A
Vector and Tensor Calculus

In relativistic theory one often encounters vector and tensor expressions in both three- and four-dimensional form. The most important of these expressions are briefly summarized in this section, where Einstein's summation convention (cf. section 3.1.2) is strictly applied for four-dimensional objects.

A.1
Three-Dimensional Expressions

A.1.1
Algebraic Vector and Tensor Operations

In chapter 2 the Kronecker delta δ_{ij} and the totally antisymmetric Levi-Cività symbol ε_{ijk} were introduced by Eqs. (2.24) and (2.9), respectively. Their relation to each other is given by

$$\sum_{i=1}^{3} \varepsilon_{ijk}\varepsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl} \tag{A.1}$$

This immediately yields

$$\sum_{i,j=1}^{3} \varepsilon_{ijk}\varepsilon_{ijm} = \sum_{j=1}^{3} \left(\delta_{jj}\delta_{km} - \delta_{jm}\delta_{jk}\right) = 2\delta_{km} \tag{A.2}$$

since the trace of the Kronecker symbol is given by

$$\sum_{i=1}^{3} \delta_{ii} = 3 \tag{A.3}$$

The Euclidean scalar product between two arbitrary three-dimensional vectors $\boldsymbol{A}$ and $\boldsymbol{B}$ is given by

$$\boldsymbol{A} \cdot \boldsymbol{B} = \sum_{i=1}^{3} A_i B_i = AB\cos\gamma \tag{A.4}$$

Relativistic Quantum Chemistry. Markus Reiher and Alexander Wolf

ISBN: 978-3-527-31292-4

with A and B being the length of the vectors $\boldsymbol{A}$ and $\boldsymbol{B}$, respectively, and γ being the angle spanned by these vectors, $\gamma = \angle(\boldsymbol{A}, \boldsymbol{B})$. The *vector product* or *cross product* between these vectors yields again a three-vector $\boldsymbol{C}$ defined as

$$\boldsymbol{C} \;=\; \boldsymbol{A} \times \boldsymbol{B} \;=\; \begin{pmatrix} A_y B_z - A_z B_y \\ A_z B_x - A_x B_z \\ A_x B_y - A_y B_x \end{pmatrix} \tag{A.5}$$

and its ith component might thus be written as

$$C_i \;=\; \big(\boldsymbol{A}\times\boldsymbol{B}\big)_i \;=\; \sum_{j,k=1}^{3} \varepsilon_{ijk} A_j B_k \tag{A.6}$$

A.1.2
Differential Vector Operations

The *gradient* of a scalar function $\phi = \phi(\boldsymbol{r})$ is defined as the three-dimensional vector of its Cartesian partial derivatives,

$$\text{grad}\,\phi(\boldsymbol{r}) \;=\; \nabla\phi(\boldsymbol{r}) \;=\; \left(\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z}\right)^T \;\in \mathbb{R}^3 \tag{A.7}$$

which is consequently interpreted as a column-vector in this book. The *divergence* of a vector field $\boldsymbol{A} = \boldsymbol{A}(\boldsymbol{r})$ is a measure of the sources defined by

$$\text{div}\boldsymbol{A} \;=\; \nabla \cdot \boldsymbol{A} \;=\; \sum_{i=1}^{3} \frac{\partial A_i}{\partial x_i} \;=\; \sum_{i=1}^{3} \partial_i A_i \;\in \mathbb{R} \tag{A.8}$$

whereas the *curl* of this vector field is itself a vector field defined by

$$\text{curl}\,\boldsymbol{A} \;=\; \nabla \times \boldsymbol{A} \;=\; \begin{pmatrix} \partial_y A_z - \partial_z A_y \\ \partial_z A_x - \partial_x A_z \\ \partial_x A_y - \partial_y A_x \end{pmatrix} \;\in \mathbb{R}^3 \tag{A.9}$$

(in the German literature, it is also common to use 'rot' instead of 'curl'). Finally, the *Laplacian* of a scalar function ϕ might be considered as a generalization of the familiar one-dimensional second derivative as is given by

$$\Delta\phi(\boldsymbol{r}) \;=\; \text{div grad}\,\phi(\boldsymbol{r}) \;=\; \sum_{i=1}^{3} \frac{\partial^2\phi(\boldsymbol{r})}{\partial x_i^2} \;=\; \sum_{i=1}^{3} \partial_i^2\phi(\boldsymbol{r}) \;\in \mathbb{R} \tag{A.10}$$

Application of the Laplacian to a vector field $\boldsymbol{A}$ has to be understood as acting separately on each component. The result is then again a three-vector, of course. We note some important identities for the above vector operations.

