Appendix A: Mathematical Tools

A.1 Solving Second-Order Linear Homogeneous Differential Equations: Special Functions

The differential equations that generate the special functions of physics are of the general form

$$\frac{d^2y}{dx^2} + p(x)\frac{dy}{dx} + q(x)y = 0. \tag{A.1}$$

If y_1 and y_2 are two independent solutions of (A.1), then any other solution can be written in the form

$$y_3 = ay_1 + by_2, \tag{A.2}$$

where a, b are arbitrary constant coefficients, which are chosen so that y_3 satisfies the required boundary conditions; y_3 is called the general solution of Eq. (A.1) (it contains already two constants of integration).

Among the most important orthogonal polynomials for this course are the Hermite polynomials, the Legendre and associated Legendre polynomials, the Laguerre and associated Laguerre polynomials, and the cylindrical and spherical Bessel functions, which we will briefly review in what follows.

A.1.1 Hermite polynomials

The Hermite[1] equation is

$$H_n'' - 2xH_n' + 2nH_n = 0. \tag{A.3}$$

The normalization is chosen so that the coefficient of x^n in H_n is 2^n; it follows that

$$H_n(x) = (2x)^n - \frac{n(n-1)}{1!}(2x)^{n-2} + \frac{n(n-1)(n-2)(n-3)}{2!}(2x)^{n-4} + \ldots; \tag{A.4}$$

the last term is proportional to x or is a constant; H_n is even or odd if n is even or odd, respectively. Hermite polynomials have the following *generating function*,

$$F(x,t) = e^{2xt-t^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!}t^n. \tag{A.5}$$

[1] Charles Hermite (1822–1901) was a famous French mathematician; the term Hermitian applies to properties of several mathematical entities.

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and the Rodrigues formula,

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n e^{-x^2}}{dx^n}. \tag{A.6}$$

By deriving the generating function it is easy to show that

$$H_n'(x) = 2n H_{n-1}(x). \tag{A.7}$$

From this expression and the differential Hermite equation follows the recurrence relation

$$H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x). \tag{A.8}$$

Using the generating function, it is possible to check that the orthogonality relation is

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = 0 \quad (n \neq m), \tag{A.9}$$

which shows that $w = e^{-x^2}$ is the weight function; for this reason the Hermite functions $e^{-x^2/2} H_n(x)$ are sometimes introduced which are orthonormal with weight 1; the normalization factor is

$$\int_{-\infty}^{\infty} e^{-x^2} H_n^2(x) dx = 2^n n! \sqrt{\pi}. \tag{A.10}$$

The first Hermite polynomials are

$$\begin{array}{ll} H_0 = 1 & H_1 = 2x \\ H_2 = 4x^2 - 2 & H_3 = 8x^3 - 12x \\ H_4 = 16x^4 - 48x^2 + 12 & H_5 = 32x^5 - 160x^3 + 120x. \end{array} \tag{A.11}$$

A.1.2 Legendre polynomials and spherical harmonics

We turn to the solutions of Eq. (11.47), obtained for the angular part of the Schrödinger equation of a central problem,

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d\Theta}{d\theta} \right) + \left(\lambda - \frac{m^2}{\sin^2\theta} \right) \Theta = 0. \tag{A.12}$$

With the change of variable $x = \cos\theta$, this equation transforms into

$$(1 - x^2) \frac{d^2\Theta}{dx^2} - 2x \frac{d\Theta}{dx} + \left(\lambda - \frac{m^2}{1 - x^2} \right) \Theta = 0. \tag{A.13}$$

A particular case is the Legendre[2] equation, when $m = 0$,

$$(1 - x^2) \frac{d^2\Theta}{dx^2} - 2x \frac{d\Theta}{dx} + \lambda\Theta = 0. \tag{A.14}$$

The regular solutions in the interval $(-1, +1)$ are obtained by a Taylor series expansion around $x = 0$, $\Theta = \sum_{k=0}^{\infty} a_k x^k$, which leads to the recurrence relation

$$a_{k+2} = \frac{k(k+1) - \lambda}{(k+1)(k+2)} a_k. \tag{A.15}$$

[2] Adrien-Marie Legendre (1752–1833) was an outstanding French mathematician.

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For $a_1 = 0$, $a_0 \neq 0$, the solution is even and for $a_0 = 0$, $a_1 \neq 0$, it is odd; in both cases $(a_{k+2}/a_k) \to 1$ when $k \to \infty$, so that both diverge for $x = \pm 1$ ($\theta = 0$ or π). The only way to obtain regular solutions is by choosing λ such that one of the series becomes a polynomial. From the recurrence relation it follows that a regular solution exists if and only if

$$\lambda = l(l+1), \quad l = 0, 1, 2, \ldots \tag{A.16}$$

The first Legendre polynomials, obtained directly from the preceding results, are the following,

$$\begin{aligned} P_0 &= 1 & P_1 &= x \\ P_2 &= \tfrac{1}{2}(3x^2 - 1) & P_3 &= \tfrac{1}{2}(5x^3 - 3x) \\ P_4 &= \tfrac{1}{8}(35x^4 - 30x^2 + 3) & P_5 &= \tfrac{1}{8}(63x^5 - 70x^3 + 15x). \end{aligned} \tag{A.17}$$

The normalization has been chosen such that

$$P_l(\pm 1) = (\pm 1)^l. \tag{A.18}$$

Using the Rodrigues formula

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l}(x^2 - 1)^l, \tag{A.19}$$

we obtain after integrating by parts,

$$\int_{-1}^{1} P_l(x) P_{l'}(x) dx = \frac{2}{2l+1} \delta_{ll'}, \tag{A.20}$$

as well as the recurrence relation

$$(n+1)P_{n+1}(x) = (2n+1)x P_n(x) - n P_{n-1}(x). \tag{A.21}$$

The generating function leads to a formula of great practical value, namely

$$F(x,t) = \frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n. \tag{A.22}$$

The regular solutions of Eq. (A.13) with $m \neq 0$ are the associated Legendre polynomials. Since the equation depends on m^2, changing the sign of m should not affect the solution; therefore if Θ_l^m is the solution for $m > 0$, the solution for $m < 0$ is taken as

$$\Theta_l^{-|m|}(x) = (-1)^m C_{lm} \Theta_l^{|m|}(x), \tag{A.23}$$

where C_{lm} is an arbitrarily chosen constant.

For $m > 0$ the associated Legendre polynomial $\Theta = P_l^m$ is given by

$$P_l^m(x) = (1 - x^2)^{m/2} \frac{d^m P_l}{dx^m}, \tag{A.24}$$

or alternatively,

$$\begin{aligned} P_l^m(x) &= \frac{1}{2^l l!}(1 - x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}}(x^2 - 1)^l \\ &= \frac{(-1)^m (l+m)!}{2^l l! (l-m)!}(1 - x^2)^{-m/2} \frac{d^{l-m}}{dx^{l-m}}(x^2 - 1)^l. \end{aligned} \tag{A.25}$$

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It is clear that only for $m \leq l$ are the solutions regular and physically acceptable. The first associated Legendre polynomials are the following,

$$P_1^1(x) = \sqrt{1-x^2}, \quad P_2^1(x) = 3x\sqrt{1-x^2}, \quad P_2^2(x) = 3(1-x^2) \tag{A.26}$$

or in terms of the angle θ, with $x = \cos\,\theta$,

$$P_1^1 = \sin\theta, \quad P_2^1 = 3\sin\theta\cos\theta, \quad P_2^2 = 3\sin^2\theta. \tag{A.27}$$

