsymbol{r}\times\boldsymbol{L})}{\hbar r^2}.$$

From $\boldsymbol{L}^2 = L_x{}^2 + L_y{}^2 + L_z{}^2$, we have

$$\boldsymbol{L}^2 = -\hbar^2[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta})],$$

where the proof is given by Mathematica. Using

$$\frac{\boldsymbol{L}^2}{\hbar^2} = -r^2\nabla^2 + \frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}),$$

we can also prove that

$$r\nabla^2 - \nabla(1 + r\frac{\partial}{\partial r}) = \frac{i}{\hbar}\nabla\times\mathbf{L}.$$

((**Note**))

$$\nabla^2 = -\frac{1}{\hbar^2 r^2}\mathbf{L}^2 + \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})$$
$$= -\frac{1}{\hbar^2 r^2}\mathbf{L}^2 + \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})$$
$$= -\frac{1}{\hbar^2 r^2}\mathbf{L}^2 + \frac{1}{r}\frac{\partial^2}{\partial r^2}(r)$$

13. Mathematica

((Arfken))

2.5.13 From Exercise 2.5.12 show that

$$-i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\frac{\partial}{\partial \varphi}.$$

This is the quantum mechanical operator corresponding to the z-component of orbital angular momentum.

((Arfken))

2.5.14 With the quantum mechanical orbital angular momentum operator defined as $\mathbf{L} = -i(\mathbf{r} \times \nabla)$, show that

(a) $L_x + iL_y = e^{i\varphi}\left(\frac{\partial}{\partial \theta} + i\cot\theta\frac{\partial}{\partial \varphi}\right)$,

(b) $L_x - iL_y = -e^{-i\varphi}\left(\frac{\partial}{\partial \theta} - i\cot\theta\frac{\partial}{\partial \varphi}\right)$.

((Arfken))

2.5.15 Verify that $\mathbf{L} \times \mathbf{L} = i\mathbf{L}$ in spherical polar coordinates. $\mathbf{L} = -i(\mathbf{r} \times \nabla)$, the quantum mechanical orbital angular momentum operator.
Hint. Use spherical polar coordinates for $\mathbf{L}$ but Cartesian components for the cross product.

((Arfken))

2.5.16 (a) From Eq. (2.46) show that

$$\mathbf{L} = -i(\mathbf{r} \times \nabla) = i\left(\hat{\boldsymbol{\theta}}\frac{1}{\sin\theta}\frac{\partial}{\partial \varphi} - \hat{\boldsymbol{\varphi}}\frac{\partial}{\partial \theta}\right).$$

(b) Resolving $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\varphi}}$ into Cartesian components, determine L_x, L_y, and L_z in terms of θ, φ, and their derivatives.

(c) From $L^2 = L_x^2 + L_y^2 + L_z^2$ show that

$$\mathbf{L}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \varphi^2}$$
$$= -r^2\nabla^2 + \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right).$$

((**Arfken**))

2.5.17 With $\mathbf{L} = -i\mathbf{r} \times \nabla$, verify the operator identities

(a) $\nabla = \hat{\mathbf{r}}\frac{\partial}{\partial r} - i\frac{\mathbf{r} \times \mathbf{L}}{r^2}$,

(b) $\mathbf{r}\nabla^2 - \nabla\left(1 + r\frac{\partial}{\partial r}\right) = i\nabla \times \mathbf{L}$.

((**Arfken**))

2.5.18 Show that the following three forms (spherical coordinates) of $\nabla^2\psi(r)$ are equivalent:

(a) $\frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{d\psi(r)}{dr}\right]$; (b) $\frac{1}{r}\frac{d^2}{dr^2}[r\psi(r)]$; (c) $\frac{d^2\psi(r)}{dr^2} + \frac{2}{r}\frac{d\psi(r)}{dr}$.

