Chapter 3

Complex Variable Theory

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I. Introduction

Complex variable theory is the differential and integral calculus of complex-valued functions of a complex-valued variable. A few elegant and powerful theorems, due mainly to Augustin Louis Cauchy (1787–1857) and to Karl Weierstrass (1815–1897) and Georg Friedrich Bernhard Riemann (1826–1866), contain the main results. Both the generality of the basic theorems and the remarkable interconnections among differentiation, integration, and power series expansion endow complex variable theory with a unique aesthetic unity.
Complex variable theory is a basic tool for many sciences. The classic application is to the solution of Laplace's equation in two dimensions, as in electrostatics, hydrodynamics, and temperature distribution. The very "language" of quantum mechanics is complex variable theory. In this chapter, two general applications are treated: the evaluation of real definite integrals, and the representation of so-called special functions by contour integrals. Specific applications are also given that are relevant to quantum chemistry.

The organization of the chapter is to proceed from the general to the specific. Sections II–V deal in turn with complex numbers, differentiation, integration, and power series. The major theorems occur in Sections III–V. Section VI introduces elementary functions and the notion of branch point. Major applications begin in Section VII with the evaluation of real definite integrals, and in Section VIII with the simpler higher transcendental functions—the gamma function, the beta function, the hypergeometric function, the confluent hypergeometric function, and special cases of these latter two. A brief excursion into Fourier transforms in Section IX leads into the evaluation of "Slater-type orbital" multicenter integrals in quantum chemistry in Section X. Finally, in Section XI "Lagrange's formula" is derived and applied to the formal solution of the nondegenerate Rayleigh–Schrödinger perturbation problem in quantum mechanics.

II. Complex Numbers

What are complex numbers? The reader is probably already able to reply: that a complex number \( z \) is composed of two real numbers, \( x \) and \( y \), and a symbol \( i \); that it is written

\[
x = x + iy = x + yi;
\]

that \( i \) satisfies,

\[
i^2 = -1;
\]

and that complex numbers otherwise obey the rules of ordinary algebra.

What is taken today for granted took hundreds of years to develop. The first implicit appearance of complex numbers is in sixteenth century formulas for the real roots of cubic and quartic polynomials, as, for instance, were published by Girolamo Cardano. That a polynomial could have complex roots, and that a polynomial of degree \( n \) has exactly \( n \)
roots, were recognized in the seventeenth century. But the birth of complex numbers was not complete until the doctoral thesis of Karl Friedrich Gauss and his proof of the fundamental theorem of algebra in 1799.

To characterize more precisely the complex number system, we first define a field. Loosely, a field is a set whose elements (numbers) can be combined by addition, subtraction, multiplication, and division. We then construct the complex field from the field of real numbers. The complex field is the smallest field that contains the real number field as a subfield and a solution of $z^2 = -1$.

A. THE COMPLEX NUMBER FIELD

A field $F$ is a set of elements closed under two binary operations, called addition and multiplication, which satisfy the following axioms ($z, z_1, z_2$, and $z_3$ denote any elements of $F$):

**Associative Laws**

\[
(z_1 + z_2) + z_3 = z_1 + (z_2 + z_3) \tag{2.3}
\]

\[
(z_1z_2)z_3 = z_1(z_2z_3). \tag{2.4}
\]

**Commutative Laws**

\[
z_1 + z_2 = z_2 + z_1 \tag{2.5}
\]

\[
z_1z_2 = z_2z_1. \tag{2.6}
\]

**Distributive Law**

\[
z_1(z_2 + z_3) = z_1z_2 + z_1z_3. \tag{2.7}
\]

**Additive Identity**

There is an element 0 in $F$ for which

\[
z + 0 = z \quad \text{for all } z \text{ in } F. \tag{2.8}
\]

**Multiplicative Identity**

There is an element 1 in $F$ for which

\[
z1 = z \quad \text{for all } z \text{ in } F. \tag{2.9}
\]
Additive Inverse

For each \( z \) in \( F \), there is an element in \( F \), usually denoted \((-z)\), for which
\[
 z + (-z) = 0. \tag{2.10}
\]

Multiplicative Inverse

For each nonzero \( z \) in \( F \), there is an element in \( F \), usually denoted \( z^{-1} \), for which
\[
 zz^{-1} = 1. \tag{2.11}
\]

The rational number system and the real number system are both examples of fields. We show how to construct the complex field from the real number field.

Let \( S \) denote the set of all ordered pairs \( (x, y) \) of real numbers \( x \) and \( y \). Define equality, addition (\( \oplus \)), and multiplication (\( \times \)) on \( S \) by
\[
(x_1, y_1) = (x_2, y_2) \iff \text{both } x_1 = x_2 \text{ and } y_1 = y_2 \tag{2.12}
\]
\[
(x_1, y_1) \oplus (x_2, y_2) = (x_1 + x_2, y_1 + y_2) \tag{2.13}
\]
\[
(x_1, y_1) \times (x_2, y_2) = (x_1x_2 - y_1y_2, x_1y_2 + y_1x_2). \tag{2.14}
\]

The additive and multiplicative identities are \((0, 0)\) and \((1, 0)\). The additive and multiplicative inverses for \((x, y) [\{x, y \neq (0, 0)\}]\) are \((-x, -y)\) and \((x/(x^2 + y^2)^{1/2}, -y/(x^2 + y^2)^{1/2})\). One may quickly verify that under \( \oplus \) and \( \times \), \( S \) is a field; that under \( \oplus \) and \( \times \), the set of all elements of \( S \) of the form \((x, 0)\) is also a field, essentially the field of real numbers; that \((x, y) \times (x, y) = (-1, 0)\) has two solutions, \((0, 1)\) and \((0, -1)\),
\[
(0, 1) \times (0, 1) = (0, -1) \times (0, -1) = (-1, 0); \tag{2.15}
\]
and that any \((x, y)\) can be written
\[
(x, y) = (x, 0) \oplus (0, 1) \times (y, 0). \tag{2.16}
\]

This field \( S \) is called the complex field, usually denoted by \( \mathbb{C} \), and the \((x, y)\) are called complex numbers.

B. Notation and Conventions. Elementary Consequences

The cumbersome \((x, y)\) notation is seldom used, except in the context of the preceding construction. Instead, a "real number" \((x, 0)\) is simply
written \( x \), the **imaginary unit** \((0, 1)\) is written \( i \), and an arbitrary \((x, y)\) is written \( x + iy \), following Eq. (2.16). A **pure imaginary** number is further shortened to \( iy \) from \( 0 + iy \), and 1 and 0 mean \((1, 0)\) and \((0, 0)\). The \( \oplus \) and \( \times \) are replaced by the usual \( + \) and \( \cdot \) (or nothing). Equations (2.13)–(2.15) are then

\[
(x_1 + iy_1) + (x_2 + iy_2) = (x_1 + x_2) + i(y_1 + y_2) \tag{2.17}
\]

\[
(x_1 + iy_1)(x_2 + iy_2) = (x_1x_2 - y_1y_2) + i(x_1y_2 + y_1x_2) \tag{2.18}
\]

\[
i^2 = (-i)^2 = -1. \tag{2.19}
\]

Subtraction and division are adaptations of addition and multiplication:

\[
z_1 - z_2 = z_1 + (\neg z_2) \tag{2.20}
\]

\[
z_1/z_2 = z_1z_2^{-1}, \quad z_2 \neq 0. \tag{2.21}
\]

It is conventional to reserve \( z \) and \( w \) to denote complex numbers and \( x, y, u, \) and \( v \) to denote real numbers. The relations,

\[
z = x + iy \tag{2.22}
\]

\[
w = u + iv \tag{2.23}
\]

shall **invariably be understood**, if not explicitly stated.

Some conventional terminology, given \( z = x + iy \), follows:

1. The **real part** of \( z \), \( \text{Re} \ z \), is \( x \):

\[
\text{Re} \ z = x. \tag{2.24}
\]

2. The **imaginary part** of \( z \), \( \text{Im} \ z \), is \( y \) (not \( iy \)):

\[
\text{Im} \ z = y. \tag{2.25}
\]

3. The **absolute value** of \( z \), \( |z| \), also called modulus, magnitude, or length, is

\[
|z| = (x^2 + y^2)^{1/2}. \tag{2.26}
\]

4. The **argument** of \( z \), \( \arg z \), is

\[
\arg z = \arctan(y/x), \quad z \neq 0, \tag{2.27}
\]

\[
= \arccos(x/|z|) = \arcsin(y/|z|), \quad z \neq 0. \tag{2.28}
\]
5. The complex conjugate of $z$, denoted both by $\bar{z}$ and by $z^*$ (especially in the scientific literature), is

$$\bar{z} = x - iy.$$  \hfill (2.29)

Note that arg $z$ is defined only up to integer multiples of $2\pi$ and that it is undefined for $z = 0$. A particular single-valued choice, denoted by Arg $z$ and called the principal value of arg $z$, is fixed by

$$-\pi < \text{Arg } z \leq \pi.$$  \hfill (2.30)