Note that the polynomials are orthogonal with respect to l, but not to m,

$$\int_{-1}^{1} P_l^m P_{l'}^m(x)dx = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'}. \tag{A.28}$$

Equation (11.45) defines the spherical harmonics as the functions normalized to unity obtained by multiplying an associated Legendre function and the function $e^{im\varphi}$. Taking into account the normalization of P_l^m, Eq. (A.28), we obtain the spherical harmonics as the following functions, for l a positive integer and m a positive or negative integer, $|m| \leq l$,[3]

$$Y_l^m(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}(-1)^m P_l^m(\cos\theta)e^{im\varphi}. \tag{A.29}$$

The first spherical harmonics are

$$\begin{aligned} &Y_0^0 = \tfrac{1}{\sqrt{4\pi}} \qquad Y_1^0 = \sqrt{\tfrac{3}{4\pi}}\cos\theta \qquad Y_1^{\pm1} = \mp\sqrt{\tfrac{3}{8\pi}}\sin\theta e^{\pm i\varphi} \\ &Y_2^0 = \sqrt{\tfrac{5}{16\pi}}(3\cos^2\theta - 1) \qquad Y_2^{\pm1} = \mp\sqrt{\tfrac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\varphi} \\ &Y_2^{\pm2} = \sqrt{\tfrac{15}{32\pi}}\sin^2\theta e^{\pm 2i\varphi}. \end{aligned} \tag{A.30}$$

A.1.3 Laguerre polynomials

The associated Laguerre[4] polynomials are the regular solutions of the differential equation

$$\rho u'' + [2(l+1) - \rho]u' + (\beta - l - 1)u = 0, \tag{A.31}$$

which is obtained for the radial part of the hydrogen-like wave function once the asymptotic solutions at the origin and infinity have been extracted. With the change of variable $\rho = 2x$ this equation transforms into

$$xu'' + 2(l+1-x)u' + 2(\beta - l - 1)u = 0. \tag{A.32}$$

According to the results given in the introduction, the point $x = 0$ is singular, so the general solution of (A.31) is singular at the origin, but there is a particular regular

[3] For $m < 0$ we use (A.23) with $C_{lm} = 1$.

[4] Edmond Nicolas Laguerre (1834–1886) was a noted French mathematician.

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solution, which is constructed from a Taylor series of the form $u = \sum_{k=0}^{\infty} a_k x^k$. This gives the recurrence relation

$$a_{k+1} = 2\frac{k+l+1-\beta}{(k+1)(k+2l+2)}a_k, \tag{A.33}$$

from which $a_{k+1}/a_k \to 2/k$ when $k \to \infty$. This is precisely the behavior of the coefficients of the power series of e^{2x}; therefore, the series diverges exponentially, unless it is cut off by reducing β to a positive integer,

$$\beta \equiv n = k + l + 1, \tag{A.34}$$

so that a_{n-l} and hence all a_k for $k > n - l$ are zero. The method gives us the associated Laguerre polynomials and the preceding relation is the most important result in connection with these polynomials.

In order to generalize a little, we write (A.31) in the form

$$xu'' + (p + 1 - x)u' + (q - p)u = 0, \tag{A.35}$$

which reduces to (A.31) with the identification $x = \rho$, $p = 2l + 1$, $q = n + l$, $\beta = n$. With $p = 0$ we get the Laguerre equation,

$$xu'' + (1 - x)u' + qu = 0. \tag{A.36}$$

By deriving it p times we obtain (A.35), therefore if $L^p_{q-p}(x)$ are the solutions of (A.35) and $L_q(x)$ those of (A.36), we have

$$L^p_{q-p}(x) = (-1)^p \frac{d^p}{dx^p} L_q(x); \tag{A.37}$$

in particular, $L^0_q = L_q$ (the sign $(-1)^p$ is conventional and has been chosen so that the coefficient of x^n is $(-1)^n$). From (A.37) we get the Rodrigues formula

$$x^p L^p_n(x) = \frac{1}{n!} e^x \frac{d^n}{dx^n} \left(e^{-x} x^{n+p}\right), \tag{A.38}$$

where $L^p_n(x)$ is a polynomial only if $p = 0, 1, 2, \ldots$. Expanding in series we get

$$L^p_n(x) = \sum_{s=0}^{n} (-1)^s \begin{pmatrix} n+p \\ n-s \end{pmatrix} \frac{x^s}{s!}, \tag{A.39}$$

where $\begin{pmatrix} n \\ r \end{pmatrix} = \frac{n!}{r!(n-r)!}$ is a binomial coefficient. The Rodrigues formula leads also to the orthogonality relation,

$$\int_0^\infty e^{-x} x^p L^p_n(x) L^p_m(x) dx = \frac{\Gamma(n+p+1)}{n!} \delta_{nm} \tag{A.40}$$

(Re $p > 0$). The most common recurrence relations are

$$xL^{p+1}_n = (n + p + 1)L^p_n - (n + 1)L^p_{n+1} = (n + p)L^p_{n-1} - (n - x)L^p_n, \tag{A.41}$$

$$\frac{d}{dx} L^p_n(x) = -L^{p+1}_{n-1}(x). \tag{A.42}$$

The generating function is

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$$e^{-\frac{tx}{1-t}} = (1-t)^{p+1} \sum_{n=0}^{\infty} L_n^p(x) t^n, \tag{A.43}$$

which shows that the exponential on the left can be expanded in terms of associated Laguerre polynomials of arbitrary index p, including $p = 0$. The simplest Laguerre polynomials are

$$L_0^p = 1 \qquad L_1 = 1 - x \qquad L_2 = 1 - 2x + \tfrac{1}{2}x^2. \tag{A.44}$$

A.1.4 Cylindrical Bessel functions

The (cylindrical) Bessel[5] functions are the solutions of the differential Bessel equation,

$$y'' + \frac{1}{x}y' + \left(1 + \frac{\nu^2}{x^2}\right) y = 0 \tag{A.45}$$

where ν is an arbitrary (real or complex) parameter. One of the solutions of this equation is called a Bessel function of the first kind and is conventionally denoted as $J_\nu(x)$; if ν is not an integer, a second independent solution is $J_{-\nu}(x)$. In this case it is customary to introduce the Bessel function of the second kind or Neumann[6] function (also called Weber function), which is usually denoted in physics by $N_\nu(x)$ (and in mathematics by $Y_\nu(x)$) and defined as

$$N_\nu(x) = \frac{1}{\sin \pi\nu} \left(\cos \pi\nu J_\nu(x) - J_{-\nu}(x)\right), \quad |\arg x| < \pi. \tag{A.46}$$

In terms of these functions, the Hankel functions or Bessel functions of the third kind are defined as

$$H_\nu^{(1,2)}(x) = J_\nu(x) \pm i N_\nu(x), \tag{A.47}$$

where the index 1(2) corresponds to the sign $+(-)$. When $\nu = n$ is an integer, J_n and J_{-n} cease to be independent,

$$J_{-n}(x) = (-1)^n J_n(x), \quad n \text{ integer}. \tag{A.48}$$

Applying the methods discussed in the introduction, it is possible to show that

$$J_\nu(x) = \left(\frac{x}{2}\right)^\nu \sum_{k=0}^{\infty} (-1)^k \frac{1}{k!\Gamma(\nu + k + 1)} \left(\frac{x}{2}\right)^{2k}. \tag{A.49}$$

The generating function of $J_n(x)$ for integer n is

$$e^{\frac{x}{2}(t - \frac{1}{t})} = \sum_{n=-\infty}^{\infty} J_n(x) t^n, \tag{A.50}$$

and the most common recurrence relations are ($Z_\nu \equiv Z_\nu(x)$ stands for any Bessel function)

$$x(Z_{\nu-1} + Z_{\nu+1}) = 2\nu Z_\nu, \tag{A.51}$$

$$xZ'_\nu = xZ_{\nu-1} - \nu Z_\nu = \nu Z_\nu - xZ_{\nu+1}. \tag{A.52}$$

The half-indexed Bessel functions reduce to a finite sum of circular functions,

[5] Friedrich Wilhelm Bessel (1784-1846) was German astronomer, mathematician, and physicist.

