Appendix AA

The Gradient and Laplacian Operators

THE GRADIENT OPERATOR

The gradient of a function is a vector that points in the direction in which the function changes most rapidly and has a magnitude equal to the rate of change of the function in that direction. It is the natural three-dimensional generalization of the derivative with respect to a single variable. In Cartesian coordinates, the gradient of the function ψ can be written

$$\nabla\psi = \mathbf{i}\frac{\partial\psi}{\partial x} + \mathbf{j}\frac{\partial\psi}{\partial y} + \mathbf{k}\frac{\partial\psi}{\partial z}, \tag{AA.1}$$

where **i**, **j**, and **k** are unit vectors pointing along the x, y, and z axes, respectively.

In spherical coordinates, which are defined in Eq. (4.3), the gradient of the function ψ is

$$\nabla\psi = \hat{\mathbf{r}}\,\frac{\partial\psi}{\partial r} + \hat{\theta}\,\frac{1}{r}\,\frac{\partial\psi}{\partial\theta} + \hat{\phi}\,\frac{1}{r\sin\theta}\,\frac{\partial\psi}{\partial\phi}, \tag{AA.2}$$

where $\hat{\mathbf{r}}$, $\hat{\theta}$, and $\hat{\phi}$ are unit vectors pointing in the direction in which $\mathbf{r}$ moves when r, θ, and ϕ increase. We note that the factor $r\partial\theta$ that occurs in the denominator of the second term is the distance the point at $\mathbf{r}$ would move if the angle θ increased by an amount $\partial\theta$ with r and ϕ held fixed, while the factor $r\sin\theta\partial\phi$ which occurs in the denominator of the third term is the distance the point at $\mathbf{r}$ would move if ϕ increased by $\partial\phi$ with r and θ held fixed. Each of the terms of the gradient operator gives the rate of change of the function on which the gradient operator acts with respect to the displacement associated with a particular spherical coordinate.

The equation defining the gradient of a function of any orthogonal set of coordinates is similar to Eq. (AA.2) defining the gradient of a function for spherical coordinates. For a system of orthogonal coordinates (q_1, q_2, q_3), a change of the first coordinate q_1 by an amount $\mathrm{d}q_1$ causes a spatial point to move a distance $\mathrm{d}s_1 = h_1\,\mathrm{d}q_1$. Similarly, changes in the second coordinate by $\mathrm{d}q_2$ and a change of the third coordinates by $\mathrm{d}q_3$ causes the point to move distances $\mathrm{d}s_2 = h_2\,\mathrm{d}q_2$ and $\mathrm{d}s_3 = h_3\,\mathrm{d}q_3$, respectively. The weights (h_1, h_2, h_3) determines how far the point moves if the corresponding coordinate changes. The gradient of a function ψ in a system with coordinate (q_1, q_2, q_3) is defined by the equation

$$\nabla\psi = \hat{\mathbf{e}}_1\frac{1}{h_1}\frac{\partial\psi}{\partial q_1} + \hat{\mathbf{e}}_2\frac{1}{h_2}\frac{\partial\psi}{\partial q_2} + \hat{\mathbf{e}}_3\,\frac{1}{h_3}\,\frac{\partial\psi}{\partial q_3}. \tag{AA.3}$$

Here as for the spherical coordinates (r, θ, ϕ) the quantities $h_1\partial q_1$, $h_2\partial q_2$, and $h_3\partial q_3$ occurring in the denominators of the above equation give the distances a point will move if the three coordinates change by the amounts ∂q_1, ∂q_2, and ∂q_3, respectively. The three weight factors for spherical coordinates are

$$h_r = 1, \quad h_\theta = r, \quad h_\phi = r\sin\theta. \tag{AA.4}$$

THE DIVERGENCE OF A VECTOR

To find the divergence of a vector **A**, we consider the infinitesimal volume $\mathrm{d}V = \mathrm{d}q_1\mathrm{d}q_2\mathrm{d}q_3$. The volume is bounded by surfaces for which the first coordinate has the values, q_1 and $q_1 + \mathrm{d}q_1$, the second coordinate has the values, q_2 and $q_2 + \mathrm{d}q_2$, and the third coordinate has the values, q_3 and $q_3 + \mathrm{d}q_3$. Gauss's theorem for the vector field $\mathbf{A}(q_1, q_2, q_3)$ is

$$\int \nabla \cdot \mathbf{A}\, \mathrm{d}V = \int \mathbf{A} \cdot \mathrm{d}\mathbf{S}.$$