Some elementary consequences of the definitions given above are

$$\text{Re } z = \frac{1}{2}(z + \bar{z})$$  \hfill (2.31)

$$\text{Im } z = -\frac{1}{2}i(z - \bar{z}),$$ \hfill (2.32)

$$\bar{x_1 + x_2} = \bar{x}_1 + \bar{x}_2$$  \hfill (2.33)

$$\bar{x_1 x_2} = \bar{x}_1 \bar{x}_2$$  \hfill (2.34)

$$z \bar{z} = |z|^2 = |z^2|,$$  \hfill (2.35)

$$|z| \geq 0, \text{ with equality only when } z = 0$$  \hfill (2.36)

$$|\bar{z}| = |z|$$  \hfill (2.37)

$$|x_1 x_2| = |x_1| \cdot |x_2|$$  \hfill (2.38)

$$|x_1/x_2| = |x_1| / |x_2|,$$  \hfill (2.39)

$$\text{arg}(x_1 x_2) = \text{arg } x_1 + \text{arg } x_2 \pmod{2\pi}$$  \hfill (2.40)

$$\text{arg}(x_1/x_2) = \text{arg } x_1 - \text{arg } x_2 \pmod{2\pi},$$  \hfill (2.41)

$$\text{Re } z \leq |z|$$  \hfill (2.42)

$$\text{Im}(z) \leq |z|,$$  \hfill (2.43)

$$|x_1 + x_2| \leq |x_1| + |x_2| \quad \text{(triangle inequality)}$$  \hfill (2.44)

$$|x_1 - x_2| \geq |x_1| - |x_2| \quad \text{(variant of triangle inequality),}$$  \hfill (2.45)

$$\left| \sum_{k=1}^{n} x_k w_k \right|^2 \leq \left( \sum_{k=1}^{n} |x_k|^2 \right) \left( \sum_{k=1}^{n} |w_k|^2 \right) \quad \text{(Cauchy's inequality),}$$  \hfill (2.46)

$$z = |z| (\cos \phi + i \sin \phi), \quad \text{where } \phi = \text{arg } z \quad \text{(polar form for } z).$$  \hfill (2.47)
To derive Eq. (2.46), note that \( \sum_{k=1}^{n} |z_k - \lambda \bar{w}_k|^2 \geq 0 \), and choose \( \lambda = \frac{1}{\lambda} \frac{\sum_{k=1}^{n} \bar{z}_k w_k}{\sum_{k=1}^{n} |w_k|^2} \). The derivations of the remaining equations are more straightforward and are left to the reader.

C. GEOMETRIC REPRESENTATION

The ordered pair notation of Section II.A suggests and provides a one-to-one correspondence between complex numbers \( z = x + iy \) and points \((x, y)\) in a plane. Figure 1a shows the position vector corresponding to \( z \). Note particularly the significance of \(|z|\) and \(\arg z\) [cf. Eq. (2.47)] and the location of the point corresponding to \( \bar{z} \). The geometric picture of addition corresponds to vector addition (Fig. 1b), as is to be expected from Eq. (2.17). That multiplication has a geometric interpretation is a surprise! The position vector corresponding to \( z_1 z_2 \) has a length equal to the product of the lengths of \( z_1 \) and \( z_2 \) [Eq. (2.38)] and an angular coordinate equal to the sum of those for \( z_1 \) and \( z_2 \) [Eq. (2.40)], as illustrated in Fig. 1c:

\[
\begin{align*}
 z_1 z_2 &= |z_1| (\cos \phi_1 + i \sin \phi_1) |z_2| (\cos \phi_2 + i \sin \phi_2) \\
 &= |z_1 z_2| [\cos(\phi_1 + \phi_2) + i \sin(\phi_1 + \phi_2)].
\end{align*}
\]

So straightforward and so conceptually useful is the geometric picture that the distinction between "complex number" and its corresponding "point" is customarily ignored. The terms complex number \( z \) and point \( z \) are used interchangeably, as are \( xy \) plane, complex plane, \( z \) plane, and complex \( z \) plane. The \( x \) axis is called the real axis, and the \( y \) axis the imaginary axis.
D. Powers and Roots

Computation of $z^n$ and $z^{1/n}$ is an instructive yet elementary exercise. Let $n$ be a positive integer. Inductive iteration of Eq. (2.48) gives

$$z^n = |z|^n(\cos \phi + i \sin \phi)^n$$

$$(2.49)$$

$$= |z|^n(\cos n\phi + i \sin n\phi), \quad n \text{ an integer.}$$

$$(2.50)$$

Equation (2.50) is also valid when $n$ is a negative integer (take reciprocals of both sides). The equation

$$(\cos \phi + i \sin \phi)^n = \cos n\phi + i \sin n\phi$$

$$(2.51)$$

is known as de Moivre’s formula.

We now seek a solution $w$ to the equation

$$w^n = z = |z|(\cos \phi + i \sin \phi), \quad z \neq 0.$$  

$$(2.52)$$

By Eq. (2.50), there are precisely $n$ solutions,

$$w = |z|^{1/n}(\cos[(\phi + 2\pi k)/n] + i \sin [(\phi + 2\pi k)/n]),$$

$$k = 0, 1, \ldots, n - 1, \quad (2.53)$$

where $|z|^{1/n}$ denotes the real, positive, $n$th root of $|z|$. There are thus $n$ $n$th roots of $z$, denoted by the $n$-fold ambiguous symbol $z^{1/n}$.

The $n$ numbers

$$(\omega_n)^k = \cos(2\pi k/n) + i \sin(2\pi k/n), \quad k = 0, 1, \ldots, n - 1,$$

$$(2.54)$$

are called the $n$th roots of unity. They lie on the unit circle at the vertices of a regular $n$-sided polygon. The case $n = 6$ is illustrated in Fig. 2.

![Fig. 2. The six sixth roots of unity.](image)
The rational powers of \( z \), \( z^{m/n} (z \neq 0, m \text{ and } n \text{ both nonzero integers}) \), can be defined by

\[
z^{m/n} = (z^m)^{1/n} = |z|^{m/n} \{ \cos[(m/n)(\phi + 2\pi k)] + i \sin[(m/n)(\phi + 2\pi k)] \}.
\]

(2.55)

If \( m \) and \( n \) are relatively prime, then there are precisely \( |n| \) such numbers.

### III. Analytic Functions of a Complex Variable

The main thrust of this section is to define "analytic function" in terms of differentiation. The concepts of limit, continuity, and differentiation are developed in some detail. The main result is the connection of analyticity with the Cauchy–Riemann equations. Conjugate coordinates and the two-dimensional Laplace equation, both being derivative topics, are included at the end.

#### A. Functions of a Complex Variable

By a function \( f \) of a complex variable \( z \), denoted by \( f(z) \), is meant: (1) a "rule" or "correspondence" by which a definite complex number is associated with each value of the complex variable \( z \); and (2) a set \( D \) of points \( z \) to which the "rule" applies. The set \( D \) is called the domain of definition of \( f \).

As in real analysis, a small liberty is taken with the definition just given, and "function" is used in a second, distinct way: \( f(z) \) may mean, as above, the "rule" itself, and implicitly the domain of definition, or \( f(z) \) may mean the number associated with the number \( z \) by the "rule", as in "\( f \) takes on the value \( f(z) \) at the point \( z \)."

The set of values taken on by \( f(z) \) is called the range of \( f \).

Inherent in part (1) of our definition of the word "function" is that \( f(z) \) have only one value at \( z \), i.e., that \( f \) should be single valued. It turns out that certain functions are so closely related to each other (in the sense of analytic continuation) that they are put under a common umbrella, multiple-valued function. An example is \( z^{1/n} \), Eq. (2.53). This third usage of "function," considered in detail in Section VI, unfortunately is accompanied by a certain amount of semantic confusion. We refrain from using the redundant expression, "single-valued function," to mean "function," but use "multiple-valued function" as an inseparable term for that object.
Some simple functions are

\[ f(z) = 1, \quad \text{with domain of definition} \quad \mathbb{C} \]  
(3.1a)

\[ = z, \quad \mathbb{C} \]  
(3.1b)

\[ = z^2, \quad \mathbb{C} \]  
(3.1c)

\[ = z^n \quad (n \text{ a positive integer}), \quad \mathbb{C} \]  
(3.1d)

\[ = \sum_{k=0}^{n} c_k z^k \quad (c_k \in \mathbb{C}, c_n \neq 0; \quad \mathbb{C}) \]  
(3.1e)

polynomial of degree \( n \),

\[ = z, \quad \mathbb{C} \]  
(3.1f)

\[ = |z|, \quad \mathbb{C} \]  
(3.1g)

\[ = z^{-n} \quad (n \text{ a positive integer}), \quad \mathbb{C} - \{0\} \]  
(3.1h)

\[ = p_n(z)/q_m(z) \quad \text{(quotient of two polynomials,} \quad \mathbb{C} - \{\text{points at which } q_m = 0\} \]  
(3.1i)

called a rational function),

\[ \quad = |z|^{1/n} \left( \cos \frac{\arg z}{n} + i \sin \frac{\arg z}{n} \right) \quad \mathbb{C} \]  
(3.1j)

\[ \quad (\quad -\pi < \arg z \leq \pi) \]

\[ \quad = |z|^{1/n} \left( \cos \frac{\arg z}{n} + i \sin \frac{\arg z}{n} \right) \quad \mathbb{C} \]  
(3.1k)

\[ \quad (0 \leq \arg z < 2\pi) \]

\[ \quad = |z_1 - z_2| \quad \mathbb{C}. \]

A complex function \( f(z) \) corresponds to two real functions, \( u \) and \( v \), of the two real variables \( x \) and \( y \):

\[ f(z) = u(x, y) + iv(x, y). \]  
(3.2)

Just as \( z = x + iy \) is a standard notation, so is Eq. (3.2). Equation (3.2) permits results for functions of two real variables to be used for functions of a complex variable.