[6] Carl Neumann (1832-1925) was a German mathematician and theoretical physicist; he is one of the initiators of the theory of integral equations.

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$$J_{n+1/2}(x) = -\sqrt{\frac{2x}{\pi}} x^n \left(\frac{d}{x dx}\right)^n \frac{\sin x}{x}, \tag{A.53}$$

$$J_{-n-1/2}(x) = \sqrt{\frac{2x}{\pi}} x^n \left(\frac{d}{x dx}\right)^n \frac{\cos x}{x}. \tag{A.54}$$

For $|x| \gg |\nu|$ the asymptotic behavior is given by

$$J_{\pm\nu}(x) = \sqrt{\frac{2}{\pi x}} \cos\left(x \mp \frac{\pi}{2}\nu - \frac{\pi}{4}\right)\left[1 + \mathcal{O}\left(\frac{1}{x^2}\right)\right] - \sqrt{\frac{2}{\pi x}} \sin\left(x \mp \frac{\pi}{2}\nu - \frac{\pi}{4}\right)\left[\frac{\Gamma(\nu + 3/2)}{\Gamma(\nu - 1/2)} \cdot \frac{1}{2x} + \mathcal{O}\left(\frac{1}{x^3}\right)\right]. \tag{A.55}$$

When the variable x is imaginary, it is often convenient to introduce the Bessel functions with imaginary argument I_ν and K_ν, according to the formulas

$$I_\nu(x) = e^{-\frac{\pi}{2}\nu i} J_\nu(ix), \tag{A.56}$$

$$K_\nu(x) = \tfrac{1}{2}\pi i e^{\frac{\pi}{2}\nu i} H_\nu^{(1)}(ix). \tag{A.57}$$

For large values of x, I diverges exponentially, whereas K tends to zero,

$$I_\nu(x) \underset{x\to\infty}{\longrightarrow} \frac{e^x}{\sqrt{2\pi x}}, \tag{A.58}$$

$$K_\nu(x) \underset{x\to\infty}{\longrightarrow} \sqrt{\frac{\pi}{2x}} e^{-x}. \tag{A.59}$$

I_ν and K_ν are called *modified Bessel functions*.

A.1.5 Spherical Bessel functions

In Section 12.1 we obtained the following differential equation for the radial wave function of a free particle in a central potential,

$$y'' + \frac{2}{x}y' + \left(1 - \frac{l(l+1)}{x^2}\right) y = 0. \tag{A.60}$$

By making the change of variable $y = Z/\sqrt{x}$, the resulting equation for the new function $Z(x)$ is

$$Z'' + \frac{1}{x}Z' + \left(1 - \frac{(l+\frac{1}{2})^2}{x^2}\right) Z = 0. \tag{A.61}$$

Comparing with (A.45), we see that Z is a cylindrical Bessel function with half-integer index $\nu = l + 1/2$; for this reason, the solutions of (A.60), which can be written in the conventional form

$$j_l(x) = \sqrt{\frac{\pi}{2x}} J_{l+1/2}(x) \tag{A.62}$$

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(and analogous expressions for the other cylindrical Bessel functions), are called *spherical Bessel* functions.[7]

Spherical Bessel functions include those specifically called spherical Bessel functions of the first kind $j_l(x)$, of the second kind or Neumann functions $n_l(x)$, and of the third kind or Hankel functions $h_l^{(1)}(x)$, $h_l^{(2)}(x)$. They are related by

$$h_l^{(1,2)}(x) = j_l(x) \pm i n_l(x); \tag{A.63}$$

the pairs (j_n, n_n) o $(h_k^{(1)}, h_n^{(2)})$ are linearly independent solutions of (A.60) for any $l = n = 0, 1, 2, \ldots$. Being proportional to the half-indexed Bessel functions, the spherical Bessel functions can be expressed as the sum of a finite number of terms, each of which contains a circular function. The first spherical Bessel functions are

$$\begin{aligned} j_0 &= \tfrac{1}{x}\sin x & n_0 &= -\tfrac{1}{x}\cos x \\ j_1 &= \tfrac{1}{x^2}\sin x - \tfrac{1}{x}\cos x & n_1 &= -\tfrac{1}{x^2}\cos x - \tfrac{1}{x}\sin x \\ j_2 &= \left(\tfrac{3}{x^3} - \tfrac{1}{x}\right)\sin x - \tfrac{3}{x^2}\cos x & n_2 &= -\left(\tfrac{3}{x^3} - \tfrac{1}{x}\right)\cos x - \tfrac{3}{x^2}\sin x, \end{aligned} \tag{A.64}$$

which shows that j_n are the regular solutions of (A.60), while n_n are singular at the origin. Their asymptotic behavior at the origin is

$$j_l(x) \simeq \frac{1}{(2l+1)!!}x^l, \quad n_l(x) \simeq -\frac{(2l-1)!!}{x^{l+1}} \quad (x \ll |l|), \tag{A.65}$$

and at $x \to \infty$,

$$j_l(x) \simeq \frac{1}{x}\cos\left[x - \frac{\pi}{2}(l+1)\right], \quad n_l(x) \simeq \frac{1}{x}\sin\left[x - \frac{\pi}{2}(l+1)\right] \quad (x \gg |l|). \tag{A.66}$$

In closed form, we have

$$j_l(x) = (-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\left(\frac{\sin x}{x}\right), \quad n_l(x) = -(-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\left(\frac{\cos x}{x}\right). \tag{A.67}$$

The generating function for the Bessel functions is

$$\frac{1}{x}\cos\sqrt{x^2 - 2xt} = \sum_{l=0}^{\infty}\frac{t^l}{l!}j_{l-1}(x), \tag{A.68}$$

and for the Neumann functions it is

$$\frac{1}{x}\sin\sqrt{x^2 + 2xt} = \sum_{l=0}^{\infty}\frac{(-t)^l}{l!}n_{l-1}(x). \tag{A.69}$$

The following recurrence relations hold for any of the functions $j_l(x)$, $n_l(x)$, $h_l^{(1,2)}(x)$,

$$(2l+1)f_l = x(f_{l-1} + f_{l+1}), \tag{A.70}$$

$$(2l+1)f_l' = lf_{l-1} - (l+1)f_{l+1}. \tag{A.71}$$

[7] The term "Bessel function" is used here to refer generically to any of the solutions of the corresponding differential equations.