For any differentiable vector fields $\boldsymbol{A}$, $\boldsymbol{B}$ and scalar functions ϕ, ψ the following relations hold:

$$\text{grad}\,(\phi\psi) = \phi\,\text{grad}\,\psi + \psi\,\text{grad}\,\phi \tag{A.11}$$

$$\text{div}\,\left(\phi \boldsymbol{A}\right) = \boldsymbol{A}\cdot\text{grad}\,\phi + \phi\,\text{div}\boldsymbol{A} \tag{A.12}$$

$$\text{curl}\,\left(\phi \boldsymbol{A}\right) = (\text{grad}\,\phi)\times\boldsymbol{A} + \phi\,\text{curl}\,\boldsymbol{A} \tag{A.13}$$

$$\text{div}\,(\boldsymbol{A}\times\boldsymbol{B}) = \boldsymbol{B}\cdot\text{curl}\,\boldsymbol{A} - \boldsymbol{A}\cdot\,\text{curl}\,\boldsymbol{B} \tag{A.14}$$

$$\text{curl}\,(\boldsymbol{A}\times\boldsymbol{B}) = \boldsymbol{A}\,\text{div}\boldsymbol{B} - \boldsymbol{B}\,\text{div}\boldsymbol{A} + (\boldsymbol{B}\cdot\nabla)\boldsymbol{A} - (\boldsymbol{A}\cdot\nabla)\boldsymbol{B} \tag{A.15}$$

$$\Delta\boldsymbol{A} = \text{grad}\,(\text{div}\boldsymbol{A}) - \text{curl}\,(\text{curl}\,\boldsymbol{A}) \tag{A.16}$$

$$\text{div}\,\text{curl}\,\boldsymbol{A} = 0 \tag{A.17}$$

$$\text{curl}\,\text{grad}\,\phi = 0 \tag{A.18}$$

The proof of all these relations is straightforward and thus omitted here. Eq. (A.17) states that any rotational vector field has no sources, and Eq. (A.18) summarizes the fact that the curl of any gradient field is zero.

A.1.3 Integral Theorems and Distributions

In classical mechanics and electrodynamics the integral theorems of Gauss and Stokes may often be employed beneficially. Given a sufficiently smooth (i.e., differentiable) and well-behaved vector field $\boldsymbol{A}$, *Gauss' theorem* may be expressed in its most elementary form as

$$\int_V \text{div}\boldsymbol{A}\,\mathrm{d}^3 r = \int_{\partial V} \boldsymbol{A}\cdot\mathrm{d}\boldsymbol{\sigma} \tag{A.19}$$

where $\partial\,V$ denotes the closed surface of the volume V and $\boldsymbol{\sigma}$ is the outer normal unit vector perpendicular to the plane ∂V. Eq. (A.19) is also denoted as the *divergence theorem* and relates the volume integral over all sinks and sources (i.e., the divergence) of a vector field $\boldsymbol{A}$ to the net flow of this vector field through the volume's boundary. Similarly, in its simplest form *Stokes' theorem* relates the vortices or curls of a vector field $\boldsymbol{A}$ within a given plane or surface S to the line integral of this vector field along the surface's boundary ∂S,

$$\int_S (\text{curl}\,\boldsymbol{A})\cdot\mathrm{d}\boldsymbol{\sigma} = \oint_{\partial S} \boldsymbol{A}\cdot\mathrm{d}\boldsymbol{r} \tag{A.20}$$

Here $\boldsymbol{\sigma}$ again denotes the outer normal unit vector perpendicular to the surface S. Eq. (A.20) is sometimes also referred to as the *curl theorem* .