**B. LIMIT, CONTINUITY**

"Limit" and "continuity" hang on the notion of distance. The distance between \( z_1 \) and \( z_2 \) is defined to be the length of the vector connecting the two points in the complex plane: \( |z_1 - z_2| \).
A *neighborhood* of $z_0$ is the interior of a circle centered on $z_0$; i.e., \( \{ z \mid |z - z_0| < r \} \). This symbol is read “the set of all points $z$ satisfying $|z - z_0| < r$.” The $r$ is usually intended to be small.

We say that $f(z)$ *approaches a limit* $f_0$ as $z$ approaches $z_0$, written,

\[
 f(z) \to f_0 \quad \text{as} \quad z \to z_0, \quad \text{or} \quad \lim_{z \to z_0} f(z) = f_0, \tag{3.3}
\]

if and only if $f(z)$ is defined at all points of some neighborhood of $z_0$, except possibly at $z_0$ itself, and $|f(z) - f_0| \to 0$ as $|z - z_0| \to 0$. Although we have tied the definition of complex limit to real limit, it is important to realize that the limit process takes place in two dimensions. $f(z)$ must approach $z_0$ independently of the relative rates of $x \to x_0$ and $y \to y_0$. It is *explicitly* stated (“neighborhood”) in the definition that $z$ can approach $x_0$ from any direction. Of course, “$f(z)$ approaches $f_0$ as $z$ approaches $z_0$ along the curve $γ$” has an obvious meaning, but such a qualified use of “limit” is the exception. Most of the general theorems refer to points that can be approached from any direction (i.e., interior points).

If $f(z) \to f_0$ at $z_0$, then $u(x, y) \to u_0$ and $v(x, y) \to v_0$ as both $x$ and $y$ approach $x_0$ and $y_0$, and conversely.

A number of elementary consequences follow from the definition of limit, the triangle inequality [Eq. (2.44)], and \( |z_1z_2| = |z_1| |z_2| \):

\[
 \lim_{z \to z_0} \left( \sum_{k=1}^{N} f_k(z) \right) = \sum_{k=1}^{N} \left( \lim_{z \to z_0} f_k(z) \right) \tag{3.4}
\]

\[
 \lim_{z \to z_0} \left( \prod_{k=1}^{N} f_k(z) \right) = \prod_{k=1}^{N} \left( \lim_{z \to z_0} f_k(z) \right) \tag{3.5}
\]

\[
 \lim_{z \to z_0} \left( \frac{f_1(z)}{f_2(z)} \right) = \frac{\left( \lim_{z \to z_0} f_1(z) \right)}{\left( \lim_{z \to z_0} f_2(z) \right)} \quad \text{if} \quad \lim_{z \to z_0} f_2(z) \neq 0. \tag{3.6}
\]

The function $f(z)$ is said to be *continuous* at $z_0$ if and only if $f(z)$ is defined at $z_0$ and

\[
 \lim_{z \to z_0} f(z) = f(z_0). \tag{3.7}
\]

### C. Derivative

The *derivative* of $f(z)$ at $z_0$, denoted variously by $(d/dz)f(z_0)$, $(d/dz)f$, $df/dz$, $f'(z_0)$, and $f'$, is defined by

\[
 f'(z_0) = \lim_{h \to 0} \frac{f(z_0 + h) - f(z_0)}{h}. \tag{3.8}
\]
provided the limit exists. This definition is formally identical with the
real case, but the fundamental difference is that the limit must not depend
on how \(h = \Re h + i \Im h\) approaches zero.

The rules for derivatives of sums, products, quotients, and compositions
are the same as for the real case, being consequences of Eqs. (3.4)–(3.6)
and (3.8):

\[
(f + g)' = f' + g' \\
(fg)' = f'g + fg' \\
(f/g)' = (f'g - fg')/g^2
\]  

\[
\frac{d}{dz} f(g(z)) = \frac{df(g)}{dg} \frac{dg(z)}{dz} \quad \text{(chain rule)}.
\]  

The proofs are virtually identical with the real case and are not restated
here.

Derivatives of polynomials and rational functions are easily obtained.
An immediate consequence of the definition [Eq. (3.8)] is that

\[
(d/dz)k = 0, \quad k \text{ a constant}, \tag{3.13}
\]

\[
(d/dz)z = 1. \tag{3.14}
\]

The sum, product, and quotient rules, applied inductively, then give

\[
(d/dz)z^n = nz^{n-1}, \quad n \text{ an integer, } \ z \neq 0 \quad \text{when } n \text{ is negative}. \tag{3.15}
\]

When the integer \(n\) is positive, Eq. (3.15) also follows from

\[
(z_1^n - z_2^n)/(z_1 - z_2) = z_1^{n-1} + z_1^{n-2}z_2 + \cdots + z_1z_2^{n-2} + z_2^{n-1}. \tag{3.16}
\]

Thus, polynomials are differentiable everywhere, and rational functions
are differentiable everywhere except where their denominators vanish, and
their derivatives are obtained formally by the same rules as in real analysis.

The complex conjugate \(\bar{z}\) of \(z\) does not have a derivative anywhere,
since

\[
(z + h - \bar{z})/h = \bar{h}/h = [\cos(\arg h) - i \sin(\arg h)]^2 \tag{3.17}
\]

approaches no limit as \(h\) approaches zero. (A “direction-dependent”
limit is not enough.)

Similarly, \(|z|\) has no derivative, and \(|z|^2 = z\bar{z}\) has a derivative only
at \(z = 0\).
D. CAUCHY–RIEMANN EQUATIONS

The Cauchy–Riemann equations are an immediate consequence of the independence of \( f'(z_0) \) on how \( h \) approaches zero in Eq. (3.8). By alternatively computing \( f' \) with real \( h \) and pure imaginary \( h \), one obtains

\[
f'(z_0) = \lim_{h_x \to 0} \frac{f(z_0 + h_x) - f(z_0)}{h_x} = \frac{\partial f(z_0)}{\partial x} \tag{3.18}
\]

\[
= \lim_{h_y \to 0} \frac{f(z_0 + ih_y) - f(z_0)}{ih_y} = -i \frac{\partial f(z_0)}{\partial y} \tag{3.19}
\]

or the Cauchy–Riemann equation in complex form,

\[
(\partial / \partial x)f(z_0) = -i(\partial / \partial y)f(z_0). \tag{3.20}
\]

In real form, the Cauchy–Riemann equations are

\[
(\partial / \partial x)u(x_0, y_0) = (\partial / \partial y)v(x_0, y_0) \tag{3.21a}
\]

\[
(\partial / \partial y)u(x_0, y_0) = -(\partial / \partial x)v(x_0, y_0). \tag{3.21b}
\]

Note: The existence of \( f'(z_0) \) guarantees the continuity of \( f, u, \) and \( v \) at \( z_0 \) and the existence of the partial derivatives \( u_x, u_y, v_x, \) and \( v_y \) at \( (x_0, y_0) \).

Of more practical importance is the reverse: Given that \( u \) and \( v \) satisfy the Cauchy–Riemann equations at \( z_0 \), does \( f = u + iv \) have a derivative at \( z_0 \)? More information is needed. If the estimate is valid,

\[
f(z_0 + h_x + ih_y) - f(z_0) = h_x(\partial / \partial x)f(z_0) + h_y(\partial / \partial y)f(z_0) + \varepsilon, \tag{3.22}
\]

where \( \varepsilon / |h| \) tends to zero as \( |h| \) tends to zero, then the Cauchy–Riemann equation (3.20) in Eq. (3.8) gives

\[
\lim_{h \to 0} \frac{f(z_0 + h_x + ih_y) - f(z_0)}{h_x + ih_y} = \lim_{h \to 0} \frac{(h_x + ih_y)(\partial / \partial x)f(z_0) + \varepsilon}{h_x + ih_y}
\]

\[
= \frac{\partial}{\partial x} f(z_0), \tag{3.23}
\]

and the answer would be yes. The "if," however, cannot always be satisfied affirmatively, as is shown by the example

\[
u(x, y) = v(x, y) = xy/(x^2 + y^2), \quad (x, y) \neq (0, 0) \tag{3.24}
\]

\[
u = 0, \quad (x, y) = (0, 0) \tag{3.25}
\]

\[
\begin{align*}
  u_x(0, 0) &= u_y(0, 0) = v_x(0, 0) = v_y(0, 0) = 0
\end{align*} \tag{3.26}
\]
The Cauchy–Riemann equations are trivially satisfied, but \( u \) and \( v \) are not even continuous at \((0, 0)\)!