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A.2 Mathematical Identities

$$\boldsymbol{A}\times(\boldsymbol{B}\times\boldsymbol{C})=(\boldsymbol{A}\cdot\boldsymbol{C})\,\boldsymbol{B}-(\boldsymbol{A}\cdot\boldsymbol{B})\,\boldsymbol{C}$$
$$(\boldsymbol{A}\times\boldsymbol{B})\times\boldsymbol{C}=(\boldsymbol{A}\cdot\boldsymbol{C})\,\boldsymbol{B}-(\boldsymbol{B}\cdot\boldsymbol{C})\,\boldsymbol{A}$$
$$\boldsymbol{A}\cdot(\boldsymbol{B}\times\boldsymbol{C})=(\boldsymbol{A}\times\boldsymbol{B})\cdot\boldsymbol{C}=(\boldsymbol{C}\times\boldsymbol{A})\cdot\boldsymbol{B}$$
$$(\boldsymbol{A}\times\boldsymbol{B})\cdot(\boldsymbol{C}\times\boldsymbol{D})=(\boldsymbol{A}\cdot\boldsymbol{C})\,(\boldsymbol{B}\cdot\boldsymbol{D})-(\boldsymbol{A}\cdot\boldsymbol{D})\,(\boldsymbol{B}\cdot\boldsymbol{D})$$
$$(\boldsymbol{A}\times\boldsymbol{B})\times(\boldsymbol{C}\times\boldsymbol{D})=[\boldsymbol{A}\cdot(\boldsymbol{B}\times\boldsymbol{D})]\,\boldsymbol{C}-[\boldsymbol{A}\cdot(\boldsymbol{B}\times\boldsymbol{C})]\,\boldsymbol{D}$$
$$=[\boldsymbol{A}\cdot(\boldsymbol{C}\times\boldsymbol{D})]\,\boldsymbol{B}-[\boldsymbol{B}\cdot(\boldsymbol{C}\times\boldsymbol{D})]\,\boldsymbol{A}$$
$$\nabla\times(\nabla u)=0,\quad \nabla\cdot(\nabla u)=\nabla^2 u$$
$$\nabla\cdot(\nabla\times\boldsymbol{A})=0,\quad \nabla\times(\nabla\times\boldsymbol{A})=\nabla(\nabla\cdot\boldsymbol{A})-\nabla^2\boldsymbol{A}$$
$$\nabla(uv)=u\nabla v+v\nabla u$$
$$\nabla\cdot(u\boldsymbol{A})=(\nabla u)\cdot\boldsymbol{A}+u\nabla\cdot\boldsymbol{A}$$
$$\nabla\times(u\boldsymbol{A})=(\nabla u)\times\boldsymbol{A}+u\nabla\times\boldsymbol{A}$$
$$\nabla\cdot(\boldsymbol{A}\times\boldsymbol{B})=\boldsymbol{B}\cdot(\nabla\times\boldsymbol{A})-\boldsymbol{A}\cdot(\nabla\times\boldsymbol{B})$$
$$\nabla(\boldsymbol{A}\cdot\boldsymbol{B})=(\boldsymbol{A}\cdot\nabla)\,\boldsymbol{B}+(\boldsymbol{B}\cdot\nabla)\,\boldsymbol{A}+\boldsymbol{A}\times(\nabla\times\boldsymbol{B})+\boldsymbol{B}\times(\nabla\times\boldsymbol{A})$$
$$\nabla\times(\boldsymbol{A}\times\boldsymbol{B})=(\boldsymbol{B}\cdot\nabla)\,\boldsymbol{A}-(\boldsymbol{A}\cdot\nabla)\,\boldsymbol{B}+\boldsymbol{A}(\nabla\cdot\boldsymbol{B})-\boldsymbol{B}(\nabla\cdot\boldsymbol{A})$$

$$\boldsymbol{F}=\hat{\mathrm{n}}\left(\boldsymbol{F}\cdot\hat{\mathrm{n}}\right)+\hat{\mathrm{n}}\times\left(\boldsymbol{F}\times\hat{\mathrm{n}}\right)=\boldsymbol{F}_{\parallel}+\boldsymbol{F}_{\perp}$$
$$\int_V(\nabla\cdot\boldsymbol{F})\,\mathrm{d}v=\oint_S\boldsymbol{F}\cdot\mathrm{d}\boldsymbol{a}\quad\text{(Gauss divergence theorem)}$$
$$\int_V(\nabla\times\boldsymbol{F})\,\mathrm{d}v=-\oint_S\boldsymbol{F}\times\mathrm{d}\boldsymbol{a}\quad\text{(a variant of Gauss theorem)}$$
$$\int_V(\nabla u)\,\mathrm{d}v=\oint_S u\,\mathrm{d}\boldsymbol{a}\quad\text{(a variant of Gauss theorem)}$$
$$\int_S(\nabla\times\boldsymbol{F})\cdot\mathrm{d}\boldsymbol{a}=\oint_C\boldsymbol{F}\cdot\mathrm{d}\boldsymbol{r}\quad\text{(Stokes theorem)}$$
$$\int_S\mathrm{d}\boldsymbol{a}\times\nabla\psi=\oint_C\psi\,\mathrm{d}\boldsymbol{r}\quad\text{(a variant of Stokes theorem)}$$
$$\int_V\left(\phi\nabla^2\psi-\psi\nabla^2\phi\right)dv=\oint_S(\phi\nabla\psi-\psi\nabla\phi)\cdot\mathrm{d}\boldsymbol{a}\quad\text{(Green theorem)}$$
$$\int_V\left(\phi\nabla^2\psi+\nabla\phi\cdot\nabla\psi\right)dv=\oint_S\phi\mathrm{d}\boldsymbol{a}\cdot\nabla\psi\quad\text{(first Green identity)}$$

Noncommuting operators

Consider two noncommuting operators P, Q that belong to a Hilbert space of linear vector operators. To third order in their commutators, a Taylor expansion gives

$$\ln(e^P e^Q)=(P+Q)+\frac{1}{2}[P,Q]+\frac{1}{12}([P,[P,Q]]+[Q,[Q,P]])-\frac{1}{24}[Q,[P,[P,Q]]]. \tag{A.72}$$

This is the (logarithm of the) *Baker–Campbell–Hausdorff formula*, including up to third-order commutators.

A.3 Curvilinear Coordinates

A.3.1 Spherical coordinates

$$x=r\sin\theta\cos\varphi,\quad y=r\sin\theta\sin\varphi,\quad z=r\cos\theta,$$
$$0\le r<\infty,\quad 0\le\theta\le\pi,\quad 0\le\varphi\le 2\pi.$$

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$$\frac{\partial r}{\partial x_i} = \frac{x_i}{r}, \quad \frac{\partial x_i}{\partial r} = \frac{x_i}{r}.$$

$$\frac{\partial \theta}{\partial x} = \frac{1}{r}\cos\theta\cos\varphi, \quad \frac{\partial \theta}{\partial y} = \frac{1}{r}\cos\theta\sin\varphi, \quad \frac{\partial \theta}{\partial z} = -\frac{1}{r}\sin\theta.$$

$$\frac{\partial \varphi}{\partial x} = -\frac{1}{r\sin\theta}\sin\varphi, \quad \frac{\partial \varphi}{\partial y} = \frac{1}{r\sin\theta}\cos\varphi, \quad \frac{\partial \varphi}{\partial z} = 0.$$

$$\hat{\mathbf{a}}_r = \widehat{\mathbf{i}}\sin\theta\cos\varphi + \widehat{\mathbf{j}}\sin\theta\sin\varphi + \hat{\mathbf{k}}\cos\theta,$$

$$\hat{\mathbf{a}}_\theta = \widehat{\mathbf{i}}\cos\theta\cos\varphi + \widehat{\mathbf{j}}\cos\theta\sin\varphi - \hat{\mathbf{k}}\sin\theta,$$