In discussions of the Coulomb potential the following relations are often useful. The gradients of a distance between two positions, $\boldsymbol{r}$ and $\boldsymbol{r}'$, read

$$\nabla_{\boldsymbol{r}} |\boldsymbol{r}-\boldsymbol{r}'| = \nabla_{\boldsymbol{r}} \sqrt{(\boldsymbol{r}-\boldsymbol{r}')^2} = \frac{1}{2}\frac{1}{\sqrt{(\boldsymbol{r}-\boldsymbol{r}')^2}}\left[2(\boldsymbol{r}-\boldsymbol{r}')\right] = \frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|} \quad \text{(A.21)}$$

$$\nabla_{\boldsymbol{r}'} |\boldsymbol{r}-\boldsymbol{r}'| = \frac{1}{2}\frac{1}{\sqrt{(\boldsymbol{r}-\boldsymbol{r}')^2}}\left[2(\boldsymbol{r}-\boldsymbol{r}')\right](-1) = -\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|} \quad \text{(A.22)}$$

and the gradient and Laplacian of the inverse distance become

$$\nabla_{\boldsymbol{r}} \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} = -\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^3} = -\nabla_{\boldsymbol{r}'}\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \quad \text{(A.23)}$$

$$\Delta \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} = -4\pi\,\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}') \quad \text{(A.24)}$$

The indices in Eq. (A.21) label the variable with respect to which the derivative is taken. We note that the proof of Eq. (A.24) is only trivial for $\boldsymbol{r}-\boldsymbol{r}' \neq 0$ for which the right-hand side becomes zero. In this case, where $\boldsymbol{r} \neq \boldsymbol{r}'$, we may simply differentiate the inverse distance and obtain this result right away,

$$\left(\Delta\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\right)_{\boldsymbol{r}\neq\boldsymbol{r}'} = \nabla_{\boldsymbol{r}}\cdot\left(\nabla_{\boldsymbol{r}}\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\right) \overset{(A.23)}{=} \nabla_{\boldsymbol{r}}\cdot\left(-\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^3}\right)$$

$$= -\left(\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^3}\underbrace{\nabla_{\boldsymbol{r}}\cdot(\boldsymbol{r}-\boldsymbol{r}')}_{3} + \underbrace{(\boldsymbol{r}-\boldsymbol{r}')\cdot\nabla_{\boldsymbol{r}}\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^3}}_{-3(\boldsymbol{r}-\boldsymbol{r}')\cdot(\boldsymbol{r}-\boldsymbol{r}')/|\boldsymbol{r}-\boldsymbol{r}'|^5}\right) = 0 \quad \text{(A.25)}$$

(Δ may equally well be resolved by a differentiation with respect to $\boldsymbol{r}'$). Eq. (A.24) states that the function

$$G(\boldsymbol{r},\boldsymbol{r}') = -\frac{1}{4\pi\,|\boldsymbol{r}-\boldsymbol{r}'|} \quad \text{(A.26)}$$

is the so-called *Green's function* of the Laplacian, since application of the differential operator Δ to G yields the three-dimensional *delta distribution* $\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}')$ [971, p. 22ff.]. The three-dimensional delta distribution is the product of three one-dimensional delta distributions,

$$\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}') = \delta(x-x')\,\delta(y-y')\,\delta(z-z') \quad \text{(A.27)}$$

which may sloppily be thought of as being zero everywhere except at $x = x'$, where it is appropriately infinite such that

$$\int_{-\infty}^{\infty} dx\,\delta(x-x')f(x) = f(x') \quad \text{(A.28)}$$

for *all* continuous and integrable test functions f. A very useful and convenient integral representation of the delta distribution is given by

$$\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k \, e^{\mathrm{i}k(x-x')} \tag{A.29}$$

which will become important in appendix E in the discussion of Fourier transforms.

A.1.4
Total Differentials and Time Derivatives

In both classical mechanics and quantum mechanics one often has to deal with *total* time derivatives of functions depending on many time-dependent arguments. For example, consider a real-valued function f depending on N time-dependent arguments $x_i(t)$ and explicitly on the time t itself,

$$f = f(x_1(t), x_2(t), \ldots, x_N(t), t) \tag{A.30}$$

The partial time derivative of the function f is simply given by

$$\partial_t f = \frac{\partial f}{\partial t} \tag{A.31}$$

i.e., the time-dependence of the arguments x_i does not matter at all for the calculation of the partial time derivative of f. Only the explicit time dependence is taken into account. For the calculation of the *total* time derivative, however, both explicit and implicit dependences on the time t have to be taken into account, i.e., the total time derivative is given by application of the chain rule of multi-dimensional calculus,

$$\dot{f} = \frac{\mathrm{d}f}{\mathrm{d}t} = \sum_{i=1}^{N} \frac{\partial f}{\partial x_i} \frac{dx_i}{dt} + \frac{\partial f}{\partial t} \tag{A.32}$$