((**Mathematica**))

Vector analysis
Angular momentum in the spherical coordinates
Here we use the angular momentum operatior in the unit of ℏ=1

```
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};
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 (Cross[(ur r), Gra[#]]) &) // Simplify;
 Lx := (ux.L[#] &) // Simplify; Ly := (uy.L[#] &) // Simplify;
 Lz := (uz.L[#] &) // Simplify;
```

Arfken 2.5 .16 (a)

$$\mathbf{L} = -i(\mathbf{r} \times \nabla) = i\left(\hat{\boldsymbol{\theta}}\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi} - \hat{\boldsymbol{\varphi}}\frac{\partial}{\partial\theta}\right).$$

```
L[ψ[r, θ, ϕ]] // Simplify
```

$\{0,\ i\,\mathrm{Csc}[\theta]\,\psi^{(0,0,1)}[r, \theta, \phi],\ -i\,\psi^{(0,1,0)}[r, \theta, \phi]\}$

Arfken 2.5.14, 2.5.16(b)

$$L_x + iL_y = e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right),$$

$$L_x - iL_y = -e^{-i\varphi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\varphi}\right).$$

Lz = $-i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\frac{\partial}{\partial\varphi}.$

```
Lx[ψ[r, θ, ϕ]] // FullSimplify

ⅈ (Cos[ϕ] Cot[θ] ψ^(0,0,1)[r, θ, ϕ] + Sin[ϕ] ψ^(0,1,0)[r, θ, ϕ])

Lx[ψ[r, θ, ϕ]] + ⅈ Ly[ψ[r, θ, ϕ]] // Simplify

(Cos[ϕ] + ⅈ Sin[ϕ]) (ⅈ Cot[θ] ψ^(0,0,1)[r, θ, ϕ] + ψ^(0,1,0)[r, θ, ϕ])

Lx[ψ[r, θ, ϕ]] - ⅈ Ly[ψ[r, θ, ϕ]] // TrigToExp // FullSimplify

(ⅈ Cos[ϕ] + Sin[ϕ]) (Cot[θ] ψ^(0,0,1)[r, θ, ϕ] + ⅈ ψ^(0,1,0)[r, θ, ϕ])

Lz[ψ[r, θ, ϕ]] // Simplify

-ⅈ ψ^(0,0,1)[r, θ, ϕ]
```

Arfkem 2.5 .15 $\mathbf{L} \times \mathbf{L} = i\mathbf{L}$

```
Lx[Ly[ψ[r, θ, ϕ]]] - Ly[Lx[ψ[r, θ, ϕ]]] - ⅈ Lz[ψ[r, θ, ϕ]] //
 Simplify
```

```
0
```

Arfken 2.5.16(c)

$$\mathbf{L}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$
$$= -r^2\nabla^2 + \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right).$$

```
eq1 = Lx[Lx[ψ[r, θ, ϕ]]] + Ly[Ly[ψ[r, θ, ϕ]]] + Lz[Lz[ψ[r, θ, ϕ]]] //
   Expand // FullSimplify
```

$-\mathrm{Csc}[\theta]^2\,\psi^{(0,0,2)}[r, \theta, \phi] - \mathrm{Cot}[\theta]\,\psi^{(0,1,0)}[r, \theta, \phi] - \psi^{(0,2,0)}[r, \theta, \phi]$

```
eq2 = - r^2 Lap[ψ[r, θ, ϕ]] + D[r^2 D[ψ[r, θ, ϕ], r], r] // Simplify
```

$-\mathrm{Csc}[\theta]^2\,\psi^{(0,0,2)}[r, \theta, \phi] - \mathrm{Cot}[\theta]\,\psi^{(0,1,0)}[r, \theta, \phi] - \psi^{(0,2,0)}[r, \theta, \phi]$

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

```
0
```

Arfken 2.5.17(a) $\nabla = \hat{\mathbf{r}}\frac{\partial}{\partial r} - i\frac{\mathbf{r}\times\mathbf{L}}{r^2},$

```
eq3 = ur D[ψ[r, θ, ϕ], r] - ⅈ Cross[1/r ur, L[ψ[r, θ, ϕ]]] // Simplify
```

$$\left\{\psi^{(1,0,0)}[r,\theta,\phi],\ \frac{\psi^{(0,1,0)}[r,\theta,\phi]}{r},\ \frac{\mathrm{Csc}[\theta]\,\psi^{(0,0,1)}[r,\theta,\phi]}{r}\right\}$$

```
eq4 = Gra[ψ[r, θ, ϕ]]
```

$$\left\{\psi^{(1,0,0)}[r,\theta,\phi],\ \frac{\psi^{(0,1,0)}[r,\theta,\phi]}{r},\ \frac{\mathrm{Csc}[\theta]\,\psi^{(0,0,1)}[r,\theta,\phi]}{r}\right\}$$

```
eq3 - eq4 // Simplify
```

