Quantum Mechanics II: Mathematical appendix

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Overview

Contents

1 Elements of differential calculus

Let a Cartesian system of coordinates (x, y, z) as in the Fig. 1.

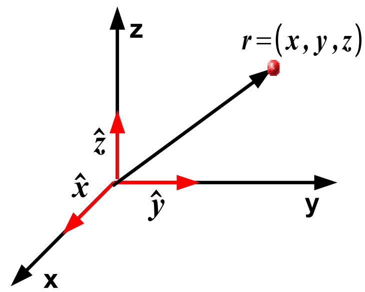

Figure 1: Cartesian system of coordinates with indicated unit vectors.

The position of a point in $\mathbb{R}^3$ with these coordinates will be denoted as

$$\mathbf{r} = x\hat{x} + y\hat{y} + z\hat{z} \,, \tag{1.1}$$

where $(\hat{x}, \hat{y}, \hat{z})$ are the corresponding orthogonal unit vectors.

The volume element in Cartesian coordinates is

$$dv = d^3\mathbf{r} = dxdydz \,. \tag{1.2}$$

The *gradient operator* is defined by its action on a function $\Phi(\mathbf{r})$ as

$$\nabla\Phi = \frac{\partial\Phi}{\partial x}\hat{x} + \frac{\partial\Phi}{\partial y}\hat{y} + \frac{\partial\Phi}{\partial z}\hat{z} \,. \tag{1.3}$$

If we move the point at $\mathbf{x}$ by a small vector to a new position $\mathbf{r} + d\mathbf{r}$ the function changes as

$$d\Phi = \nabla\Phi \cdot d\mathbf{r} \,. \tag{1.4}$$

In the following $\mathbf{A}$ and $\mathbf{B}$ are vectors. In addition, it will be convenient to denote the Cartesian coordinates x, y, z by x_i, $i = 1, 2, 3$. Accordingly the components of a vector A_x, A_y and A_z will be denoted by A_1, A_2 and A_2, respectively.

The *divergence* of a vector is given by

$$\nabla \cdot \mathbf{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} = \partial_i A_i \,. \tag{1.5}$$

The *curl* of a vector is given by

$$
\begin{aligned}
\nabla \times \mathbf{A} &= \det \begin{pmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_x \end{pmatrix} . \\
&= (\partial_y A_z - \partial_z A_y)\hat{\mathbf{x}} + (\partial_z A_x - \partial_x A_z)\hat{\mathbf{y}} + (\partial_x A_y - \partial_y A_x)\hat{\mathbf{z}} \, . \qquad (1.6)
\end{aligned}
$$

The *Laplace operator* on a function $\Phi(\mathbf{x})$ acts as

$$
\nabla^2 \Phi = \nabla \cdot \nabla \Phi = \partial_i \partial_i \Phi \, . \tag{1.7}
$$

An arbitrary *unit vector* is of the form

$$
\hat{\mathbf{n}} = n_x \hat{x} + n_y \hat{y} + n_z \hat{z} \, , \qquad n_x^2 + n_y^2 + n_z^2 = 1 \, . \tag{1.8}
$$

Then the directional derivative along $\hat{n}$ is defined as

$$
\frac{\partial}{\partial n} = \hat{\mathbf{n}} \cdot \nabla \, . \tag{1.9}
$$

The ith component of the outer product $\mathbf{A} \times \mathbf{B}$ is given by

$$
(\mathbf{A} \times \mathbf{B})_i = \epsilon_{ijk} A_j B_k \, , \tag{1.10}
$$

for any two vectors in $\mathbb{R}^3$.

<u>Exercise</u>: Using properties of determinants prove that the definition

$$
\mathbf{A} \times \mathbf{B} = \det \begin{pmatrix} \hat{x} & \hat{y} & \hat{z} \\ A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \end{pmatrix} , \tag{1.11}
$$

is consistent with (1.10).

