Appendix B

Angular Momentum in Spherical Coordinates

In this appendix, we will show how to derive the expressions of the gradient $\vec{\nabla}$, the Laplacian ∇^2 , and the components of the orbital angular momentum in spherical coordinates.

B.1 Derivation of Some General Relations

The Cartesian coordinates (x, y, z) of a vector \vec{r} are related to its spherical polar coordinates (r, θ, φ) by

$$x = r \sin \theta \cos \varphi, \quad y = r \sin \theta \sin \varphi, \quad z = r \cos \theta.$$
 (B.1)

The orthonormal Cartesian basis $(\hat{x}, \hat{y}, \hat{z})$ is related to its spherical counterpart $(\hat{r}, \hat{\theta}, \hat{\varphi})$ by

$$\hat{x} = \hat{r}\sin\theta\cos\varphi + \hat{\theta}\cos\theta\cos\varphi - \hat{\varphi}\sin\varphi, \qquad (B.2)$$

$$\hat{y} = \hat{r}\sin\theta\sin\varphi + \theta\cos\theta\sin\varphi + \hat{\phi}\cos\varphi, \qquad (B.3)$$

$$\hat{z} = \hat{r}\cos\theta - \theta\sin\theta.$$
 (B.4)

Differentiating (B.1), we obtain

$$dx = \sin\theta\cos\varphi\,dr + r\cos\theta\cos\varphi\,d\theta - r\sin\theta\sin\varphi\,d\varphi, \tag{B.5}$$

$$dy = \sin\theta \sin\varphi \, dr + r \cos\theta \sin\varphi \, d\theta + r \sin\theta \cos\varphi \, d\varphi, \tag{B.6}$$

$$dz = \cos\theta \, dr - r \sin\theta \, d\theta. \tag{B.7}$$

Solving these equations for dr, $d\theta$, and $d\varphi$, we obtain

$$dr = \sin\theta\cos\varphi \, dx + \sin\theta\sin\varphi \, dy + \cos\theta \, dz, \tag{B.8}$$

$$d\theta = \frac{1}{r}\cos\theta\cos\varphi\,dx + \frac{1}{r}\cos\theta\sin\varphi\,dy - \frac{1}{r}\sin\theta\,dz,\tag{B.9}$$

$$d\varphi = -\frac{\sin\varphi}{r\sin\theta}dx + \frac{\cos\varphi}{r\sin\theta}dy.$$
 (B.10)

We can verify that (B.5) to (B.10) lead to

$$\frac{\partial r}{\partial x} = \sin\theta\cos\varphi, \qquad \frac{\partial\theta}{\partial x} = \frac{1}{r}\cos\varphi\cos\theta, \qquad \frac{\partial\varphi}{\partial x} = -\frac{\sin\varphi}{r\sin\theta}, \qquad (B.11)$$
$$\frac{\partial r}{\partial x} = -\frac{\sin\varphi}{r\sin\theta}, \qquad (B.11)$$

$$\frac{\partial y}{\partial y} = \sin\theta\sin\varphi, \qquad \frac{\partial y}{\partial y} = -\sin\phi\cos\theta, \qquad \frac{\partial y}{\partial y} = -\sin\phi, \qquad (B.12)$$

$$\frac{\partial r}{\partial z} = \cos\theta, \qquad \frac{\partial \theta}{\partial z} = -\frac{1}{r}\sin\theta, \qquad \frac{\partial \phi}{\partial z} = 0,$$
 (B.13)

which, in turn, yield

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial x}$$
$$= \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\varphi\frac{\partial}{\partial \theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial \varphi}, \tag{B.14}$$

$$\frac{\partial}{\partial y} = \frac{\partial}{\partial r}\frac{\partial r}{\partial y} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial y} + \frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial y}$$
$$= \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial \theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial \varphi}, \qquad (B.15)$$

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial r}\frac{\partial r}{\partial z} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial z} + \frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}.$$
(B.16)

B.2 Gradient and Laplacian in Spherical Coordinates

We can show that a combination of (B.14) to (B.16) allows us to express the operator $\vec{\nabla}$ in spherical coordinates:

$$\vec{\nabla} = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}, \quad (B.17)$$

and also the Laplacian operator ∇^2 :

$$\nabla^2 = \vec{\nabla}.\vec{\nabla} = \left(\hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial\theta} + \frac{\hat{\varphi}}{r\sin\varphi}\frac{\partial}{\partial\varphi}\right) \cdot \left(\hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial\theta} + \frac{\hat{\varphi}}{r\sin\theta}\frac{\partial}{\partial\varphi}\right).$$
(B.18)