{0, 0, 0}

Arfken 2.5.17 (b) $\mathbf{r}\nabla^2 - \nabla\left(1 + r\frac{\partial}{\partial r}\right) = i\nabla \times \mathbf{L}.$

```
eq5 = ur r Lap[ψ[r, θ, ϕ]] // Simplify
```

$$\left\{\frac{1}{r}\left(\mathrm{Csc}[\theta]^2\,\psi^{(0,0,2)}[r,\theta,\phi] + \mathrm{Cot}[\theta]\,\psi^{(0,1,0)}[r,\theta,\phi] + \psi^{(0,2,0)}[r,\theta,\phi] + 2\,r\,\psi^{(1,0,0)}[r,\theta,\phi] + r^2\,\psi^{(2,0,0)}[r,\theta,\phi]\right),\ 0,\ 0\right\}$$

```
eq6 = Gra[ψ[r, θ, ϕ] + r D[ψ[r, θ, ϕ], r]] // Simplify
```

$$\left\{2\,\psi^{(1,0,0)}[r,\theta,\phi] + r\,\psi^{(2,0,0)}[r,\theta,\phi],\ \frac{\psi^{(0,1,0)}[r,\theta,\phi]}{r} + \psi^{(1,1,0)}[r,\theta,\phi],\ \frac{\mathrm{Csc}[\theta]\left(\psi^{(0,0,1)}[r,\theta,\phi] + r\,\psi^{(1,0,1)}[r,\theta,\phi]\right)}{r}\right\}$$

```
eq7 = ⅈ Curla[L[ψ[r, θ, ϕ]]] // Simplify
```

$$\left\{\frac{1}{r}\left(\mathrm{Csc}[\theta]^2\,\psi^{(0,0,2)}[r,\theta,\phi] + \mathrm{Cot}[\theta]\,\psi^{(0,1,0)}[r,\theta,\phi] + \psi^{(0,2,0)}[r,\theta,\phi]\right),\ -\frac{\psi^{(0,1,0)}[r,\theta,\phi] + r\,\psi^{(1,1,0)}[r,\theta,\phi]}{r},\ -\frac{\mathrm{Csc}[\theta]\left(\psi^{(0,0,1)}[r,\theta,\phi] + r\,\psi^{(1,0,1)}[r,\theta,\phi]\right)}{r}\right\}$$

```
seq1 = eq5 - eq6 - eq7 // Simplify
```

{0, 0, 0}

The form of $\nabla^2\psi(r)$ can be expressed by

Arfken 2.5.18 (a) $\frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{d\psi(r)}{dr}\right]$; (b) $\frac{1}{r}\frac{d^2}{dr^2}[r\psi(r)]$; (c) $\frac{d^2\psi(r)}{dr^2}+\frac{2}{r}\frac{d\psi(r)}{dr}$.

```
eq8 = Lap[χ[r]] // FullSimplify
```

$$\frac{2\,\chi'[r]}{r} + \chi''[r]$$

```
eq9 = 1/r^2 D[r^2 D[χ[r], r], r] // FullSimplify
```

$$\frac{2\,\chi'[r]}{r} + \chi''[r]$$

```
eq10 = 1/r D[r χ[r], {r, 2}] // FullSimplify
```

$$\frac{2\,\chi'[r]}{r} + \chi''[r]$$

14. Radial momentum operator in the quantum mechanics

(a) In classical mechanics, the radial momentum of the radius r is defined by

$$p_{rc} = \frac{1}{r}(\boldsymbol{r} \cdot \boldsymbol{p}) .$$

(b) In quantum mechanics, this definition becomes ambiguous since the component of p and r do not commute. Since pr should be Hermitian operator, we need to define as the radial momentum of the radius r is defined by

$$p_{rq} = \frac{1}{2}(\frac{\boldsymbol{r}}{r} \cdot \boldsymbol{p} + \boldsymbol{p} \cdot \frac{\boldsymbol{r}}{r}) .$$