$$\hat{\mathbf{a}}_\varphi = -\widehat{\mathbf{i}}\sin\varphi + \widehat{\mathbf{j}}\cos\varphi.$$

$$\widehat{\mathbf{i}} = \hat{\mathbf{a}}_r\sin\theta\cos\varphi + \hat{\mathbf{a}}_\theta\cos\theta\cos\varphi - \hat{\mathbf{a}}_\varphi\sin\varphi,$$

$$\widehat{\mathbf{j}} = \hat{\mathbf{a}}_r\sin\theta\sin\varphi + \hat{\mathbf{a}}_\theta\cos\theta\sin\varphi + \hat{\mathbf{a}}_\varphi\cos\varphi,$$

$$\hat{\mathbf{k}} = \hat{\mathbf{a}}_r\cos\theta - \hat{\mathbf{a}}_\theta\sin\theta.$$

$$\hat{\mathbf{a}}_r \times \hat{\mathbf{a}}_\theta = \hat{\mathbf{a}}_\varphi, \quad \hat{\mathbf{a}}_r \times \hat{\mathbf{a}}_\varphi = -\hat{\mathbf{a}}_\theta, \quad \hat{\mathbf{a}}_\theta \times \hat{\mathbf{a}}_\varphi = \hat{\mathbf{a}}_r,$$

$$\frac{\partial \hat{\mathbf{a}}_r}{\partial \theta} = \hat{\mathbf{a}}_\theta, \quad \frac{\partial \hat{\mathbf{a}}_\theta}{\partial \theta} = -\hat{\mathbf{a}}_r, \quad \frac{\partial \hat{\mathbf{a}}_\varphi}{\partial \theta} = 0,$$

$$\frac{\partial \hat{\mathbf{a}}_r}{\partial \varphi} = \hat{\mathbf{a}}_\varphi\sin\theta, \quad \frac{\partial \hat{\mathbf{a}}_\theta}{\partial \varphi} = \hat{\mathbf{a}}_\varphi\cos\theta, \quad \frac{\partial \hat{\mathbf{a}}_\varphi}{\partial \varphi} = -\hat{\mathbf{a}}_r\sin\theta - \hat{\mathbf{a}}_\theta\cos\theta$$

$$d\mathbf{r} = \hat{\mathbf{a}}_r\,dr + \hat{\mathbf{a}}_\theta r\,d\theta + \hat{\mathbf{a}}_\varphi r\sin\theta\,d\varphi$$

$$da = r^2\sin\theta\,d\theta\,d\varphi$$

$$dv = r^2\sin\theta\,dr\,d\theta\,d\varphi.$$

$$\mathrm{grad}u = \nabla u = \hat{\mathbf{a}}_r\frac{\partial u}{\partial r} + \hat{\mathbf{a}}_\theta\frac{1}{r}\frac{\partial u}{\partial \theta} + \hat{\mathbf{a}}_\varphi\frac{1}{r\sin\theta}\frac{\partial u}{\partial \varphi},$$

$$\mathrm{div}\boldsymbol{A} = \nabla\cdot\boldsymbol{A} = \frac{1}{r^2}\frac{\partial}{\partial r}r^2A_r + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}\sin\theta A_\theta + \frac{1}{r\sin\theta}\frac{\partial A_\varphi}{\partial \varphi},$$

$$\mathrm{rot}\boldsymbol{A} = \nabla\times\boldsymbol{A} = \hat{\mathbf{a}}_r\frac{1}{r\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta A_\varphi - \frac{\partial A_\theta}{\partial\varphi}\right) +$$

$$+\frac{\hat{\mathbf{a}}_\theta}{r}\left(\frac{1}{\sin\theta}\frac{\partial A_r}{\partial\varphi} - \frac{\partial}{\partial r}rA_\varphi\right) + \frac{\hat{\mathbf{a}}_\varphi}{r}\left(\frac{\partial}{\partial r}rA_\theta - \frac{\partial A_r}{\partial\theta}\right),$$

$$\nabla^2 u = \frac{1}{r}\frac{\partial^2}{\partial r^2}ru + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial u}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 u}{\partial\varphi^2},$$

$$\nabla^2\boldsymbol{A}\,|_r = \left(-\frac{2}{r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} + \frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)A_r$$

$$+\left(-\frac{2}{r^2}\frac{\partial}{\partial\theta} - \frac{2\cos\theta}{r^2\sin\theta}\right)A_\theta + \left(-\frac{2}{r^2\sin\theta}\frac{\partial}{\partial\varphi}\right)A_\varphi =$$

$$= \nabla^2 A_r - \frac{2}{r^2}A_r - \frac{2}{r^2}\frac{\partial A_\theta}{\partial\theta} - \frac{2\cos\theta}{r^2\sin\theta}A_\theta - \frac{2}{r^2\sin\theta}\frac{\partial A_\varphi}{\partial\varphi},$$

$$\nabla^2\boldsymbol{A}\,|_\theta = \nabla^2 A_\theta - \frac{1}{r^2\sin^2\theta}A_\theta + \frac{2}{r^2}\frac{\partial A_r}{\partial\theta} - \frac{2\cos\theta}{r^2\sin^2\theta}\frac{\partial A_\varphi}{\partial\varphi},$$

$$\nabla^2\boldsymbol{A}\,|_\varphi = \nabla^2 A_\varphi - \frac{1}{r^2\sin^2\theta}A_\varphi + \frac{2}{r^2\sin\theta}\frac{\partial A_r}{\partial\varphi} + \frac{2\cos\theta}{r^2\sin^2\theta}\frac{\partial A_\theta}{\partial\varphi}.$$

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$$\nabla = \hat{\mathbf{a}}_r \frac{\partial}{\partial r} - \frac{i}{\hbar r^2} \boldsymbol{r} \times \hat{\boldsymbol{L}}$$
$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r - \frac{\hat{\boldsymbol{L}}^2}{\hbar^2 r^2}.$$