The problem is the same as the "differentiability" or existence of a "total differential" for a real function of two real variables. It is (more than) sufficient to assume additionally that \( u_x, u_y, v_x, \) and \( v_y \) are continuous at \((x_0, y_0)\). Then by the mean value theorem,

\[
\begin{align*}
  u(x_0 + h_x, y_0 + h_y) - u(x_0, y_0) &= u(x_0 + h_x, y_0 + h_y) - u(x_0, y_0 + h_y) + u(x_0, y_0 + h_y) - u(x_0, y_0) \\
  &= u_x(x_0 + \theta_1 h_x, y_0 + h_y)h_x + u_y(x_0, y_0 + \theta_2 h_y)h_y,
\end{align*}
\]

\[0 \leq \theta_1 \leq 1, \quad 0 \leq \theta_2 \leq 1,
\]

and further, by continuity,

\[
\begin{align*}
  u(x_0 + h_x, y_0 + h_y) - u(x_0, y_0) &= u_x(x_0, y_0)h_x + u_y(x_0, y_0)h_y + \varepsilon_1 h_x + \varepsilon_2 h_y
\end{align*}
\]

where both \( \varepsilon_1 \) and \( \varepsilon_2 \) tend to zero as \(| h | \) tends to zero. Equation (3.29) and a similar one for \( v \) clinch Eq. (3.22).

Thus, if \( f \) has a derivative at \( z_0 \), the Cauchy–Riemann equations are satisfied. If the first partial derivatives satisfy the Cauchy–Riemann equations and are continuous at \( z_0 \), then \( f \) has a derivative at \( z_0 \).

### E. Analytic Functions

A function \( f(z) \) is said to be analytic at a point \( z_0 \) if \( f'(z) \) exists at every point of some neighborhood of \( z_0 \). \( f(z) \) is said to be analytic in a region (region used loosely for some portion of the complex plane) if \( f(z) \) is analytic at every point of the region. Complex analysis is indeed the theory of analytic functions.

Polynomials are analytic in the entire \( z \) plane; rational functions are analytic for all \( z \) except where their denominators vanish (see Section III.C).

Analytic functions can be constructed from real functions with the aid of the Cauchy–Riemann equations. For instance, \( f(z) = e^x \cos y + ie^x \sin y \) satisfies the Cauchy–Riemann equation and has continuous partial derivatives everywhere. It is therefore analytic for all \( z \).

If the derivative of an analytic function vanishes identically in some neighborhood of \( z_0 \), \( f'(z) \equiv 0 \) for \(| z - z_0 | < r \), then

\[
u_x = u_y = v_x = v_y \equiv 0, \quad |z - z_0| < r,
\]
and $f(z)$ is a constant in that neighborhood. Moreover, if $f$ is identically real or identically imaginary, then either $f$ is not analytic or $f' = 0$ and $f$ is constant.

F. CONJUGATE COORDINATES

This amusing, sometimes useful subject gives an interesting insight into analyticity. Note that $x = \frac{1}{2}(z + \bar{z})$, $y = -\frac{i}{2}(z - \bar{z})$ have the same form as a coordinate transformation. If one regards an arbitrary complex function, $f = u(x, y) + iv(x, y)$, to be a function of the "independent" variables $z$ and $\bar{z}$, one may compute formally

$$\frac{\partial f}{\partial z} = \frac{\partial x}{\partial z} \frac{\partial f}{\partial x} + \frac{\partial y}{\partial z} \frac{\partial f}{\partial y} = \frac{1}{2} \left( \frac{\partial f}{\partial x} - i \frac{\partial f}{\partial y} \right) \tag{3.31}$$

$$\frac{\partial f}{\partial \bar{z}} = \frac{\partial x}{\partial \bar{z}} \frac{\partial f}{\partial x} + \frac{\partial y}{\partial \bar{z}} \frac{\partial f}{\partial y} = \frac{1}{2} \left( \frac{\partial f}{\partial x} + i \frac{\partial f}{\partial y} \right). \tag{3.32}$$

The Cauchy–Riemann equation (3.20) is just $(\partial f/\partial \bar{z}) = 0$.

One can add rigor to these remarks and present some results of complex variable theory from this point of view. [See, for instance, Nehari (1968).] An old and interesting application related to spherical harmonics is found in Hobson (1955).

G. TWO-DIMENSIONAL LAPLACE EQUATION

The basis for using complex variable theory to solve Laplace's equation in two dimensions is the Cauchy–Riemann equations. For an analytic function $f$, $(\partial f/\partial x) = -i(\partial f/\partial y)$, or $(\partial f/\partial x)^2 = -(\partial f/\partial y)^2$, so that $f$, $u$, and $v$ are all solutions of the two-dimensional Laplace equation

$$\frac{\partial^2 f}{\partial x^2} f(z) + \frac{\partial^2 f}{\partial y^2} f(z) = 0, \quad f(z) \text{ analytic} \tag{3.33}$$

$$\frac{\partial^2}{\partial x^2} u(x, y) + \frac{\partial^2}{\partial y^2} u(x, y) = 0 \tag{3.34}$$

$$\frac{\partial^2}{\partial x^2} v(x, y) + \frac{\partial^2}{\partial y^2} v(x, y) = 0. \tag{3.35}$$

A solution of Laplace's equation is called a harmonic function. The real functions $u$ and $v$ (or $v$ and $-u$) are said to be conjugate harmonic.
functions when \( u + iv \) is an analytic function. Solving Laplace’s equation is equivalent to finding an analytic function satisfying specified boundary conditions. This important application is discussed in many standard texts (e.g., Ahlfors, 1966; Churchill, 1960; Nehari, 1968) and by Henderson in Chapter 4, Section IX, of this volume.

We complete this section with an entertainingly useful exercise involving conjugate coordinates: how to find the conjugate harmonic function \( v(x, y) \) and the analytic function \( f(z) \) when given the harmonic function \( u(x, y) \). Start with

\[
f(z) = 2u(x, y) - \overline{f(z)}. \tag{3.36}
\]

Since \( f(z) \) is analytic, \( (\partial/\partial \bar{z}) f(z) = 0 \), i.e., \( \overline{(\partial/\partial z)f(z)} = 0 \), so that \( f(z) \) is a function only of \( \bar{z} \):

\[
\overline{f(z)} = g(\bar{z}) = g(x - iy). \tag{3.37}
\]

We use Eq. (3.37) to rewrite Eq. (3.36),

\[
f(x + iy) = 2u(x, y) - g(x - iy), \tag{3.38}
\]

into which we substitute formally

\[
x = z/2, \quad y = z/2i \tag{3.39}
\]

and find

\[
f(z) = 2u(z/2, z/2i) - \overline{f(0)}. \tag{3.40}
\]

The usefulness of Eq. (3.40) hangs on the meaningfulness of \( u(z/2, z/2i) \). The meaning is clear if \( u(x, y) \) is a polynomial in \( x \) and \( y \). Note that \( v(x, y) \) is determined only up to an arbitrary additive constant.

IV. Complex Integration

The most important theorems in complex analysis, Cauchy’s theorem and Cauchy’s integral formula, are derived in this section. After defining the complex integral, we show that the usual rules of ordinary calculus are valid for the complex calculus. We derive Cauchy’s theorem and integral formula, and then explore their immediate consequences.
A. Definition of the Complex Integral

In ordinary calculus, the definite integral of a function \( f(x) \), piecewise continuous on the closed interval \((a, b)\), is defined by

\[
\int_a^b f(x) \, dx = \lim_{n \to \infty} \sum_{k=1}^{n} f(\xi_k) \Delta x_k,
\]

(4.1)

where

\[
a = x_0 < x_1 < x_2 \cdots < x_n = b,
\]

\[
x_{k-1} \leq \xi_k \leq x_k, \quad \text{and} \quad \Delta x_k = x_k - x_{k-1}.
\]

(4.2)

In the complex case there is the added freedom of specifying the path \( \gamma \) connecting the complex numbers \( a \) and \( b \).

A path or curve \( \gamma \) in the complex plane is a geometric object. Its analytical description is called a parametric representation:

\[
\gamma : z = z(t), \quad t_a \leq t \leq t_b, \quad z(t) \text{ continuous},
\]

(4.3)

\[
z(t_a) = a, \quad z(t_b) = b.
\]

(4.4)

\( \gamma \) can be conveniently subdivided by subdividing \([t_a, t_b]\):

\[
t_a = t_0 < t_1 < t_2 \cdots < t_n = t_b, \quad t_{k-1} \leq \xi_k \leq t_k,
\]

(4.5)

\[
z_k = z(t_k), \quad \xi_k = z(\xi_k), \quad \Delta z_k = z_k - z_{k-1}.
\]

(4.6)

The integral of the complex function \( f(z) \) over the path \( \gamma \) is then defined by

\[
\int_{\gamma} f(z) \, dz = \lim_{n \to \infty} \sum_{k=1}^{n} f(\xi_k) \Delta z_k,
\]

(4.7)

provided that the limit exists.

1. Concerning Paths

A complex integral depends on the path \( \gamma \), as well as on the endpoints and on \( f(z) \). If \( \gamma \) is divided at a point into two paths, \( \gamma_1 \) and \( \gamma_2 \), then we write \( \gamma = \gamma_1 + \gamma_2 \), and

\[
\int_{\gamma_1 + \gamma_2} f(z) \, dz = \int_{\gamma_1} f(z) \, dz + \int_{\gamma_2} f(z) \, dz.
\]

(4.8)
3. Complex Variable Theory

The length of a path \( \gamma \), denoted by \( L_\gamma \), is defined by

\[
L_\gamma = \lim_{n \to \infty} \sum_{k=1}^{n} |\Delta z_k|,
\]

provided that the limit exists.