This symmetric expression is indeed the canonical conjugate of r.

$$p_{rq} r - r p_{rq} = \frac{\hbar}{i} .$$

Note that

$$p_{rq} = (-i\hbar)(\frac{\partial}{\partial r} + \frac{1}{r}) = (-i\hbar)\frac{1}{r}\frac{\partial}{\partial r} r .$$

((**Mathematica**))

```
Clear["Global`"]; ur = {1, 0, 0};
Gra := Grad[#, {r, θ, ϕ}, "Spherical"] &;
Diva := Div[#, {r, θ, ϕ}, "Spherical"] &;
prc := (ℏ/ⅈ ur.Gra[#] &);
```

```
prc[ψ[r, θ, ϕ]]
```

$-i\hbar\,\psi^{(1,0,0)}[r, \theta, \phi]$

```
prq := (-ⅈ ℏ/2 ur .Gra[#] + -ⅈ ℏ/2 Diva[# ur]) &;
```

```
prq[ψ[r, θ, ϕ]] // Simplify
```

$-\frac{i\hbar\left(\psi[r,\theta,\phi]+r\,\psi^{(1,0,0)}[r,\theta,\phi]\right)}{r}$

Commutation relation

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

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

15. Expression of the Laplacian in the spherical coordinate

Here we redefine p_{rq} simplily as

$$p_r = \frac{1}{2}\left(\frac{\boldsymbol{r}}{r}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\frac{\boldsymbol{r}}{r}\right).$$

We show that

$$-\hbar^2\nabla^2 = p_r^{\;2} + \frac{\boldsymbol{L}^2}{r^2},$$

by using the Mathematica. The total Hamiltonian H can be expressed by

$$H = \frac{1}{2m}\boldsymbol{p}^2 + V(r) = -\frac{\hbar^2}{2m}\nabla^2 + V(r) = \frac{1}{2m}p_r^{\;2} + \frac{\boldsymbol{L}^2}{2mr^2} + V(r).$$

The effective potential $V_{\mathrm{eff}}(r)$ is defined as

$$V_{eff}(r) = V(r) + \frac{\hbar^2}{2mr^2} l(l+1) .$$

((**Mathematica**)) Spherical coordinate

```
Clear["Global`"]; Clear[r]
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};
L :=
 (-ⅈ ℏ
    (Cross[(ur r), Grad[#, {r, θ, ϕ},
       "Spherical"]]) &) // Simplify;
Lx := (ux.L[#]) &; Ly := (uy.L[#]) &;
Lz := (uz.L[#]) &;
Lap := Laplacian[#, { r, θ, ϕ}, "Spherical"] &;
Gra := Grad[#, { r, θ, ϕ}, "Spherical"] &;
Diva := Div[#, { r, θ, ϕ}, "Spherical"] &;
Cur := Curl[#, {r, θ, ϕ}, "Spherical"] &;

prq :=
 (-ⅈ ℏ/2 {1, 0, 0}.Gra[#] -
    ⅈ ℏ/2 Diva[# {1, 0, 0}] &);
```

```
prq[χ[r, θ, ϕ]] // Simplify
```

$$-\frac{i\hbar\left(\chi[r,\theta,\phi]+r\,\chi^{(1,0,0)}[r,\theta,\phi]\right)}{r}$$

```
eq1 = Nest[prq, χ[r, θ, ϕ], 2] // Simplify;
```

```
eq2 =
  1/r^2 (Lx[Lx[χ[r, θ, ϕ]]] + Ly[Ly[χ[r, θ, ϕ]]] +
      Lz[Lz[χ[r, θ, ϕ]]]) // FullSimplify;
```

```
eq12 = eq1 + eq2 // Simplify
```

