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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

$$x = r\sin\theta\cos\varphi, \qquad y = r\sin\theta\sin\varphi, \qquad z = r\cos\theta \tag{B.1}$$

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

$$\hat{x} = \hat{r}\sin\theta\cos\varphi + \hat{\theta}\cos\theta\cos\varphi - \hat{\varphi}\sin\varphi \tag{B.2}$$

$$\hat{y} = \hat{r}\sin\theta\sin\varphi + \hat{\theta}\cos\theta\sin\varphi + \hat{\varphi}\cos\varphi, \tag{B.3}$$

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

Differentiating (B.1), we obtain

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

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

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

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

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

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

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

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

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

$$\frac{\partial r}{\partial y} = \sin\theta\sin\varphi, \qquad \frac{\partial \theta}{\partial y} = \frac{1}{r}\sin\varphi\cos\theta, \qquad \frac{\partial \varphi}{\partial y} = \frac{\cos\varphi}{r\sin\theta}, \tag{B.12}$$

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

which, in turn, yield

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

$$\begin{aligned}\frac{\partial}{\partial y} &= \frac{\partial}{\partial r}\frac{\partial r}{\partial y} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial y} + \frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial y} \\ &= \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial \theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial \varphi},\end{aligned} \tag{B.15}$$

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

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:

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

and also the Laplacian operator ∇^2

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

Now, using the relations

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

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

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

we can show that the Laplacian operator reduces to

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

B.3 Angular Momentum in Spherical Coordinates

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

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

or as

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

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

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

Similarly, we can easily obtain

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

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

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

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

$$\hat{L}_- = \hat{L}_x - i\hat{L}_y = \hbar e^{-i\varphi}\left(\frac{\partial}{\partial \theta} - i\cot\theta\frac{\partial}{\partial \varphi}\right). \tag{B.29}$$

The expression for $\vec{L}^2$ is

$$\vec{L}^2 = -\hbar^2 r^2(\hat{r} \times \vec{\nabla})\cdot(\hat{r} \times \vec{\nabla}) = -\hbar^2 r^2\left[\nabla^2 - \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right]; \tag{B.30}$$

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

$$\vec{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \varphi^2}\right]; \tag{B.31}$$

this expression was derived by substituting (B.22) into (B.30).

Note that, using the expression (B.30) for $\vec{L}^2$, we can rewrite ∇^2 as

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\vec{L}^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{1}{\hbar^2 r^2}\vec{L}^2. \tag{B.32}$$