Exercise: Using (**??**) show (some of) the following identities

$$
\begin{aligned}
\nabla(\mathbf{A}\cdot\mathbf{B}) &= (\mathbf{A}\cdot\nabla)\mathbf{B} + (\mathbf{B}\cdot\nabla)\mathbf{A} + \mathbf{A}\times(\nabla\times\mathbf{B}) + \mathbf{B}\times(\nabla\times\mathbf{A})\,, \\
\nabla(\Phi\mathbf{A}) &= \Phi\nabla\cdot\mathbf{A} + \mathbf{A}\cdot\nabla\Phi\,, \\
\nabla\cdot(\mathbf{A}\times\mathbf{B}) &= \mathbf{B}\cdot(\nabla\times\mathbf{A}) - \mathbf{A}\cdot(\nabla\times\mathbf{B})\,, \\
\nabla\times(\Phi\mathbf{A}) &= \Phi(\nabla\times\mathbf{A}) + \nabla\Phi\times\mathbf{A}\,, \\
\nabla\times(\mathbf{A}\times\mathbf{B}) &= \mathbf{A}(\nabla\cdot\mathbf{B}) - \mathbf{B}(\nabla\cdot\mathbf{A}) + (\mathbf{B}\cdot\nabla)\mathbf{A} - (\mathbf{A}\cdot\nabla)\mathbf{B}\,, \qquad (1.12) \\
\nabla\times(\nabla\times\mathbf{A}) &= \nabla(\nabla\cdot\mathbf{A}) - \nabla^2\mathbf{A}\,, \\
\nabla\times(\nabla\Phi) &= 0\,, \\
\nabla\cdot(\nabla\times\mathbf{A}) &= 0\,.
\end{aligned}
$$

Exercise: Show that

$$
\begin{aligned}
&\mathbf{A}\times(\mathbf{B}\times\mathbf{C}) = (\mathbf{A}\cdot\mathbf{C})\mathbf{B} - (\mathbf{A}\cdot\mathbf{B})\mathbf{C}\,, \\
&(\mathbf{A}\times\mathbf{B})\cdot(\mathbf{C}\times\mathbf{D}) = (\mathbf{A}\cdot\mathbf{C})(\mathbf{B}\cdot\mathbf{D}) - (\mathbf{A}\cdot\mathbf{D})(\mathbf{B}\cdot\mathbf{C}) \qquad (1.13)
\end{aligned}
$$

and that the exterior product is non-associative, but the Jacobi identity is obeyed

$$
\mathbf{A}\times(\mathbf{B}\times\mathbf{C}) + \mathbf{B}\times(\mathbf{C}\times\mathbf{A}) + \mathbf{C}\times(\mathbf{A}\times\mathbf{B}) = 0\,. \qquad (1.14)
$$

2 Fundamental theorems

2.1 The fundamental theorem for gradients

Consider the infinitesimal change (1.4) along a curve from the point $\mathbf{a}$ to the point $\mathbf{b}$ The total change in Φ is

$$
\int_{\mathbf{a}}^{\mathbf{b}} \nabla\Phi\cdot d\mathbf{r} = \Phi(\mathbf{b}) - \Phi(\mathbf{a})\,. \qquad (2.1)
$$

This states that the total change of a function depends on the difference of values of the function at the end points and not on the details of the path between them. If the path is closed then the integral vanishes.

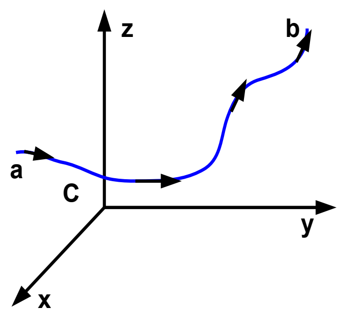

Figure 2: A curve C with end points **a** and **b**. Arrows indicate small tangent displacements.

2.2 The fundamental theorem for divergences

Consider a volume V bounded by a surface S. The divergence (or Gauss's) theorem states that

$$\int_V dv \nabla \cdot \mathbf{A} = \oint_S dS \hat{\mathbf{n}} \cdot \mathbf{A} \,, \tag{2.2}$$

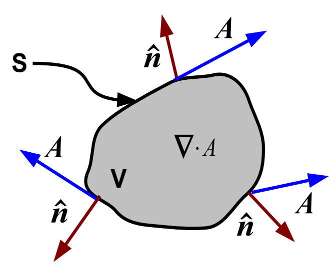

Figure 3: The divergence of a vector **A** over a volume V can be computed from its projection on the normal $\hat{\mathbf{n}}$ (pointing outwards) to the surface S bounding V.

2.3 The fundamental theorem for curls

Consider a surface S bounded by a closed curve C. The curl (or Stoke's) theorem states that

$$\int dS \hat{\mathbf{n}} \cdot (\nabla \times \mathbf{A}) = \oint_C \mathbf{A} \cdot d\mathbf{r} \,. \tag{2.3}$$

3 Curvilinear coordinates

In many problems there are present special symmetries we would like to take advantage in trying to solve them. Hence, using Cartesian coordinates is not always

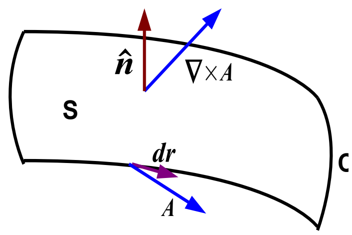

Figure 4: The projection of the curl of a vector $\mathbf{A}$ on the normal $\hat{\mathbf{n}}$ to a surface S can be computed from the circulation of $\mathbf{A}$ on the curve C (anticlockwise) bounding S.

the most convenient choice. The most common other coordinates systems are the so called cylindrical and spherical.