$$-\frac{1}{r^2}\hbar^2\left(\mathrm{Csc}[\theta]^2\chi^{(0,0,2)}[r,\theta,\phi]+\mathrm{Cot}[\theta]\chi^{(0,1,0)}[r,\theta,\phi]+\chi^{(0,2,0)}[r,\theta,\phi]+2r\chi^{(1,0,0)}[r,\theta,\phi]+r^2\chi^{(2,0,0)}[r,\theta,\phi]\right)$$

```
eq3 = -ħ^2 Lap[χ[r, θ, ϕ]] // Simplify
```

$$-\frac{1}{r^2}\hbar^2\left(\mathrm{Csc}[\theta]^2\chi^{(0,0,2)}[r,\theta,\phi]+\mathrm{Cot}[\theta]\chi^{(0,1,0)}[r,\theta,\phi]+\chi^{(0,2,0)}[r,\theta,\phi]+2r\chi^{(1,0,0)}[r,\theta,\phi]+r^2\chi^{(2,0,0)}[r,\theta,\phi]\right)$$

```
eq12 - eq3 // FullSimplify
```

0

16 Cylindrical coordinates

The position of a point in space P having Cartesian coordinates x, y, and z may be expressed in terms of cylindrical co-ordinates

$$x=\rho\cos\phi,\qquad y=\rho\sin\phi,\qquad z=z.$$

The position vector r is written as

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

$$d\mathbf{r}=\sum_{j=1}^{3}\mathbf{e}_j h_j dq_j=\mathbf{e}_\rho d\rho+\mathbf{e}_\phi\rho d\phi+\mathbf{e}_z dz,$$

where

$$h_1 = h_\rho = 1$$
$$h_2 = h_\phi = \rho$$
$$h_3 = h_z = 1$$

The unit vectors are written as

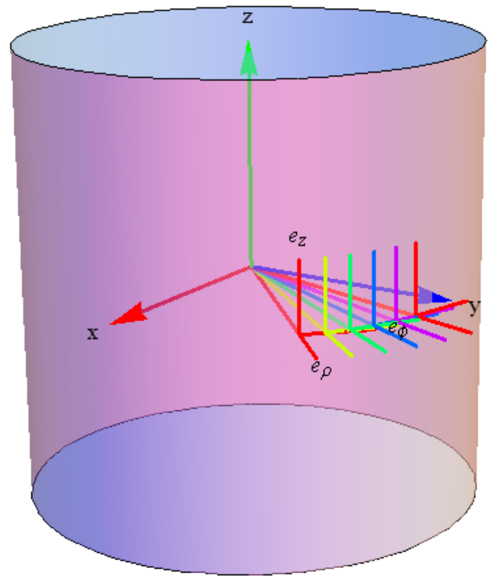
$$\mathbf{e}_\rho = \frac{1}{h_\rho}\frac{\partial \mathbf{r}}{\partial \rho} = \frac{\partial \mathbf{r}}{\partial \rho} = \cos\phi \mathbf{e}_x + \sin\phi \mathbf{e}_y$$
$$\mathbf{e}_\phi = \frac{1}{h_\phi}\frac{\partial \mathbf{r}}{\partial \phi} = \frac{1}{\rho}\frac{\partial \mathbf{r}}{\partial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

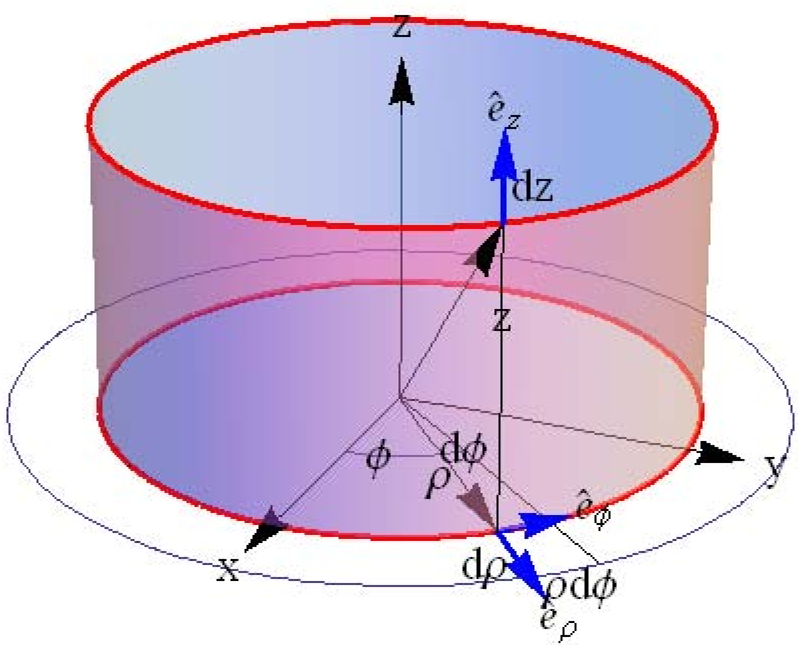
The above expression can be described using a matrix A as