The integral of the out-going normal of $\mathbf{A}$ over the two surfaces for which the first coordinate has the values q_1 and $q_1 + \mathrm{d}q_1$ is

$$(A_1 \mathrm{d}s_2 \mathrm{d}s_3)_{q_1+\mathrm{d}q_1} - (A_1 \mathrm{d}s_2 \mathrm{d}s_3)_{q_1} = \frac{\partial (A_1 \mathrm{d}s_2 \mathrm{d}s_3)}{\partial q_1} \mathrm{d}q_1.$$

Using the fact that the displacements, $\mathrm{d}s_1, \mathrm{d}s_2$, and $\mathrm{d}s_3$, are equal to $h_1 \mathrm{d}q_1, h_2 \mathrm{d}q_2$, and $h_3 \mathrm{d}q_3$, respectively, the above equation can be written

$$(A_1 \mathrm{d}s_2 \mathrm{d}s_3)_{q_1+\mathrm{d}q_1} - (A_1 \mathrm{d}s_2 \mathrm{d}s_3)_{q_1} = \frac{1}{h_1 h_2 h_3} \frac{\partial (h_2 h_3 A_1)}{\partial q_1} \mathrm{d}V.$$

Analogous expressions hold for the other two sets of surfaces. According to Gauss's theorem, the sum of these three terms is equal to $\mathbf{A} \cdot \mathbf{A} \mathrm{d}V$. Hence the divergence of $\mathbf{A}$ is given by the equation

$$\nabla \cdot \mathbf{A} = \frac{1}{h_1 h_2 h_3} \left(\frac{\partial (h_2 h_3 A_1)}{\partial q_1} + \frac{\partial (h_3 h_1 A_2)}{\partial q_2} + \frac{\partial (h_1 h_2 A_3)}{\partial q_3} \right). \tag{AA.5}$$

THE LAPLACIAN OF A FUNCTION

The Laplacian of a scalar function ψ is the divergence of the gradient of the function. We can write

$$\nabla^2 \psi = \nabla \cdot \nabla \psi.$$

Using Eq. (AA.5) for the divergence of a vector and Eq. (AA.3) for the gradient of a function, the above equation can be written

$$\nabla^2 \psi = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial q_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial \psi}{\partial q_1} \right) + \frac{\partial}{\partial q_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial \psi}{\partial q_2} \right) + \frac{\partial}{\partial q_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial \psi}{\partial q_3} \right) \right]. \tag{AA.6}$$

For spherical polar coordinates, the three weight factors are given by Eq. (AA.4) and the equation for the Laplacian operator in spherical coordinates is

$$\nabla^2 \psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2 \psi}{\partial \phi^2} \right]. \tag{AA.7}$$

THE ANGULAR MOMENTUM OPERATORS

The operator associated with the angular momentum of a particle can be obtained by writing the angular momentum in terms of the momentum

$$\mathbf{l} = \mathbf{r} \times \mathbf{p}$$

and then making the replacement $\mathbf{p} \rightarrow -\mathrm{i}\nabla$ to obtain

$$\mathbf{l} = -\mathrm{i}\hbar \mathbf{r} \times \nabla. \tag{AA.8}$$

The angular momentum operator in spherical coordinates can be obtained by using Eq. (AA.2) and the relations

$$\hat{\mathbf{r}} \times \hat{\theta} = \hat{\phi} \quad \text{and} \quad \hat{\mathbf{r}} \times \hat{\phi} = -\hat{\theta}$$

to give

$$\mathbf{l} = -\mathrm{i}\hbar \left(\hat{\phi} \frac{\partial}{\partial \theta} - \hat{\theta} \frac{1}{\sin\theta} \frac{\partial}{\partial \phi} \right).$$

The operator corresponding to the z-component of the angular momentum can then be obtained by taking the dot product of this last expression with the unit vector $\hat{\mathbf{k}}$ pointing along the z-axis to obtain

$$l_z = -\mathrm{i}\hbar \frac{\partial}{\partial \phi}. \tag{AA.9}$$

The square of the angular momentum operator is related to the second term on the right-hand side of Eq. (AA.7) by the equation

$$\mathbf{l}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]. \tag{AA.10}$$

Using Eqs. (AA.7) and (AA.10), the Lapalcian operator in spherical coordinates can be written simply

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial\psi}{\partial r} \right) - \frac{1}{r^2} \frac{\mathbf{l}^2}{\hbar^2}. \tag{AA.11}$$

The angular part of the Laplacian operator in spherical coordinates is equal to $\mathbf{l}^2/\hbar^2 r^2$.