Paths have a sense or direction. Some authors use \(-\gamma\) to denote the path whose points are the same as for \( \gamma \), but whose sense is from \( b \) to \( a \). If \( \gamma \) is given by \( z = z(t) \ (t_a \leq t \leq t_b) \), then a representation for \(-\gamma\) is

\[
-\gamma: z = z(t_a + t_b - t), \quad t_a \leq t \leq t_b.
\]

Clearly,

\[
\int_{-\gamma} f(z) \, dz = -\int_{\gamma} f(z) \, dz.
\]

If \( a = b \), \( \gamma \) is said to be closed. If \( \gamma \) is nonself-intersecting, i.e.,

\[
z(t_1) = z(t_2) \iff t_1 = t_2,
\]

then \( \gamma \) is said to be simple. If \( a = b \) is the only exception to Eq. (4.12), then \( \gamma \) is called a simple closed curve. By convention, the positive direction on a simple closed curve is counterclockwise.

When \( \int_{\gamma} f(z) \, dz \) depends only on the endpoints of \( \gamma \), we may write without ambiguity,

\[
\int_{\gamma} f(z) \, dz = \int_{a}^{b} f(z) \, dz.
\]

When \( \gamma \) is a simple closed curve with counterclockwise sense, one may use the notation

\[
\int_{\gamma} f(z) \, dz = \oint_{\gamma} f(z) \, dz.
\]

The statements "\( \int_{\gamma} f(z) \, dz \) depends only on the endpoints" and "\( \int_{\gamma} f(z) \, dz = 0 \) for all closed curves \( \gamma \)" are equivalent, for if \( \gamma_1 \) and \( \gamma_2 \) are any two paths connecting \( a \) to \( b \), then \( \gamma_1 - \gamma_2 \) is a closed curve, and

\[
\int_{\gamma_1 - \gamma_2} f(z) \, dz = \int_{\gamma_1} f(z) \, dz - \int_{\gamma_2} f(z) \, dz.
\]

The importance of instantly associating these two statements together, when only one is read, cannot be overemphasized.
\( \gamma \) is said to be \textit{piecewise differentiable} if
\[
\frac{dz(t)}{dt} = \frac{dx(t)}{dt} + i \frac{dy(t)}{dt} \tag{4.16}
\]
even exists and is continuous for \( t_a \leq t \leq t_b \), except for a finite number of jump discontinuities. We shall only consider piecewise differentiable \( \gamma \).

The terms path, curve, arc, and contour are used synonymously.

\section*{2. Existence of the Complex Integral}

If it is assumed that \( f(z) \) is piecewise continuous for \( z \) on \( \gamma \), and that \( \gamma \) has finite length, then the existence of \( \int_{\gamma} f(z) \, dz \) can be proved by the same method used to prove the existence of the real definite integral (4.1), \textit{mutatis mutandis}. It is more instructive in a practical sense to assume additionally that \( \gamma \) is piecewise differentiable and to reduce the complex integral to two real integrals, whose existence is proved in elementary calculus. For piecewise differentiable \( \gamma \), with an assist from the mean value theorem and Eqs. (4.1) and (4.16), and with due care to be taken at any finite discontinuities, we may recast Eq. (4.7) as
\[
\int_{\gamma} f(z) \, dz = \lim_{n \to \infty} \sum_{k=1}^{n} f(z_k) \frac{z_k - z_{k-1}}{t_k - t_{k-1}} (t_k - t_{k-1}) \tag{4.17}
\]
\[
= \int_{t_a}^{t_b} \left[ u(x(t), y(t)) \frac{dx(t)}{dt} - v(x(t), y(t)) \frac{dy(t)}{dt} \right] dt
+ i \int_{t_a}^{t_b} \left[ u(x(t), y(t)) \frac{dy(t)}{dt} + v(x(t), y(t)) \frac{dx(t)}{dt} \right] dt, \tag{4.18}
\]
or, more compactly and suggestively,
\[
\int_{\gamma} f(z) \, dz = \int_{t_a}^{t_b} f(z(t)) \frac{dz(t)}{dt} \, dt = \int_{t_a}^{t_b} f \frac{dz}{dt} \, dt. \tag{4.19}
\]

It remains only to show that Eqs. (4.18) and (4.19) are independent of the parameterization of \( \gamma \). Let \( z = Z(s), s_a \leq s \leq s_b \), be another piecewise differentiable representation of \( \gamma \). Then \( z(t(s)) = Z(s) \) implicitly defines a piecewise differentiable function
\[
t = t(s), \quad s_a \leq s \leq s_b. \tag{4.20}
\]
Starting with Eq. (4.19) [as shorthand for Eq. (4.18)] and using the usual rules for changing integration variables in ordinary calculus, we obtain
\[ \int_{\gamma} f(z) \, dz = \int_{s_a}^{s_b} f(z(t(s))) \frac{dz(t)}{dt} \frac{dt}{ds} \, ds. \]  
(4.21)

By the chain rule of ordinary calculus,
\[ \frac{dz}{dt} \frac{dt}{ds} = \frac{dZ}{ds}, \]  
(4.22)

so that
\[ \int_{\gamma} f(z) \, dz = \int_{s_a}^{s_b} f(Z(x)) \frac{dZ(t)}{ds} \, ds, \]  
(4.23)

which has the same form as Eq. (4.19).

3. When \( \gamma \) Runs to Infinity

If one or both of the endpoints \( a \) and \( b \) are at \( \infty \), the integral is to be regarded as the limit of the integral for finite \( a \) and \( b \), as \( a \) and/or \( b \) approach \( \infty \) appropriately, provided that the limit exists.

B. Inequalities

The analog of
\[ \left| \int_{\gamma}^{b} f(z) \, dz \right| \leq \int_{a}^{b} |f(x)| \, dx \leq \max \{ |f(x)| \} \cdot |b - a| \]  
(4.24)
is enormously useful. First define, in the notation of Section IV.A.1,
\[ \int_{\gamma} |f(z)| \, dz = \lim_{n \to \infty} \sum_{k=1}^{n} |f(z_k)| \, |\Delta z_k|, \]  
(4.25)
or, equivalently for piecewise differentiable \( \gamma \),
\[ \int_{\gamma} |f(z)| \, dz = \int_{t_a}^{t_b} |f(z(t))| \left| \frac{dz(t)}{dt} \right| \, dt. \]  
(4.26)

Then the triangle inequality (2.44) applied to the absolute value of Eq. (4.7) gives
\[ \left| \int_{\gamma} f(z) \, dz \right| \leq \int_{\gamma} |f(z)| \, |dz|. \]  
(4.27)
If $|f(z)| \leq M$ on $\gamma$, then by Eqs. (4.25) and (4.9),

$$\left| \int_{\gamma} f(z) \, dz \right| \leq \int_{\gamma} |f(z)| \, |dz| \leq ML|\gamma|. \quad (4.28)$$

C. OPEN SETS. CONNECTIVITY. DOMAINS

The main theorems of complex analysis pertain to functions analytic in a kind of region in the complex plane called a domain. This use of “domain” is distinct from “domain of definition.”

A set $S$ of points in the complex plane is said to be open if, for each point $z$ in $S$, there is a neighborhood of $z$ contained entirely in $S$.

A set $S$ of points in the complex plane is said to be connected if, for any two points $z_1$ and $z_2$ in $S$, there is a continuous path from $z_1$ to $z_2$ lying entirely in $S$.

A domain is an open, connected set.

A connected set is said to be simply connected if it has no holes. More precisely, simple connectivity means that any two paths joining the same endpoints can be continuously deformed, via paths in $S$, into each other. Otherwise the set is said to be multiply connected.

The open unit disk, $\{z \mid |z| < 1\}$, is a simply connected domain. The punctured disk, $\{z \mid 0 < |z| < 1\}$, is a multiply connected domain. The closed disk, $\{z \mid |z| \leq 1\}$, is neither open nor a domain.

The relevance of domain is best appreciated from the theorem on convergence of power series (Section V.B) and the theorem on the representation of analytic functions by power series (Section V.D).

D. THE FUNDAMENTAL THEOREM OF CALCULUS

We now prove the complex analog of the central result of ordinary calculus, the fundamental theorem,

$$\int_{a}^{b} \frac{df(x)}{dx} \, dx = f(b) - f(a). \quad (4.29)$$

1. Fundamental Theorem. Part 1

**Theorem** If $f(z)$ is analytic and $(d/dz)f(z)$ continuous in a domain $D$, and if $\gamma$ is any piecewise differentiable path lying in $D$ and having endpoints $a$ and $b$, then

$$\int_{\gamma} \frac{df(z)}{dz} \, dz = f(b) - f(a). \quad (4.30)$$
Observe that the integral in Eq. (4.30) depends only on the endpoints \( a \) and \( b \), and not on any other details of \( \gamma \). The gist of the proof is to justify Eq. (4.32) in the sequence of equations:

\[
\int_{\gamma} f(z) \, dz = \int_{t_a}^{t_b} f(z(t)) \frac{dz(t)}{dt} \, dt
\]

\[
= \int_{t_a}^{t_b} \frac{d}{dt} f(z(t)) \, dt
\]

\[
= f(z(t)) \bigg|_{t_a}^{t_b} = f(b) - f(a),
\]

for Eq. (4.33) follows from Eq. (4.32) by the fundamental theorem of ordinary calculus applied separately to Re\( f \) and Im\( f \). To evaluate \((d/dt)f(z(t))\), use Eq. (3.22), which was justified for continuous \((df/dz)\). To state the argument loosely, divide Eq. (3.22) by \( \Delta t \) and take the limit as \( \Delta t \to 0 \):

\[
\frac{d}{dt} f(z(t)) = \frac{dx}{dt} \frac{\partial f(z)}{\partial x} + \frac{dy}{dt} \frac{\partial f(z)}{\partial y}.
\]

Then the Cauchy–Riemann equation (3.20) and Eq. (4.16) give

\[
\frac{d}{dt} f(z(t)) = \frac{df(z)}{dz} \frac{dz}{dt}.
\]

An instructive exercise for the reader is to work through the equivalent derivation using the real functions \( u \) and \( v \), and the Cauchy–Riemann equations (3.21).

\[2. \text{ A Few Simple Integrals}\]

From Eq. (3.15),

\[
\int_{a}^{b} z^n \, dz = \frac{(b^{n+1} - a^{n+1})}{n + 1}, \quad n \text{ an integer, } n \neq -1.
\]

When \( n \) is negative, the integration path must avoid the origin.