A.3.2 Cylindrical coordinates

$$x = \rho \cos\varphi, \quad y = \rho \sin\varphi, \quad z = z,$$
$$0 \le \rho < \infty, \quad 0 \le \varphi \le 2\pi, \quad -\infty < z < \infty.$$
$$\hat{\mathbf{a}}_\rho = \widehat{\mathbf{i}} \cos\varphi + \widehat{\mathbf{j}} \sin\varphi, \quad \hat{\mathbf{a}}_\varphi = -\widehat{\mathbf{i}} \sin\varphi + \widehat{\mathbf{j}} \cos\varphi, \quad \hat{\mathbf{k}} = \hat{\mathbf{k}},$$
$$\widehat{\mathbf{i}} = \hat{\mathbf{a}}_\rho \cos\varphi - \hat{\mathbf{a}}_\varphi \sin\varphi, \quad \widehat{\mathbf{j}} = \hat{\mathbf{a}}_\rho \sin\varphi + \hat{\mathbf{a}}_\varphi \cos\varphi.$$
$$\hat{\mathbf{a}}_\rho \times \hat{\mathbf{a}}_\varphi = \hat{\mathbf{k}}, \quad \hat{\mathbf{a}}_\varphi \times \hat{\mathbf{k}} = \hat{\mathbf{a}}_\rho, \quad \hat{\mathbf{k}} \times \hat{\mathbf{a}}_\rho = \hat{\mathbf{a}}_\varphi,$$
$$\frac{\partial \hat{\mathbf{a}}_\rho}{\partial \varphi} = \hat{\mathbf{a}}_\varphi, \quad \frac{\partial \hat{\mathbf{a}}_\varphi}{\partial \varphi} = -\hat{\mathbf{a}}_\rho.$$
$$d\mathbf{r} = \hat{\mathbf{a}}_\rho \, d\rho + \hat{\mathbf{a}}_\varphi \, \rho d\varphi + \hat{\mathbf{k}} \, dz.$$
$$dv = \rho \, d\rho \, d\varphi \, dz.$$
$$\nabla u = \hat{\mathbf{a}}_\rho \frac{\partial u}{\partial \rho} + \hat{\mathbf{a}}_\varphi \frac{1}{\rho} \frac{\partial u}{\partial \varphi} + \hat{\mathbf{k}} \frac{\partial u}{\partial z},$$
$$\nabla \cdot \boldsymbol{F} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho F_\rho\right) + \frac{1}{\rho} \frac{\partial F_\varphi}{\partial \varphi} + \frac{\partial F_z}{\partial z},$$
$$\nabla \times \boldsymbol{F} = \frac{1}{\rho} \begin{vmatrix} \hat{\mathbf{a}}_\rho & \rho \hat{\mathbf{a}}_\varphi & \hat{\mathbf{k}} \\ \frac{\partial}{\partial \rho} & \frac{\partial}{\partial \varphi} & \frac{\partial}{\partial z} \\ F_\rho & \rho F_\varphi & F_z \end{vmatrix},$$
$$\nabla^2 u = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial u}{\partial \rho}\right) + \frac{1}{\rho^2} \frac{\partial^2 u}{\partial \varphi^2} + \frac{\partial^2 u}{\partial z^2},$$
$$\nabla^2 \boldsymbol{F}|_\rho = \nabla^2 F_\rho - \frac{1}{\rho^2} F_\rho - \frac{2}{\rho^2} \frac{\partial F_\varphi}{\partial \varphi},$$
$$\nabla^2 \boldsymbol{F}|_\varphi = \nabla^2 F_\varphi - \frac{1}{\rho^2} F_\varphi + \frac{2}{\rho^2} \frac{\partial F_\rho}{\partial \varphi},$$
$$\nabla^2 \boldsymbol{F}|_z = \nabla^2 F_z,$$
$$\nabla = \hat{\mathbf{a}}_\rho \frac{\partial}{\partial \rho} + \hat{\mathbf{a}}_\varphi \frac{1}{\rho} \frac{\partial}{\partial \varphi} + \hat{\mathbf{k}} \frac{\partial}{\partial z}.$$

A.3.3 Parabolic coordinates

$$x = \xi \eta \cos\varphi, \quad y = \xi \eta \sin\varphi, \quad z = \tfrac{1}{2}\left(\xi^2 - \eta^2\right),$$
$$0 \le \xi < \infty, \quad 0 \le \eta < \infty, \quad 0 \le \varphi \le 2\pi.$$
$$\frac{\partial \xi}{\partial x} = \frac{\eta \cos\varphi}{\xi^2 + \eta^2}, \quad \frac{\partial \xi}{\partial y} = \frac{\eta \sin\varphi}{\xi^2 + \eta^2}, \quad \frac{\partial \xi}{\partial z} = \frac{\xi}{\xi^2 + \eta^2}.$$
$$\hat{\mathbf{a}}_\xi = \widehat{\mathbf{i}} \eta \cos\varphi + \widehat{\mathbf{j}} \eta \sin\varphi + \hat{\mathbf{k}} \xi,$$

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$$\hat{\mathbf{a}}_\eta = \hat{\mathbf{i}}\xi\cos\varphi + \hat{\mathbf{j}}\xi\ \sin\varphi - \hat{\mathbf{k}}\eta,$$
$$\hat{\mathbf{a}}_\varphi = -\hat{\mathbf{i}}\xi\,\eta\,\mathrm{sen}\,\varphi + \hat{\mathbf{j}}\xi\,\eta\cos\varphi.$$
$$dv = \xi\,\eta\left(\xi^2+\eta^2\right)d\xi\,d\eta\,d\varphi.$$
$$\nabla^2 u = \frac{1}{\xi^2+\eta^2}\left(\frac{1}{\xi}\frac{\partial}{\partial\xi}\xi\frac{\partial u}{\partial\xi} + \frac{1}{\eta}\frac{\partial}{\partial\eta}\eta\frac{\partial u}{\partial\eta}\right) + \frac{1}{\xi^2\eta^2}\frac{\partial^2 u}{\partial\varphi^2}.$$

A.4 Dirac's Delta

$$\delta(x) = 0,\ x\neq 0, \qquad \int_{-\infty}^{\infty} f(x)\,\delta(x)\,dx = f(0),$$
$$\delta(ax-b) = \frac{1}{|a|}\delta\left(x-\frac{b}{a}\right),$$
$$f(x)\delta(x) = f(0)\delta(x), \qquad x\delta(x) = 0,$$
$$f(x)\delta'(x) = f(0)\delta'(x) - f'(0)\delta(x),$$
$$x\delta^{(m)}(x) = -m\delta^{(m-1)}(x),$$
$$x^n\delta^{(m)}(x) = 0 \qquad n\geq m+1,$$
$$\delta(x) = \frac{d}{dx}H(x), \qquad H(x)\ \text{the Heaviside function}$$
$$\delta\left[f(x)\right] = \sum_n \frac{1}{|f'(x_n)|}\delta\left[x-x_n\right], \qquad f(x_n)=0,\ f'(x_n)\neq 0,$$
$$\delta\left(x^2-a^2\right) = \frac{1}{2|a|}\left[\delta(x-a)+\delta(x+a)\right],$$
$$\delta((x-a)(x-b)) = \frac{1}{|a-b|}[\delta(x-a)+\delta(x-b)]$$
$$\lim_{\eta\to 0^+}\frac{1}{\eta}e^{-x^2/\eta^2} = \sqrt{\pi}\delta(x), \qquad \lim_{\eta\to 0^+}\frac{\eta}{\eta^2+x^2} = \pi\delta(x),$$
$$\delta(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\omega t}dt,$$
$$\delta_+(\omega) = \frac{1}{2\pi}\int_0^\infty e^{i\omega t}dt = \frac{i}{2\pi}\lim_{\varepsilon\to 0^+}\frac{1}{\omega+i\varepsilon} = \frac{i}{2\pi}\mathrm{P}\frac{1}{\omega}+\frac{1}{2}\delta(\omega),$$
$$\delta_-(\omega) = \frac{1}{2\pi}\int_0^\infty e^{-i\omega t}dt = -\frac{i}{2\pi}\lim_{\varepsilon\to 0^+}\frac{1}{\omega-i\varepsilon} = -\frac{i}{2\pi}\mathrm{P}\frac{1}{\omega}+\frac{1}{2}\delta(\omega),$$

where the operator P represents the principal value.

$$\nabla^2|x| = 2\delta(x), \qquad \nabla^2\frac{1}{|\boldsymbol{r}-\boldsymbol{r}_0|} = -4\pi\delta(\boldsymbol{r}-\boldsymbol{r}_0).$$
$$\delta(\boldsymbol{r}-\boldsymbol{r}_0) = \frac{1}{r^2\sin\theta}\delta(r-r_0)\,\delta(\theta-\theta_0)\,\delta(\varphi-\varphi_0), \qquad x_0,y_0,z_0\neq 0;$$
$$= \frac{1}{2\pi r^2\sin\theta}\delta(r-r_0)\,\delta(\theta), \qquad x_0,y_0=0,\ z_0\neq 0;$$