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

or by using the inverse matrix A^{-1} as

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





17. Differential operations in the cylindrical coordinate

The differential operations involving ∇ are as follows.

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

$$\nabla \cdot \boldsymbol{V} = \frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho V_\rho) + \frac{1}{\rho}\frac{\partial}{\partial \phi}V_\phi + \frac{\partial}{\partial z}V_z,$$

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

$$\nabla^2 \psi = \frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho \frac{\partial \psi}{\partial \rho}) + \frac{1}{\rho^2}\frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial^2 \psi}{\partial z^2}.$$

where $\boldsymbol{V}$ is a vector and ψ is a scalar.

18 Mathematica for the cylindrical coordinate

Vector analysis
Angular momentum in the cylindrical coordinates
Here we use the angular momentum operatior in the unit of $\hbar$=1

```
Clear["Global`"]; r1 = Sqrt[z^2 + ρ^2]; ux = {Cos[ϕ], -Sin[ϕ], 0};
uy = { Sin[ϕ], Cos[ϕ], 0}; uz = {0, 0, 1}; r = {ρ, 0, z};
ur = 1/r1 {ρ, 0, z}; Gra := Grad[#, {ρ, ϕ, z}, "Cylindrical"] &;
Lap := Laplacian[#, {ρ, ϕ, z}, "Cylindrical"] &;
Curla := Curl[#, {ρ, ϕ, z}, "Cylindrical"] &;
Diva := Div[#, {ρ, ϕ, z}, "Cylindrical"] &;
```

Vector analysis in the cylindrical coordinate

```
eq1 = Lap[ψ[ρ, ϕ, z]] // Simplify
```

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

```
eq2 = Gra[ψ[ρ, ϕ, z]] // Simplify
```

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

```
B = {Bρ[ρ, ϕ, z], Bϕ[ρ, ϕ, z], Bz[ρ, ϕ, z]};
eq3 = Curla[B] // Simplify
```

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

```
eq4 = Diva[B] // Simplify
```

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

Angular momentum in the cylindrical coordinate

```
L := (-ⅈ Cross[r, Gra[#]]) &; Lx := (ux.L[#] &) // Simplify;
Ly := (uy.L[#] &) // Simplify;
Lz := (uz.L[#] &) // Simplify;
L[ψ[ρ, ϕ, z]] // Simplify
```

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

Lx[ψ[ρ, ϕ, z]] // FullSimplify

$$i\left(-\rho\,\mathrm{Sin}[\phi]\,\psi^{(0,0,1)}[\rho,\phi,z]+\frac{z\,\mathrm{Cos}[\phi]\,\psi^{(0,1,0)}[\rho,\phi,z]}{\rho}+z\,\mathrm{Sin}[\phi]\,\psi^{(1,0,0)}[\rho,\phi,z]\right)$$

Ly[ψ[ρ, ϕ, z]] // FullSimplify

$$i\left(\rho\,\mathrm{Cos}[\phi]\,\psi^{(0,0,1)}[\rho,\phi,z]+\frac{z\,\mathrm{Sin}[\phi]\,\psi^{(0,1,0)}[\rho,\phi,z]}{\rho}-z\,\mathrm{Cos}[\phi]\,\psi^{(1,0,0)}[\rho,\phi,z]\right)$$