3.1 Cylindrical coordinates

The change of variables from Cartesian coordinates is

$$
\begin{aligned}
& x = \rho\cos\phi\,, \qquad y = \rho\sin\phi\,, \qquad z = z\,, \\
& \rho \geqslant 0\,, \qquad 0 \leqslant \phi \leqslant 2\pi\,, \qquad -\infty < z < \infty\,.
\end{aligned} \tag{3.1}
$$

The relation between the orthogonal unit vectors is

$$
\begin{aligned}
\hat{\rho} &= \cos\phi\,\hat{x} + \sin\phi\,\hat{y}\,, \\
\hat{\phi} &= -\sin\phi\,\hat{x} + \cos\phi\,\hat{y}\,, \\
\hat{z} &= \hat{z}\,.
\end{aligned} \tag{3.2}
$$

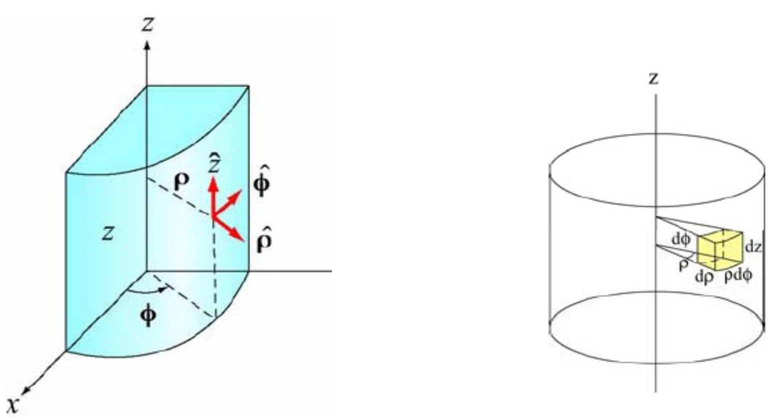

Figure 5: Cylindrical coordinates and the corresponding volume element.

Then for a function $\Phi = \Phi(\rho,\phi,z)$ and a vector $\mathbf{A} = A_\rho\hat{\rho} + A_\phi\hat{\phi} + A_z\hat{z}$ we have the following operations

$$
\begin{aligned}
\nabla\Phi &= \partial_\rho\Phi\hat{\rho} + \frac{1}{\rho}\partial_\phi\Phi\hat{\phi} + \partial_z\Phi\hat{z}\ , \\
\nabla\cdot\mathbf{A} &= \frac{1}{\rho}\partial_\rho(\rho A_\rho) + \frac{1}{\rho}\partial_\phi A_\phi + \partial_z A_z\ , \\
\nabla\times\mathbf{A} &= \frac{1}{\rho}(\partial_\phi A_z - \rho\partial_z A_\phi)\hat{\rho} + (\partial_z A_\rho - \partial_\rho A_z)\hat{\phi} + \frac{1}{\rho}\left[\partial_\rho(\rho A_\phi) - \partial_\phi A_\rho\right]\hat{z}\ , \\
\nabla^2\Phi &= \frac{1}{\rho}\partial_\rho(\rho\partial_\rho\Phi) + \frac{1}{\rho^2}\partial_\phi^2\Phi + \partial_z^2\Phi\ .
\end{aligned}
\tag{3.3}
$$

By replacing in (3.2) the unit vectors by vector components, $\hat{\rho}\to A_\rho$, etc and $\hat{x}\to A_x$, etc, we get the relation between components of vectors in the Cartesian and the polar coordinate systems.

The volume element in polar coordinates is

$$
dv = d^3\mathbf{r} = \rho d\rho dz d\phi\ . \tag{3.4}
$$

In cylindrical coordinates the normal unit vector on the curved surface of a cylinder is $\hat{\mathbf{n}} = \hat{\rho}$, whereas on the upper (lower) cap is $\hat{\mathbf{n}} = \hat{z}$ ($\hat{\mathbf{n}} = -\hat{z}$).