The integration-by-parts formula remains valid. If in a domain \( D \), \( f(z) \) and \( g(z) \) are analytic, and \( f'(z) \) and \( g'(z) \) are continuous, then by Eq. (3.10),

\[
\int_{\gamma} f'(z)g(z) \, dz = f(b)g(b) - f(a)g(a) - \int_{\gamma} f(z)g'(z) \, dz.
\]
A nice counterexample is given by $\int_\gamma (1/z) \, dz$. We have not given a function whose derivative is $1/z$, so we cannot use the fundamental theorem. We can compute the integral directly, however, when $\gamma$ is the circle $z = r \cos t + ir \sin t$ ($0 \leq t \leq 2\pi$, $r$ real and positive). Note that $dz/dt = iz$.

$$\oint_{|z|=r} (1/z) \, dz = \int_0^{2\pi} (1/z)iz \, dt = \int_0^{2\pi} i \, dt = 2\pi i. \quad (4.38)$$

This important result is independent of $r$. If $1/z$ is the derivative of an analytic function, the domain of analyticity cannot contain the circle $|z| = r$. Otherwise $\oint_{|z|=r} (1/z) \, dz$ could not be nonzero.

3. Fundamental Theorem. Part 2

The real definite integral is a differentiable function of its upper limit. So is the complex integral, if it is otherwise independent of the path.

**Theorem** (Converse of the theorem of Section IV.D.1.) If in a domain $D$, $f(z)$ is continuous and $\int_\gamma f(z) \, dz$ depends only on the endpoints of $\gamma$, for all $\gamma$ in $D$, then $f(z)$ is the derivative of a function $F(z)$ analytic in $D$.

**Proof** Fix $z_0$ and define $F(z)$ by

$$F(z) = \int_{z_0}^z f(\zeta) \, d\zeta. \quad (4.39)$$

As long as $z_0$, $z$, and $\gamma$ are in $D$, the integral depends only on the endpoints. Two special paths facilitate verifying the Cauchy–Riemann equations and computing $F'(z)$. Let $z_1$ and $z_2$ ($z_1 = x_1 + iy$ and $z_2 = x + iy_2$) both belong to a neighborhood of $z = x + iy$, entirely contained in $D$. Then one can write

$$F(z) = \int_{z_0}^{z_1} f(\zeta) \, d\zeta + \int_{z_1}^z f(\zeta) \, d\zeta = \int_{z_0}^{z_2} f(\zeta) \, d\zeta + \int_{z_2}^z f(\zeta) \, d\zeta \quad (4.40)$$

$$= F(z_1) + \int_{z_1}^z [u(\xi, y) + iv(\xi, y)] \, d\xi \quad (4.41)$$

$$= F(z_2) + i \int_{y_1}^y [u(x, \eta) + iv(x, \eta)] \, d\eta. \quad (4.42)$$

The fundamental theorem of ordinary calculus, applied separately to the
real and imaginary parts of Eq. (4.41), and then similarly to Eq. (4.42), yields
\[ \frac{\partial F(z)}{\partial x} = f(z) \]

which verifies that the Cauchy–Riemann equations are satisfied. Since 
\( f(z) \) was assumed continuous, by Section III.D and E, \( F(z) \) is analytic 
with derivative \( f(z) \), for all \( z \) in \( D \).

E. Cauchy’s Theorem

Independence of path is generally an inconvenient criterion. Cauchy’s 
theorem makes the criterion the analyticity of \( f(z) \).

1. Cauchy’s Theorem in a Simply Connected Domain. Statement

Cauchy’s Theorem Let \( f(z) \) be analytic in a simply connected do-
main \( D \), and let \( \gamma \) be any closed path in \( D \). Then
\[ \oint_{\gamma} f(z) \, dz = 0. \]  

(4.45)

If \( f'(z) \) is also assumed to be continuous, then a simple proof follows 
from the theory of real line integrals (see Section IV.1). A proof not re-
quiring the continuity of \( f'(z) \) was given by E. Goursat, and Cauchy’s 
theorem is often referred to as the Cauchy–Goursat theorem. We shall 
see in Section IV.F.2 that \( f'(z) \) itself is analytic and ipso facto continuous 
whenever \( f(z) \) is analytic.

2. Cauchy’s Theorem in a Simply Connected Domain. Proof

The proof proceeds in stages. By first taking \( \gamma \) to be a rectangle, 
we focus on relating the local behavior of \( f(z) \) at a point (analyticity) 
to its global behavior (integral about \( \gamma \)). The fundamental theorem pro-
vides the extension from rectangular to arbitrary \( \gamma \) when the domain is 
a disk. Finally, a simple procedure takes care of an arbitrarily shaped 
domain.

a. Rectangular \( \gamma \). We start with \( \gamma \) as a rectangle and immediately 
cut it into four equal rectangles, \( \gamma_1^{(1)}, \gamma_1^{(2)}, \gamma_1^{(3)}, \gamma_1^{(4)} \), as illustrated in Fig. 3.
In the sense of Eq. (4.8), both \( \gamma = \gamma^{(1)} + \gamma^{(2)} + \gamma^{(3)} + \gamma^{(4)} \) and
\[
\int_{\gamma} f(z) \, dz = \sum_{k=1}^{4} \int_{\gamma^{(k)}} f(z) \, dz. \tag{4.46}
\]
By the triangle inequality,
\[
\left| \int_{\gamma} f(z) \, dz \right| \leq \sum_{k=1}^{4} \left| \int_{\gamma^{(k)}} f(z) \, dz \right| \leq 4 \max \left\{ \left| \int_{\gamma^{(k)}} f(z) \, dz \right| \right\}. \tag{4.47}
\]
Denote by \( \gamma_1 \) the small rectangle for which \( \left| \int_{\gamma_1} f(z) \, dz \right| \) is maximum. Then
\[
\left| \int_{\gamma} f(z) \, dz \right| \leq 4 \left| \int_{\gamma_1} f(z) \, dz \right|. \tag{4.48}
\]
After carrying out this procedure \( n \) times, each time ending up with a rectangle \( \gamma_k \) that is one-quarter of the preceding \( \gamma_{k-1} \), we obtain a nested sequence of rectangles,
\[
\gamma \supset \gamma_1 \supset \gamma_2 \supset \cdots \supset \gamma_n. \tag{4.49}
\]
The sides of \( \gamma_n \) are \( 2^{-n} \) times the sides of \( \gamma \), and
\[
\left| \int_{\gamma} f(z) \, dz \right| \leq 4^n \left| \int_{\gamma_n} f(z) \, dz \right|. \tag{4.50}
\]
As \( n \to \infty \), the dimensions of \( \gamma_n \) tend to 0, and there is precisely one point \( z_0 \) contained in (or on) every rectangle of the sequence.

The analyticity of \( f \) at \( z_0 \) yields an estimate of \( \left| \int_{\gamma_n} f(z) \, dz \right| \) for sufficiently large \( n \). Given \( \varepsilon > 0 \), there is a \( \delta > 0 \), such that
\[
\left| \frac{f(z) - f(z_0)}{z - z_0} \right| - f'(z_0) \right| < \varepsilon, \quad \text{when} \quad |z - z_0| < \delta. \tag{4.51}
\]
For all sufficiently large \( n \), \( \gamma_n \) will be contained within the disk, \( |z - z_0| < \delta \). By Eq. (4.36),
\[
\int_{\gamma_n} \, dz = \int_{\gamma_n} (z - z_0) \, dz = 0 \tag{4.52}
\]
\[
\int_{\gamma_n} f(z) \, dz = \int_{\gamma_n} \left[ f(z) - f(z_0) - f'(z_0)(z - z_0) \right] \, dz. \tag{4.53}
\]
Then by the inequality (4.28),

$$\left| \oint_{\gamma_n} f(z) \, dz \right| < \varepsilon \max\{ |z - z_0| \}_{z \text{ on } \gamma_n} L_{\gamma_n}. \quad (4.54)$$

Since $L_{\gamma_n} = 2^{-n}L_\gamma$, and $\max\{ |z - z_0| \} \leq \frac{1}{2}L_{\gamma_n} = 2^{-n-1}L_\gamma$,

$$\left| \oint_{\gamma} f(z) \, dz \right| \leq 4^n \left| \oint_{\gamma_n} f(z) \, dz \right| \leq \frac{1}{2}\varepsilon L_\gamma^2. \quad (4.55)$$

But $\varepsilon$ is arbitrary, so $\oint_{\gamma} f(z) \, dz$ must vanish.