This rule has, for example, been extensively applied in the discussion of Hamiltonian mechanics in section 2.3. By formal multiplication of Eq. (A.32) by $\mathrm{d}t$ the total differential of the function f is recovered,

$$\mathrm{d}f = \sum_{i=1}^{N} \frac{\partial f}{\partial x_i} \mathrm{d}x_i + \frac{\partial f}{\partial t} \mathrm{d}t \tag{A.33}$$

A.2
Four-Dimensional Expressions

A.2.1
Algebraic Vector and Tensor Operations

As a generalization of the three-dimensional Levi-Cività symbol defined in chapter 2 by Eq. (2.9) we have introduced the four-dimensional totally antisymmetric (pseudo-)tensor $\varepsilon^{\alpha\beta\gamma\delta}$, whose contravariant components have been defined by

$$\varepsilon^{\alpha\beta\gamma\delta} = \left\{ \begin{array}{rcl} +1 & & (\alpha\beta\gamma\delta) \text{ is an even permutation of } (0123) \\ -1 & \text{if} & (\alpha\beta\gamma\delta) \text{ is an odd permutation of } (0123) \\ 0 & & \text{else} \end{array} \right\} \tag{A.34}$$

We have further introduced the four-dimensional generalization of the scalar product between any two 4-vectors a and b by

$$a \cdot b \;=\; a^T g\, b \;=\; a^\mu b_\mu \;=\; a^0 b^0 - a^i\, b^i \;=\; a^0 b^0 - \boldsymbol{a} \cdot \boldsymbol{b} \tag{A.35}$$

As a consequence, the four-dimensional distance between 2 infinitesimal neighboring events can now be expressed as

$$ds^2 \;=\; dx \cdot dx \;=\; dx^T g\, dx \;=\; g_{\mu\nu}\, dx^\mu\, dx^\nu \tag{A.36}$$

A.2.2
Differential Vector Operations

Similarly to the nonrelativistic situation [cf. Eq. (2.28)], the components of the Lorentz transformation matrix Λ may be expressed as derivatives of the new coordinates with respect to the old ones or vice versa. However, since we have to distinguish contra- and covariant components of vectors in the relativistic framework, there are now four different possibilities to express these derivatives:

$$x'^\mu \;=\; \Lambda^\mu{}_\nu x^\nu \;\longrightarrow\; \Lambda^\mu{}_\nu \;=\; \frac{\partial x'^\mu}{\partial x^\nu} \;=\; \partial_\nu x'^\mu \tag{A.37}$$

$$x^\mu \;=\; \Lambda_\nu{}^\mu x'^\nu \;\longrightarrow\; \Lambda_\mu{}^\nu \;=\; \frac{\partial x^\nu}{\partial x'^\mu} \;=\; \partial'_\mu x^\nu \tag{A.38}$$

$$x'_\mu \;=\; \Lambda_\mu{}^\nu x'_\nu \;\longrightarrow\; \Lambda_\mu{}^\nu \;=\; \frac{\partial x'_\mu}{\partial x_\nu} \;=\; \partial^\nu x'_\mu \tag{A.39}$$

$$x_\nu \;=\; \Lambda^\mu{}_\nu x'_\mu \;\longrightarrow\; \Lambda^\mu{}_\nu \;=\; \frac{\partial x_\nu}{\partial x'_\mu} \;=\; \partial'^\mu x_\nu \tag{A.40}$$

where we have employed a shorthand notation for the 4-gradient defined by

$$\partial_\mu \;\equiv\; \frac{\partial}{\partial x^\mu} \;=\; \left(\frac{1}{c}\frac{\partial}{\partial t}, \nabla\right) \;=\; \left(\frac{1}{c}\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \tag{A.41}$$

The 4-gradient has been written as a row vector above solely for our convenience; it still is to be interpreted mathematically as a column vector, of course. Being defined as the derivative with respect to the contravariant components x^μ, the 4-gradient ∂_μ is *naturally* a covariant vector whose contravariant components may be obtained by application of the metric g and read

$$\partial^\mu = g^{\mu\nu}\partial_\nu = \frac{\partial}{\partial x_\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\nabla\right) \tag{A.42}$$

The four-dimensional generalization of the Laplacian has been identified to be the d'Alembert operator

$$\Box = \partial_\mu \partial^\mu = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta \tag{A.43}$$