Lx[ψ[ρ, ϕ, z]] + i Ly[ψ[ρ, ϕ, z]] // FullSimplify

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

Lx[ψ[ρ, ϕ, z]] - i Ly[ψ[ρ, ϕ, z]] // FullSimplify

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

Lz[ψ[ρ, ϕ, z]] // Simplify

$$-i\,\psi^{(0,1,0)}[\rho,\phi,z]$$

The commutation of the angular momentum in the cylindrical coordinate

```
eq5 = Lx[Ly[ψ[ρ, ϕ, z]]] - Ly[Lx[ψ[ρ, ϕ, z]]] - ⅈ Lz[ψ[ρ, ϕ, z]] //
  Simplify
```

```
0
```

L^2 in the cylindrical coordinate

```
eq6 = Lx[Lx[ψ[ρ, ϕ, z]]] + Ly[Ly[ψ[ρ, ϕ, z]]] +
   Lz[ Lz[ψ[ρ, ϕ, z]]] // FullSimplify
```

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

Schrodionger equation with a speific wavefunction in the cylindrical coorrdinate

```
H1 = χ[ρ] Exp[ⅈ kz z] Exp[ⅈ m ϕ];
```

$$\left(\frac{-1}{2 \mu} \text{Lap}[\text{H1}] + \text{V}[\rho] \text{ H1}\right) \text{ // Simplify}$$

$$\frac{e^{i (kz\, z + m \phi)} \left(\left(m^2 + kz^2 \rho^2 + 2 \mu \rho^2 V[\rho]\right) \chi[\rho] - \rho \left(\chi'[\rho] + \rho \chi''[\rho]\right)\right)}{2 \mu \rho^2}$$

19. Expression of the Laplacian in the cylindrical coordinate

Here we redefine p_{rq} simply as

$$p_r = \frac{1}{2}\left(\frac{\boldsymbol{r}}{r} \cdot \boldsymbol{p} + \boldsymbol{p} \cdot \frac{\boldsymbol{r}}{r}\right),$$

with the commutation relation

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

where

$$r = \sqrt{\rho^2 + z^2}\ , \qquad \boldsymbol{r} = \rho \boldsymbol{e}_\rho + z \boldsymbol{e}_z .$$

We show that

$$-\hbar^2\nabla^2 = p_r^{\ 2} + \frac{L^2}{r^2},$$

by using the Mathematica.

((**Mathematica**))

```
Clear["Global`"]; r1 = Sqrt[z^2 + ρ^2]; ux = {Cos[ϕ], -Sin[ϕ], 0};
uy = { Sin[ϕ], Cos[ϕ], 0}; uz = {0, 0, 1}; r = {ρ, 0, z}; ur = 1/r1 {ρ, 0, z};
Gra := Grad[#, {ρ, ϕ, z}, "Cylindrical"] &;
Lap := Laplacian[#, {ρ, ϕ, z}, "Cylindrical"] &;
Curla := Curl[#, {ρ, ϕ, z}, "Cylindrical"] &;
Diva := Div[#, {ρ, ϕ, z}, "Cylindrical"] &;
```

Angular momentum in the cylindrical coordinate

```
L := (-ⅈ ℏ Cross[r, Gra[#]]) &; Lx := (ux.L[#] &) // Simplify;
Ly := (uy.L[#] &) // Simplify;
Lz := (uz.L[#] &) // Simplify;
```

The linear momentum in the cylindrical coordinate

```
prq := ((-ⅈ ℏ)/2 ur.Gra[#] - (ⅈ ℏ)/2 Diva[# ur] &);

prq[χ[ρ, ϕ, z]] // Simplify
```

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

Commutation relation in the cylindrical coordinate

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

$$i\hbar\,\chi[\rho,\phi,z]$$

Proof of

$-\hbar^2\nabla^2 = p_r\,2 + \frac{L^2}{r^2}$

```
eq1 = Nest[prq, χ[ρ, ϕ, z], 2] // Simplify
```

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

```
eq20 = (Lx[Lx[χ[ρ, ϕ, z]]] + Ly[Ly[χ[ρ, ϕ, z]]] + Lz[Lz[χ[ρ, ϕ, z]]]) //
  FullSimplify;
eq2 = eq20/r1^2 // Simplify
```