Now, using the relations

$$\frac{\partial \hat{r}}{\partial r} = 0, \qquad \qquad \frac{\partial \theta}{\partial r} = 0, \qquad \qquad \frac{\partial \hat{\varphi}}{\partial r} = 0, \tag{B.19}$$

$$\frac{\partial \hat{r}}{\partial \theta} = \hat{\theta}, \qquad \qquad \frac{\partial \hat{\theta}}{\partial \theta} = -\hat{r}, \qquad \qquad \frac{\partial \hat{\varphi}}{\partial \theta} = 0, \tag{B.20}$$

$$\frac{\partial \hat{r}}{\partial \varphi} = \hat{\varphi} \sin \theta, \qquad \frac{\partial \theta}{\partial \varphi} = \hat{\varphi} \cos \theta, \qquad \frac{\partial \hat{\varphi}}{\partial \varphi} = -\hat{r} \sin \theta - \hat{\theta} \cos \theta, \qquad (B.21)$$

we can show that the Laplacian operator reduces to

$$\nabla^2 = \frac{1}{r^2} \left[\frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right].$$
(B.22)

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B.3 Angular Momentum in Spherical Coordinates

The orbital angular momentum operator \vec{L} can be expressed in spherical coordinates as

$$\hat{\vec{L}} = \hat{\vec{R}} \times \hat{\vec{P}} = (-i\hbar r)\hat{r} \times \vec{\nabla} = (-i\hbar r)\hat{r} \times \left[\hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial \theta} + \frac{\hat{\varphi}}{r\sin\theta}\frac{\partial}{\partial\varphi}\right], \quad (B.23)$$

or as

$$\hat{\vec{L}} = -i\hbar \left(\hat{\varphi} \frac{\partial}{\partial \theta} - \frac{\hat{\theta}}{\sin \theta} \frac{\partial}{\partial \varphi} \right).$$
(B.24)

Using (B.24) along with (B.2) to (B.4), we express the components \hat{L}_x , \hat{L}_y , \hat{L}_z within the context of the spherical coordinates. For instance, the expression for \hat{L}_x can be written as follows:

$$\hat{L}_{x} = \hat{x}.\vec{L} = -i\hbar \left(\hat{r}\sin\theta\cos\varphi + \hat{\theta}\cos\theta\cos\varphi - \hat{\varphi}\sin\varphi\right) \cdot \left(\hat{\varphi}\frac{\partial}{\partial\theta} - \frac{\hat{\theta}}{\sin\theta}\frac{\partial}{\partial\varphi}\right)$$
$$= i\hbar \left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right). \tag{B.25}$$

Similarly, we can easily obtain

$$\hat{L}_{y} = i\hbar \left(-\cos\varphi \frac{\partial}{\partial\theta} + \cot\theta \sin\varphi \frac{\partial}{\partial\varphi} \right), \qquad (B.26)$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}.$$
(B.27)

From the expressions (B.25) and (B.26) for \hat{L}_x and \hat{L}_y , we infer that

$$\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y = \pm \hbar e^{\pm i\varphi} \left(\frac{\partial}{\partial \theta} \pm i \cot \theta \frac{\partial}{\partial \varphi}\right).$$
(B.28)

The expression for \vec{L}^2 is

$$\vec{L}^2 = -\hbar^2 r^2 (\hat{r} \times \vec{\nabla}) \cdot (\hat{r} \times \vec{\nabla}) = -\hbar^2 r^2 \left[\nabla^2 - \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right]; \tag{B.29}$$

it can be easily written in terms of the spherical coordinates as

$$\vec{L}^{2} = -\hbar^{2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^{2}\theta} \frac{\partial^{2}}{\partial\varphi^{2}} \right].$$
(B.30)

This expression was derived by substituting (B.22) into (B.29).

Note that, using the expression (B.29) for \vec{L}^2 , we can rewrite ∇^2 as

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{1}{\hbar^2 r^2} \vec{L}^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r - \frac{1}{\hbar^2 r^2} \vec{L}^2.$$
(B.31)