b. When $D$ is a Disk. With the result just obtained, we construct $F(z)$ such that $F'(z) = f(z)$. Let $z_0$ be the center of the disk and $z$ any point in the disk. The rectangle whose sides are parallel to the $x$ and $y$ axes, with opposite corners at $z_0$ and $z$, lies inside $D$, and

$$F(z) = \int_{y_0}^y f(x_0 + i\eta) \, d\eta + \int_{x_0}^x f(\xi + iy) \, d\xi \quad (4.56)$$

$$= \int_{x_0}^x f(\xi + iy_0) \, d\xi + i \int_{y_0}^y f(x + i\eta) \, d\eta. \quad (4.57)$$

We compute $(\partial/\partial x)F(z)$ from Eq. (4.56) and $(\partial/\partial y)F(z)$ from Eq. (4.57) via the fundamental theorem of ordinary calculus:

$$(\partial/\partial x)F(z) = f(z) \quad (4.58)$$

$$(\partial/\partial y)F(z) = if(z). \quad (4.59)$$

Since $f(z)$ is continuous and Eqs. (4.58) and (4.59) are the Cauchy–Riemann equations, $F(z)$ is analytic, and $F'(z) = f(z)$, for all $z$ in $D$. By the complex fundamental theorem, $\oint_{\gamma} f(z) \, dz = 0$, for all closed $\gamma$ in $D$.

c. When $D$ is an Arbitrary Simply Connected Domain. Since any closed curve may be considered to be a sum of simple closed curves, we may without loss of generality consider a simple closed curve $\gamma$ in $D$. Let $d$ denote the shortest distance from $\gamma$ to the boundary of $D$. Superimpose on $D$ a grid of lines parallel to the coordinate axes and spaced $\frac{1}{2}d$ apart. We may write $\gamma = \sum_{n} \gamma^{(n)}$, where each $\gamma^{(n)}$ is a $\frac{1}{2}d \times \frac{1}{2}d$ square lying entirely inside $\gamma$ or a partial square (part square inside $\gamma$, and part $\gamma$), and

$$\oint_{\gamma} f(z) \, dz = \sum_{n} \oint_{\gamma^{(n)}} f(z) \, dz. \quad (4.60)$$
The number of $\gamma^{(n)}$ is finite. Each $\gamma^{(n)}$ is contained in a disk of radius $\frac{1}{4}d$, lying entirely in $D$, so each term on the right-hand side of Eq. (4.60) vanishes.

3. Cauchy's Theorem in a Multiply Connected Domain

That $\int_{|z|=r} \frac{1}{z} \; dz = 2\pi i$, Eq. (4.38), shows the necessity of simple connectivity for Cauchy's theorem. There is, nevertheless, a very useful adaptation for multiply connected domains. Consider first the situation in which $\gamma_1$ and $\gamma_2$ are nonintersecting, simple closed curves, with $\gamma_2$ lying inside of $\gamma_1$, and both curves having counterclockwise sense. Let $f(z)$ be analytic both in the domain bounded on the outside by $\gamma_1$ and on the inside by $\gamma_2$, and at every point of $\gamma_1$ and $\gamma_2$. It is not necessary for $f(z)$ to be analytic everywhere inside of $\gamma_2$. Then

$$\int_{\gamma_1} f(z) \; dz = \int_{\gamma_2} f(z) \; dz.$$  \hspace{1cm} (4.61)

The essence of the proof is illustrated in Fig. 4. Additional lines are introduced to form simple closed contours, $\Gamma_1$ and $\Gamma_2$. Each of $\Gamma_1$ and $\Gamma_2$ lies in simply connected domains in which $f(z)$ is analytic, and

$$\int_{\gamma_1} f(z) \; dz - \int_{\gamma_2} f(z) \; dz = \int_{\Gamma_1} f(z) \; dz + \int_{\Gamma_2} f(z) \; dz = 0.$$  \hspace{1cm} (4.62)

![Fig. 4. Contours for multiply connected domains. (a) $\gamma_1$ and $\gamma_2$; (b) addition of two lines joining $\gamma_1$ and $\gamma_2$, so that $\Gamma_1 + \Gamma_2 = \gamma_1 - \gamma_2$; (c) a more general situation.](image)

The general situation, illustrated in Fig. 4c, is that $\gamma_1$ surrounds the disjoint simple closed curves $\gamma_2, \gamma_3, \ldots, \gamma_n$, all taken counterclockwise, and $f(z)$ is analytic on each curve and in the multiply connected domain they bound. The adaptation of Cauchy's theorem is

$$\int_{\gamma_1} f(z) \; dz = \sum_{k=2}^{n} \int_{\gamma_k} f(z) \; dz.$$  \hspace{1cm} (4.63)

A major use of Eqs. (4.61) and (4.63) in the practical evaluation of integrals is to replace a given contour $\gamma_1$ by a more tractable contour $\gamma_2$
(or $\gamma_2 + \cdots + \gamma_n$). Picturesque jargon is often employed, namely, "the contour $\gamma_1$ is deformed into the contour $\gamma_2$." As a simple example, let $\gamma$ be a simple closed curve, and let $z_0$ and the circle $|z - z_0| = r$ lie entirely inside $\gamma$. We deform $\gamma$ into $|z - z_0| = r$, then use Eq. (4.38):

$$\oint_{\gamma} (z - z_0)^{-1} \, dz = 2\pi i, \quad z_0 \text{ inside } \gamma.$$  \hspace{1cm} (4.64)

If $z_0$ were outside $\gamma$, the integral would vanish.

F. Cauchy's Integral Formula

Cauchy's integral formula, the single most important formula in complex variable theory, is the key to developing several important aspects of complex variable theory.

1. Cauchy's Integral Formula

**Theorem** Let $f(z)$ be analytic on and within a simple closed curve $\gamma$ (i.e., in a simply connected domain that contains $\gamma$). Let $z_0$ lie inside (but not on) $\gamma$. Then

$$f(z_0) = \frac{1}{2\pi i} \oint_{\gamma} \frac{f(z)}{z - z_0} \, dz \quad \text{(Cauchy's integral formula).} \quad (4.65)$$

Note that if $z_0$ were outside $\gamma$, the integral would vanish.

**Proof** Use successively: Eq. (4.64); $\oint_{\gamma} dz = 0$; $\gamma = \gamma_1$ and $\gamma_2$ = the circle, $|z - z_0| = \delta$, in Eq. (4.61); and a choice of $\epsilon$ and $\delta$ as in Eq. (4.51), to obtain

$$\frac{1}{2\pi i} \oint_{\gamma} \frac{f(z)}{z - z_0} \, dz - f(z_0) = \frac{1}{2\pi i} \oint_{\gamma} \frac{f(z) - f(z_0)}{z - z_0} \, dz$$

$$= \frac{1}{2\pi i} \oint_{\gamma} \left[ \frac{f(z) - f(z_0)}{z - z_0} - f'(z_0) \right] \, dz \quad (4.66)$$

$$\left| \frac{1}{2\pi i} \oint_{\gamma} \frac{f(z)}{z - z_0} \, dz - f(z_0) \right| < \frac{1}{2\pi} \epsilon \cdot 2\pi \delta = \epsilon \delta. \quad (4.68)$$

Clearly, the left-hand side of Eq. (4.68) vanishes.
Cauchy’s integral formula displays some of the remarkable tightness of complex variable theory. The values of an analytic function on the boundary of a region completely determine the value at every interior point!

2. Formula for \( f^{(n)}(z) \)

We now show, via Cauchy’s integral formula, that the derivative of an analytic function is itself analytic, and that an analytic function possesses derivatives of all orders.

\( a. \) Formula for \( f'(z) \). In Cauchy’s integral formula, Eq. (4.65), put \( z \) for \( z_0 \) and \( \zeta \) for \( z \). Use also

\[
\frac{1}{h} \left[ \frac{1}{\zeta - z - h} - \frac{1}{\zeta - z} \right] = \left( \frac{1}{\zeta - z} \right)^2 + h \left( \frac{1}{\zeta - z} \right)^2 \left( \frac{1}{\zeta - z - h} \right).
\]

(4.69)

Then

\[
f'(z) = \lim_{h \to 0} \frac{1}{2\pi i} \oint_{\gamma} f(\zeta) \frac{1}{h} \left[ \frac{1}{\zeta - z - h} - \frac{1}{\zeta - z} \right] d\zeta \tag{4.70}
\]

\[
= \frac{1}{2\pi i} \oint_{\gamma} \frac{f(\zeta)}{(\zeta - z)^2} \, d\zeta + \lim_{h \to 0} \frac{h}{2\pi i} \oint_{\gamma} \frac{f(\zeta)}{(\zeta - z)^2(\zeta - z - h)} \, d\zeta. \tag{4.71}
\]

Since \( z \) is inside \( \gamma \), \( |\zeta - z| \) has a nonzero minimum for \( \zeta \) on \( \gamma \), and

\[
\lim_{h \to 0} \left| \frac{h}{2\pi i} \oint_{\gamma} \frac{f(\zeta)}{(\zeta - z)^2(\zeta - z - h)} \, d\zeta \right|
\]

\[
\leq \lim_{h \to 0} \frac{|h|}{2\pi} \frac{\max\{|f(\zeta)|\} L_{\gamma}}{\min\{|\zeta - z|^2\} \min\{|\zeta - z| - |h|\}} = 0. \tag{4.72}
\]