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

```
eq12 = eq1 + eq2 // FullSimplify
```

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

L^2 in the cylindrical coordinate

```
eq3 = - ℏ^2 Lap[χ[ρ, ϕ, z]] // Expand // FullSimplify
```

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

```
eq12 - eq3 // Simplify
```

0

19 Jacobian

$$dV = dxdydz = \frac{\partial(x,y,z)}{\partial(q_1,q_2,q_3)} dq_1 dq_2 dq_3 = h_1 h_2 h_3 dq_1 dq_2 dq_3 .$$

Jacobian determinant is defined as;

$$\frac{\partial(x,y,z)}{\partial(q_1,q_2,q_3)} = \begin{vmatrix} \frac{\partial x}{\partial q_1} & \frac{\partial x}{\partial q_2} & \frac{\partial x}{\partial q_3} \\ \frac{\partial y}{\partial q_1} & \frac{\partial y}{\partial q_2} & \frac{\partial y}{\partial q_3} \\ \frac{\partial z}{\partial q_1} & \frac{\partial z}{\partial q_2} & \frac{\partial z}{\partial q_3} \end{vmatrix} .$$

(a) Spherical coordinate

$$h_1 h_2 h_3 dq_1 dq_2 dq_3 = h_r h_\theta h_\phi dr d\theta d\phi = r^2 \sin\theta dr d\theta d\phi .$$

(b) Cylindrical co-ordinate

$$h_1 h_2 h_3 dq_1 dq_2 dq_3 = h_\rho h_\phi h_z d\rho d\phi dz = \rho d\rho d\phi dz .$$

((**Mathematica**))

This is the program to determine the Jacobian determinant.

JacobianDeterminant[pt, coordsys]:

to give the determinant of the Jacobian matrix of the transformation from the coordinate system coordinate system to the Cartesian coordinate system at the point pt.

```
Clear["Gobal`"]
```

Jacobian determinant for transformation from cylindrical to Cartesian coordinates:

```
jdet = JacobianDeterminant[{ρ, ϕ, z}, Cylindrical]
```

ρ

Jacobian determinant for transformation from cylindrical to Spherical coordinates:

```
jdet = JacobianDeterminant[{r, θ, ϕ}, Spherical]
```

r^2 Sin[θ]

APPENDIX

Formula

$$\hat{\mathbf{x}} = \hat{\mathbf{r}} \sin\theta \cos\varphi + \hat{\boldsymbol{\theta}} \cos\theta \cos\varphi - \hat{\boldsymbol{\varphi}} \sin\varphi,$$

$$\hat{\mathbf{y}} = \hat{\mathbf{r}} \sin\theta \sin\varphi + \hat{\boldsymbol{\theta}} \cos\theta \sin\varphi + \hat{\boldsymbol{\varphi}} \cos\varphi,$$

$$\hat{\mathbf{z}} = \hat{\mathbf{r}} \cos\theta - \hat{\boldsymbol{\theta}} \sin\theta.$$

$$\nabla\psi = \hat{\mathbf{r}}\frac{\partial\psi}{\partial r} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial\psi}{\partial\theta} + \hat{\boldsymbol{\varphi}}\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\varphi},$$

$$\nabla\cdot\mathbf{V} = \frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}(r^2V_r) + r\frac{\partial}{\partial\theta}(\sin\theta V_\theta) + r\frac{\partial V_\varphi}{\partial\varphi}\right],$$

$$\nabla\cdot\nabla\psi = \frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right],$$

$$\nabla\times\mathbf{V} = \frac{1}{r^2\sin\theta}\begin{vmatrix} \hat{\mathbf{r}} & r\hat{\boldsymbol{\theta}} & r\sin\theta\hat{\boldsymbol{\varphi}} \\ \dfrac{\partial}{\partial r} & \dfrac{\partial}{\partial\theta} & \dfrac{\partial}{\partial\varphi} \\ V_r & rV_\theta & r\sin\theta V_\varphi \end{vmatrix}.$$