3.2 Spherical coordinates

The change of variables from Cartesian coordinates is

$$
\begin{aligned}
&x = r\sin\theta\cos\phi\ , \qquad y = r\sin\theta\sin\phi\ , \qquad z = r\cos\theta\ , \\
&r \geqslant 0\ , \qquad 0\leqslant\theta\leqslant\pi\ , \qquad 0\leqslant\phi\leqslant 2\pi\ .
\end{aligned}
\tag{3.5}
$$

The relation between the orhtogonal unit vectors is

$$
\begin{aligned}
\hat{r} &= \sin\theta\cos\phi\ \hat{x} + \sin\theta\sin\phi\ \hat{y} + \cos\theta\ \hat{z}\ , \\
\hat{\theta} &= \cos\theta\cos\phi\ \hat{x} + \cos\theta\sin\phi\ \hat{y} - \sin\theta\ \hat{z}\ , \\
\hat{\phi} &= -\sin\phi\ \hat{x} + \cos\phi\ \hat{y}\ .
\end{aligned}
\tag{3.6}
$$

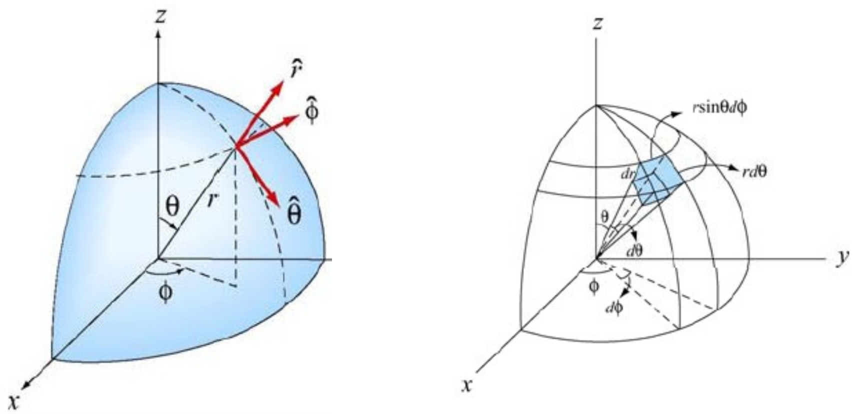

Figure 6: Spherical coordinates and the corresponding volume element.

Then for a function $\Phi = \Phi(r,\theta,\phi)$ and a vector $\mathbf{A} = A_r\hat{r} + A_\theta\hat{\theta} + A_\phi\hat{\phi}$ we have

$$
\begin{aligned}
\nabla\Phi &= \partial_r\Phi\hat{r} + \frac{1}{r}\partial_\theta\Phi\hat{\theta} + \frac{1}{r\sin\theta}\partial_\phi\Phi\hat{\phi}\,, \\
\nabla\cdot\mathbf{A} &= \frac{1}{r^2}\partial_r(r^2A_r) + \frac{1}{r\sin\theta}\partial_\theta(\sin\theta A_\theta) + \frac{1}{r\sin\theta}\partial_\phi A_\phi\,, \\
\nabla\times\mathbf{A} &= \frac{1}{r\sin\theta}\left[\partial_\theta(\sin\theta A_\phi) - \partial_\phi A_\theta\right]\hat{r} + \frac{1}{r\sin\theta}\left[\partial_\phi A_r - \sin\theta\partial_r(rA_\phi)\right]\hat{\theta} \\
&\quad + \frac{1}{r}\left[\partial_r(rA_\theta) - \partial_\theta A_r\right]\hat{\phi}\,, \qquad (3.7) \\
\nabla^2\Phi &= \frac{1}{r^2}\partial_r(r^2\partial_r\Phi) + \frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\partial_\theta\Phi) + \frac{1}{r^2\sin^2\theta}\partial_\phi^2\Phi\,.
\end{aligned}
$$

By replacing the unit vectors in (3.6) by vector components, $\hat{r} \to A_r$, etc and $\hat{x} \to A_x$, we get the relation between components of vectors.

The volume element in polar coordinates is

$$
dv = d^3\mathbf{r} = r^2 dr d\Omega\,, \qquad d\Omega = \sin\theta d\theta d\phi\,. \qquad (3.8)
$$

The element $d\Omega$ is the elementary surface of the unit sphere, i.e. the sphere of radius. The finite element is called *solid angle* and is depicted in Fig. 6. Also note that

$$
\int d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta = 4\pi\,. \qquad (3.9)
$$

In spherical coordinates the normal unit vector on the surface of a sphere is $\hat{\mathbf{n}} = \hat{r}$.