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$$= \frac{1}{4\pi r^2}\delta(r), \quad x_0, y_0, z_0 = 0,$$

$$\delta(\boldsymbol{r} - \boldsymbol{r}_0) = \frac{1}{|J(x_i, \xi_i)|}\delta\left(\xi_1 - \xi_1^0\right)\delta\left(\xi_2 - \xi_2^0\right)\delta\left(\xi_3 - \xi_3^0\right).$$

Transverse delta function:

$$\delta_{ij}^{\perp}(\boldsymbol{r} - \boldsymbol{r}_0) = \frac{1}{(2\pi)^3}\int d^3k\,\delta_{ij}^{\perp}e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)},$$

$$\delta_{ij}^{\perp} = \left(\delta_{ij} - \frac{k_i k_j}{k^2}\right).$$

A.5 The Gamma Function

$$\Gamma(z) \equiv \lim_{n\to\infty}\frac{1\cdot 2\cdot 3\cdots n}{z(z+1)(z+2)\cdots(z+n)}n^z, \quad z \neq 0, -1-2, \ldots, \operatorname{Re} z > 0 \quad \text{(Euler)},$$

$$\Gamma(z) \equiv \int_0^\infty e^{-t}t^{z-1}dt, \quad \operatorname{Re} z > 0 \quad \text{(Euler)},$$

$$\frac{1}{\Gamma(z)} \equiv ze^{\gamma z}\prod_{n=1}^{\infty}\left(1 + \frac{z}{n}\right)e^{-z/n} \quad \text{(Weierstrass)};$$

γ is the Euler–Mascheroni constant $\gamma = 0.577216\ldots$

For $-(n+1) < \operatorname{Re}(z) \leq -n, z \neq 0, -1, -2, \ldots$, the Γ function is defined by the recurrence relation

$$\Gamma(z) = \frac{\Gamma(z+1)}{z} = \frac{\Gamma(z+n+1)}{z(z+1)\cdots(z+n)}.$$

The points $z = 0, -1, -2, \ldots$ are simple poles of $\Gamma(z)$.

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\operatorname{sen}\pi z},$$

$$|\Gamma(1+i\beta)|^2 = \frac{\pi\beta}{\operatorname{senh}\pi\beta}, \quad \beta \text{ real}.$$

$$\Gamma(x+1) = x\Gamma(x).$$

$$\Gamma(n) = (n-1)!, \quad \Gamma\left(n + \tfrac{1}{2}\right) = \frac{(2n-1)!!}{2^n}\sqrt{\pi}, \quad \Gamma\left(\tfrac{1}{2}\right) = \sqrt{\pi},$$

where

$$(2n+1)!! = 1\cdot 3\cdot 5\cdots(2n+1) = \frac{(2n+1)!}{2^n n!},$$

$$(2n)!! = 2\cdot 4\cdot 6\cdots 2n = 2^n n!.$$

For $|z| \to \infty$,

$$\Gamma(z) \sim \sqrt{2\pi}z^{z-1/2}e^{-z}\left(1 + \frac{1}{12z} + \frac{1}{288z^2} - \cdots\right), \quad |\arg z| \leq \pi - \delta, \quad 0 < \delta \ll 1.$$

For x real, $x \to \infty$,

$$\Gamma(x) \sim \sqrt{2\pi}x^{x-1/2}e^{-x}.$$

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A.6 Solving Eigenvalue Problems by Means of Algebraic Consistency Conditions

Throughout the book we have encountered situations where the conditions imposed on the function to be a physical solution of Schrödinger's equation lead to quantization. The conditions usually arise from the requirement that the wave function has the correct properties to correspond to a statistical amplitude of probability, and from the boundary conditions appropriate to the problem. In the case of bound systems, this procedure usually leads to quantization. Here we explore an alternative possibility that does not require knowing the solution of the Schrödinger equation for the problem, but instead requires considering certain algebraic relations between elements of two of the most important dynamical variables (operators) that should hold in any quantum mechanical system. More specifically, given the two reference variables, certain matrix elements of them are considered, which should be related by a set of specific (and simple) relations.

The operators are usually either bilinear forms of appropriate raising and lowering operators, or else auxiliary operators constructed by resorting to the factorization of the Hamiltonian. The quantization rules follow from the solution of the (generally elementary) condition obtained. A couple of examples will illustrate the clarity and simplicity of the procedure.

A.6.1 State-dependent and state-independent ladder operators

We consider the eigenvector basis $\{|k\rangle\}$ of a certain Hermitian operator P of interest with discrete spectrum and use this basis to construct a pair of operators $\eta^\dagger, \eta$ as follows,

$$\eta^\dagger = \sum_i C_i |i+1\rangle\langle i| = \sum_i C_i \eta_i^\dagger, \tag{A.73}$$

$$\eta = \sum_i C_i^* |i\rangle\langle i+1| = \sum_i C_i^* \eta_i, \tag{A.74}$$

where the constants C_i are to be determined, and

$$\eta_i^\dagger = |i+1\rangle\langle i|, \ \eta_i = |i\rangle\langle i+1|. \tag{A.75}$$

From this equation we note that

$$\eta_i^\dagger |n\rangle = |n+1\rangle\delta_{in}, \ \eta_i |n\rangle = |n-1\rangle\delta_{i,n-1}. \tag{A.76}$$

The raising and lowering operators $\eta_i^\dagger, \eta_i$ may depend explicitly or not on the state i on which they operate. We see that the basis $\{|k\rangle\}$ corresponds to the eigenvectors of the operators $\eta\eta^\dagger$ and $\eta^\dagger\eta$, and of the linear combinations of these operators,

$$S \equiv \eta\eta^\dagger + \eta^\dagger\eta = \{\eta, \eta^\dagger\}, \quad A \equiv \eta\eta^\dagger - \eta^\dagger\eta = [\eta, \eta^\dagger], \tag{A.77}$$

which are respectively the anticommutator and the commutator of η and $\eta^\dagger$. Therefore, S and A satisfy the eigenvalue equations

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$$S\,|k\rangle = s_k\,|k\rangle\,,\ A\,|k\rangle = a_k\,|k\rangle\,, \tag{A.78}$$

whence

$$s_k + a_k = s_{k+1} - a_{k+1} \tag{A.79}$$

and

$$s_{k+1} - s_k = a_{k+1} + a_k. \tag{A.80}$$

These basic consistency conditions between the eigenvalues of S and A corresponding to adjacent states will play an important role in what follows. In particular, it is clear from Eqs. (A.78) that

$$s_k \geq |a_k|. \tag{A.81}$$

From Eqs. (A.73), (A.74), (A.77), and (A.78) we get

$$s_k = |C_k|^2 + |C_{k-1}|^2\,, \tag{A.82}$$

$$a_k = |C_k|^2 - |C_{k-1}|^2\,. \tag{A.83}$$

We will consider that the spectrum of interest is bounded from below. As is customary, we denote the ground state with $|k_{\min}\rangle = |0\rangle$ unless otherwise specified, so that $C_{-1} = 0$ and $s_0 = a_0$. Successive application of Eq. (A.80) leads then to the recurrence relation

$$s_k = a_k + 2\sum_{i=0}^{k-1}(-1)^{i-(k-1)}s_i, \tag{A.84}$$

establishing the relationship between the eigenvalues of A and those of S.

