Quantum Mechanics 2

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Partial Derivatives

Cartesian to Polar

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The coordinate transformation between Cartesian and spherical coordinates are as follows:

$$x = r\sin\theta\cos\varphi$$
$$y = r\sin\theta\sin\varphi$$
$$z = r\cos\theta$$

A

Using Chain Rule,

$$\frac{\partial}{\partial r} = \frac{\partial x}{\partial r}\frac{\partial}{\partial x} + \frac{\partial y}{\partial r}\frac{\partial}{\partial y} + \frac{\partial z}{\partial r}\frac{\partial}{\partial z}$$
$$\frac{\partial}{\partial \theta} = \frac{\partial x}{\partial \theta}\frac{\partial}{\partial x} + \frac{\partial y}{\partial \theta}\frac{\partial}{\partial y} + \frac{\partial z}{\partial \theta}\frac{\partial}{\partial z}$$
$$\frac{\partial}{\partial \varphi} = \frac{\partial x}{\partial \varphi}\frac{\partial}{\partial x} + \frac{\partial y}{\partial \varphi}\frac{\partial}{\partial y} + \frac{\partial z}{\partial \varphi}\frac{\partial}{\partial z}$$

Using the transformation equations A,

$$\frac{\partial x}{\partial r} = \sin\theta\cos\varphi\,; \qquad \frac{\partial y}{\partial r} = \sin\theta\sin\varphi\,; \qquad \frac{\partial z}{\partial r} = \cos\theta\,;$$

$$\frac{\partial x}{\partial \theta} = r\cos\theta\cos\varphi; \qquad \frac{\partial y}{\partial \theta} = r\cos\theta\sin\varphi\,; \qquad \frac{\partial z}{\partial \theta} = -r\sin\theta;$$

$$\frac{\partial x}{\partial \varphi} = -r\sin\theta\sin\varphi; \qquad \frac{\partial y}{\partial \varphi} = r\sin\theta\cos\varphi; \qquad \frac{\partial z}{\partial \varphi} = 0$$

Thus

$$\begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \varphi} \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta \\ r\cos\theta\cos\varphi & r\cos\theta\sin\varphi & -r\sin\theta \\ -r\sin\theta\sin\varphi & r\sin\theta\cos\varphi & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix}$$

If we let

$$B = \begin{pmatrix} \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta \\ r\cos\theta\cos\varphi & r\cos\theta\sin\varphi & -r\sin\theta \\ -r\sin\theta\sin\varphi & r\sin\theta\cos\varphi & 0 \end{pmatrix}$$

then,

$$\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} = B^{-1} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \varphi} \end{pmatrix}$$

From [Inverse], the matrix elements of the inverse of B may be obtained using

$$(B^{-1})^n_m = \frac{C^m_n}{\Delta}$$

where Δ is the determinant of B, and C^m_n is the cofactor of the element B^m_n of the matrix B (note that this is the transpose).

The determinant of B is

$$\begin{aligned}
\Delta &= 0 + (\sin\theta\sin\varphi)(-r\sin\theta)(-r\sin\theta\sin\varphi) + \cos\theta\,(r\cos\theta\cos\varphi)(r\sin\theta\cos\varphi) \\
&- (-r\sin\theta\sin\varphi)(r\cos\theta\sin\varphi)\cos\theta - (r\sin\theta\cos\varphi)(-r\sin\theta)(\sin\theta\cos\varphi) - 0 \\
&= r^2\sin^2\theta\ \sin\theta\ \sin^2\varphi + r^2\cos^2\theta\sin\theta\cos^2\varphi + r^2\cos^2\theta\sin\theta\sin^2\varphi + r^2\sin^2\theta\ \sin\theta\ \cos^2\varphi \\
&= r^2\sin^2\theta\ \sin\theta\ \sin^2\varphi + r^2\cos^2\theta\sin\theta + r^2\sin^2\theta\ \sin\theta\ \cos^2\varphi \\
&= r^2\sin^2\theta\sin\theta + r^2\cos^2\theta\sin\theta = r^2\sin\theta
\end{aligned}$$

and the cofactors are

$$C_1^1 = \begin{vmatrix} r\cos\theta\sin\varphi & -r\sin\theta \\ r\sin\theta\cos\varphi & 0 \end{vmatrix} = r^2\sin^2\theta\cos\varphi$$

$$C_1^2 = -\begin{vmatrix} r\cos\theta\cos\varphi & -r\sin\theta \\ -r\sin\theta\sin\varphi & 0 \end{vmatrix} = r^2\sin^2\theta\sin\varphi$$

$$C_1^3 = \begin{vmatrix} r\cos\theta\cos\varphi & r\cos\theta\sin\varphi \\ -r\sin\theta\sin\varphi & r\sin\theta\cos\varphi \end{vmatrix} = r^2\sin\theta\cos\theta$$

$$C_2^1 = -\begin{vmatrix} \sin\theta\sin\varphi & \cos\theta \\ r\sin\theta\cos\varphi & 0 \end{vmatrix} = r\sin\theta\cos\theta\cos\varphi$$

$$C_2^2 = \begin{vmatrix} \sin\theta\cos\varphi & \cos\theta \\ -r\sin\theta\sin\varphi & 0 \end{vmatrix} = r\sin\theta\cos\theta\sin\varphi$$

$$C_2^3 = -\begin{vmatrix} \sin\theta\cos\varphi & \sin\theta\sin\varphi \\ -r\sin\theta\sin\varphi & r\sin\theta\cos\varphi \end{vmatrix} = -r\sin^2\theta$$

$$C_3^1 = \begin{vmatrix} \sin\theta\sin\varphi & \cos\theta \\ r\cos\theta\sin\varphi & -r\sin\theta \end{vmatrix} = -r\sin\varphi$$

$$C_3^2 = -\begin{vmatrix} \sin\theta\cos\varphi & \cos\theta \\ r\cos\theta\cos\varphi & -r\sin\theta \end{vmatrix} = r\cos\varphi$$

$$C_3^2 = \begin{vmatrix} \sin\theta\cos\varphi & \sin\theta\sin\varphi \\ r\cos\theta\cos\varphi & r\cos\theta\sin\varphi \end{vmatrix} = 0$$

Thus,

$$B^{-1} = \frac{1}{r^2\sin\theta}\begin{pmatrix} r^2\sin^2\theta\cos\varphi & r\sin\theta\cos\theta\cos\varphi & -r\sin\varphi \\ r^2\sin^2\theta\sin\varphi & r\sin\theta\cos\theta\sin\varphi & r\cos\varphi \\ r^2\sin\theta\cos\theta & -r\sin^2\theta & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \sin\theta\cos\varphi & \frac{1}{r}\cos\theta\cos\varphi & -\frac{\sin\varphi}{r\sin\theta} \\ \sin\theta\sin\varphi & \frac{1}{r}\cos\theta\sin\varphi & \frac{\cos\varphi}{r\sin\theta} \\ \cos\theta & -\frac{1}{r}\sin\theta & 0 \end{pmatrix}$$

and

$$\frac{\partial}{\partial x} = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$