For some applications it is convenient to introduce a couple of auxiliary operators α, β, indirectly defined through the relations

$$\eta^\dagger = \tfrac{1}{\sqrt{2}}(\alpha - i\beta), \text{ and} \tag{A.85}$$

$$\eta = \tfrac{1}{\sqrt{2}}(\alpha + i\beta). \tag{A.86}$$

From Eqs. (A.77) it follows that

$$A = i[\beta, \alpha], \tag{A.87}$$

$$S = \alpha^2 + \beta^2. \tag{A.88}$$

In this form, when the ladder operators are known, the consistency conditions allow us to determine the spectrum of A in terms of the spectrum of S or vice versa. This is particularly useful when either one of these operators is identified with a dynamical variable of interest, as is the case in the following example.

A.6.1.1 The radial problem

There is a family of problems for which a factorization method allows one to construct appropriate state-independent operators A and S, which can be used to solve the eigenvalue problem with the help of the consistency relations. These are

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N-dimensional radial problems, that is, central-force problems in N dimensions ($N = 1, 2, 3$) reduced to the radial variable only. The procedure is briefly presented for the 3D case ($N = 3$).

To study the spectrum associated with the radial factor, we introduce two operators that depend on a continuous dimensionless variable q as follows (where Λ is a real parameter)

$$B_{n\pm} = q^n \pm \left(\frac{-\Lambda}{q^n} + \frac{1}{q^{n-2}} \frac{d^2}{dq^2} \right), \tag{A.89}$$

with the properties

$$\left[q \frac{d}{dq}, B_{n\pm} \right] = n B_{n\mp}, \tag{A.90}$$

$$B_{n+} = 2q^n - B_{n-}. \tag{A.91}$$

This procedure is justified by the fact that for certain values of the exponent n, B_{n-} happens to take the form of an important quantum-mechanical radial Hamiltonian, as will be seen below. A careful examination of the above equations suggests the choice of

$$\alpha = B_{n+}, \tag{A.92}$$

$$i\beta = q \frac{d}{dq} - \left(q \frac{d}{dq} \right)^\dagger = 2q \frac{d}{dq} + (n-1)\mathbb{I}, \tag{A.93}$$

so that, after some simple transformations, one gets

$$S = \alpha^2 + \beta^2 = B_{n-}^2 + (n^2 - 1 - 4\Lambda)\mathbb{I}, \tag{A.94}$$

$$A = i[\beta, \alpha] = 2n B_{n-}. \tag{A.95}$$

These equations show that the eigenvalues of the operators A and S are related by the eigenvalues of the operator B_{n-}, which are the ones of interest. Denoting these eigenvalues by b_k, we obtain, from the consistency condition (A.80),

$$b_{k+1}^2 - b_k^2 = 2n(b_{k+1} + b_k). \tag{A.96}$$

Upon elimination of the common factor $b_{k+1} + b_k$ (assuming it is different from zero, which is true in the cases of interest), this equation simplifies into $b_{k+1} - b_k = 2n$, with solution

$$b_k = b_0 + 2nk. \tag{A.97}$$

For $n > 0$, which is the only case we shall study here, there is no upper bound. Equation (A.84) gives $2nb_0 = b_0^2 + n^2 - 1 - 4\Lambda$, whence

$$b_0 = n \pm \sqrt{1 + 4\Lambda} \geq 0. \tag{A.98}$$

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We see that the proposed choice of the operators α, β has led to the general solution expressed in Eq. (A.97). The essence of the method was to obtain a nonlinear relationship between s_k and a_k, with $a_k \propto b_k$, and to use the consistency condition to determine b_k. In the following we apply the procedure to Schrödinger's hydrogen-like atom, and in exercise E19.3 to Dirac's hydrogen-like atom.

The hydrogen-like atom

The radial Schrödinger equation for the hydrogen-like atom is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{Ze^2}{r}\right] u = Eu, \tag{A.99}$$

where $u = rR$, $R(r)$ being the radial part of the wave function. Multiplying by r, in terms of the variable $q = \beta_E r$ with $\beta_E = \sqrt{2m\,|E|}/\hbar$, the radial Hamiltonian reduces, after some simple rearrangements, to the operator B_{n-} for $n = 1$,

$$\left(-q\frac{d^2}{dq^2} + \frac{l(l+1)}{q} + q\right) u = B_{1-}u = \frac{Ze^2}{\hbar}\sqrt{\frac{2m}{|E|}}u. \tag{A.100}$$

To determine $b_0 = (Ze^2/\hbar)\sqrt{2m/|E_0|}$ we proceed, using (A.98) now with $n = 1$ and $\Lambda = l(l+1)$, thus obtaining $b_0 = 2(l+1)$ (the minus sign in Eq. (A.98) is ruled out since $b_0 \geq 0$ for any l). Using Eq. (A.97), we get $b_k = 2(l+k+1)$, which combined with $b_k = (Ze^2/\hbar)\sqrt{2m/|E_k|}$ gives, for the energy eigenvalues,[8]

$$E_{kl} = -\frac{Z^2e^4m}{2\hbar^2(k+l+1)^2} = -\frac{Z^2e^4m}{2\hbar^2\mathrm{n}^2}. \tag{A.101}$$

Bibliographical Notes

Clear, elegant and comprehensive textbooks on mathematical methods in physics are Morse and Feshbach (1953), and Hassani (2013). Another recommended book is Margenau and Murphy (2009).

The handbooks of integrals and special functions by Abramowitz and Stegun (1972), and Gradshteyn and Ryzhik (2007) are a necessary and very useful general reference.

For early work on the algebraic consistency method, see de la Peña and Montemayor (1980). An elaboration of the method is given in Fernández and Castro (1984), and further applications are given in de la Peña et al. (2022).

[8] The principal quantum number $\mathrm{n} = k + l + \frac{N-1}{2}$, is an integer in the 1D and 3D cases, and a half-integer in the 2D case. Although central-force problems can be reduced to 1D (radial) problems regardless of their physical dimension N, the energy spectrum explicitly depends on the number of dimensions.

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Physical Constants

Electron charge	e	-1.6021×10^{-19} C
Electron mass	m_e	9.10938×10^{-31} kg 0.510998 MeV/c^2
Proton mass	m_p	1836.152 m_e 1.67262×10^{-27} kg 938.272 MeV/c^2 1.007276 u.a.m.
Velocity of light in vacuum	c	2.99792458×10^8 m/s 137.036 u.a.
Planck constant	$\hbar$	1.0546×10^{-34} J · s 6.5821×10^{-15} eV · s
	$\hbar c$	3.1613×10^{-26} J · m 1.9732×10^{-11} MeV·cm
	$\hbar\omega_{\text{visible}}$	~ 2 eV
Avogadro number	N_A	6.02214×10^{23} part/mol
Free space permeability	μ_0	$4\pi \times 10^{-7}$ H/ m
Free space permittivity	$\varepsilon_0 = 1/\mu_0 c^2$	8.85418×10^{-12} F/m
Classical electron radius	$r_0 = e^2/4\pi\varepsilon_0 mc^2$	2.8179×10^{-15} m
Fine structure constant	$\alpha = e^2/\hbar c$	1/137.036
Compton electron wavelength	$\lambda_C = h/m_e c$	2.4263×10^{-12} m
Bohr radius	$a_0 = \lambda_C/\alpha$	0.5291 Å
Rydberg constant	R_H	109737.315 1/ cm
Bohr magneton	$\mu_B = \lvert e\rvert\, \hbar/2m_0$	9.2740×10^{-24} J/tesla
Boltzmann constant	k_B	1.3806×10^{-23} J/ K 8.6173×10^{-5} eV/K
	$k_B T_{\text{room temp}}$	~ 0.025 eV

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