Thus, \( f'(z) \) is given by the formula obtained by differentiating Cauchy’s integral formula under the integral sign:

\[
f'(z) = \frac{1}{2\pi i} \oint_{\gamma} \frac{f(\zeta)}{(\zeta - z)^2} \, d\zeta, \quad z \text{ inside } \gamma. \tag{4.73}
\]
b. Formula for $f^{(2)}(z)$. Does $f'(z)$ have a derivative?

\[
\lim_{h \to 0} \frac{f'(z + h) - f'(z)}{h} = \lim_{h \to 0} \frac{1}{2\pi i} \oint_{\gamma} f(\zeta) \frac{1}{h} \left[ \frac{1}{(\zeta - z - h)^2} - \frac{1}{(\zeta - z)^2} \right] d\zeta
\]

\[(4.74)\]

\[
= \frac{2}{2\pi i} \oint_{\gamma} \frac{f(\zeta)}{(\zeta - z)^3} d\zeta + \lim_{h \to 0} \frac{h}{2\pi i} \oint_{\gamma} f(\zeta)
\times \left[ \frac{2}{(\zeta - z - h)(\zeta - z)^2} + \frac{1}{(\zeta - z - h)^2(\zeta - z)^2} \right] d\zeta.
\]

\[(4.75)\]

As in Eqs. (4.71) and (4.72), the second integral in Eq. (4.75) vanishes, and

\[
f^{(2)}(z) = \frac{2}{2\pi i} \oint_{\gamma} \frac{f(\zeta)}{(\zeta - z)^3} d\zeta, \quad z \text{ inside } \gamma.
\]

\[(4.76)\]

c. Formula for $f^{(n)}(z)$. By induction, $f^{(n)}(z)$ exists and is analytic wherever $f(z)$ is analytic. Further,

\[
f^{(n)}(z) = \frac{n!}{2\pi i} \oint_{\gamma} \frac{f(\zeta)}{(\zeta - z)^{n+1}} d\zeta, \quad z \text{ inside } \gamma,
\]

\[(4.77)\]
as is obtained by integrating $(2\pi i)^{-1} \oint_{\gamma} f^{(n)}(\zeta)(\zeta - z)^{-1} d\zeta$ by parts, $n$ times. [This argument was not used to obtain Eq. (4.76), because the analyticity of both $f'(z)$ and $f^{(2)}(z)$ was not yet shown.]

The integral formula (4.77) displays the remarkable interconnection between complex integration and differentiation. It is also the formula obtained by differentiating Cauchy's integral formula $n$ times and interchanging the order of integration and differentiation.

G. SOME CONSEQUENCES OF CAUCHY'S INTEGRAL FORMULA, INCLUDING THE FUNDAMENTAL THEOREM OF ALGEBRA

One consequence is that analytic functions are infinitely differentiable. A few more quick consequences follow.

1. Bound for $|f^{(n)}(z)|$

Let $f(z)$ be analytic on and within a circle of radius $r$, centered on $z$, and let $|f(\zeta)| \leq M$, for $\zeta$ on the circle. By Eqs. (4.77) and (4.28),

\[
|f^{(n)}(z)| \leq Mn!r^{-n} \quad \text{(Cauchy's estimate).}
\]

\[(4.78)\]
2. Liouville's Theorem

If \( f(z) \) is analytic and bounded everywhere in the complex plane, then \( f(z) \) is constant.

**Proof** Take \( n = 1 \), and let \( r \to \infty \) in Cauchy's estimate. A main use of Liouville's theorem is to prove the fundamental theorem of algebra.

3. Fundamental Theorem of Algebra

A polynomial \( p_n(z) \), of degree \( n > 0 \), has at least one complex root.

**Proof** If \( p_n(z) \) were never zero, \( 1/p_n(z) \) and \( p_n(z) \) itself would be constant.

4. Morera's Theorem

If \( f(z) \) is continuous in a domain \( D \), and if \( \int_\gamma f(z) \, dz = 0 \), for all closed \( \gamma \) in \( D \), then \( f(z) \) is analytic in \( D \).

Section IV.D.3 implies that the integral of \( f(z) \) is analytic, and \( f(z) \) is its derivative. But the derivative of an analytic function is analytic.

5. Theorem

Let \( g(\zeta) \) be piecewise continuous on a simple closed curve \( \gamma \). Then

\[
    f(z) = \frac{1}{2\pi i} \int_\gamma \frac{g(\zeta)}{\zeta - z} \, d\zeta, \quad z \text{ inside } \gamma,
\]

(4.79)
defines a function analytic in the simply connected domain bounded by \( \gamma \).

**Proof** The integral clearly exists, and the derivation of Eq. (4.73), *mutatis mutandis*, provides a formula for \( f'(z) \). Note that Eq. (4.79) may not be used for \( z \) on \( \gamma \), and that \( f(z) \) does not necessarily approach \( g(\zeta) \) as \( z \) approaches \( \zeta \) on \( \gamma \).

6. Maximum Modulus Theorem

Let \( f(z) \) be analytic in a domain \( D \). Then \( |f(z)| \) has no maximum in \( D \).
Proof

\[ |f(z_0)| \leq |(2\pi i)^{-1} \oint_{|z-z_0|=\varepsilon} f(z)(z-z_0)^{-1} \, dz| \leq \max \{ |f(z)| \}_{|z-z_0|=\varepsilon}, \]

for all \( z_0 \) in \( D \), and for all sufficiently small \( \varepsilon \).

H. SUBSTITUTION FORMULA

The complex version of the substitution formula is a consequence of both Cauchy's theorem and the fundamental theorem, part 2.

Let \( z = z(\zeta) \), considered as a mapping, map the curve \( \gamma_{\zeta} \) one to one onto the curve \( \gamma_z \). Let \( f(z) \) and \( z(\zeta) \) be analytic functions of \( z \) and \( \zeta \) in appropriate domains. Then

\[ \int_{\gamma_z} f(z) \, dz = \int_{\gamma_{\zeta}} f(z(\zeta)) \frac{dz(\zeta)}{d\zeta} \, d\zeta. \]  

(4.80)

Proof Both \( \oint f(z) \, dz \) and \( \oint f(z(\zeta)) \frac{dz(\zeta)}{d\zeta} \, d\zeta \) have the same derivative with respect to \( \zeta \).

I. CONNECTION WITH REAL LINE INTEGRALS

The complex integral is composed of two real line integrals. In the notation of Section IV.A, a line integral in two dimensions over the piecewise differentiable path \( \gamma \) is given by

\[ \int_{t_a}^{t_b} \left[ p(x(t), y(t)) \frac{dx(t)}{dt} + q(x(t), y(t)) \frac{dy(t)}{dt} \right] \, dt \]

\[ = \int_{\gamma} [p(x, y) \, dx + q(x, y) \, dy], \]  

(4.81)

where \( p \) and \( q \) are continuous on \( \gamma \). Via Eq. (4.18) in line integral notation, namely,

\[ \int_{\gamma} f(z) \, dz = \int_{\gamma} [u(x, y) \, dx - v(x, y) \, dy] \]

\[ + i \int_{\gamma} [v(x, y) \, dx + u(x, y) \, dy], \]  

(4.82)

results for real line integrals can be applied to complex integrals.
The following are relevant results for real line integrals: If \( p, q, p_y, \)
and \( q_x \) are continuous functions of \( x \) and \( y \) in a domain \( D \), then

1. the line integral \( \int_\gamma (p \, dx + q \, dy) \) depends only on the endpoints of \( \gamma \), if and only if there is a function \( \phi(x, y) \), differentiable in \( D \), for which \( p = \phi_x \) and \( q = \phi_y \);
2. further, if \( D \) is simply connected, and \( \gamma \) is any simple closed curve in \( D \), then \( \oint_\gamma (p \, dx + q \, dy) = 0 \), if and only if \( p_y = q_x \) everywhere in \( D \);
3. still further (with \( D \) simply connected),

\[
\oint_\gamma (p \, dx + q \, dy) = \iint_{\text{area enclosed by } \gamma} (q_x - p_y) \, dx \, dy \tag{4.83}
\]

(Green's theorem or Gauss's theorem, restricted to two dimensions).

Result 1 is essentially the same result as the fundamental theorem, part 2 (Section IV.D.3). Either result 2 or 3 provides an immediate proof of Cauchy's theorem, if \( f'(z) \) is assumed to be continuous. In either case, one first takes \( p = u \) and \( q = -v \), then \( p = v \) and \( q = u \), and obtains results separately for each term in Eq. (4.82).

V. Power Series

A main result of this section is that convergent power series and analytic function are synonymous. Other important results concern the convergence, differentiation, and integration of power series, the existence of Laurent series, and the concept of analytic continuation.

A. Elementary Definitions and Results

The definitions of infinite series and convergence are virtually the same as in real analysis.

The expressions \( \sum_{k=0}^{\infty} c_k \), \( \sum_{k=0}^{\infty} f_k(z) \), where \( c_k \in \mathbb{C} \) and \( f_k(z) \in \mathbb{C} \), are called infinite series.

The expressions \( \sum_{k=0}^{\infty} c_k z^k \), \( \sum_{k=0}^{\infty} c_k (z - z_0)^k \), where \( c_k \in \mathbb{C} \), are called power series in \( z \) and in \( z - z_0 \).

The \( n \)th partial sum of an infinite series is the sum of the terms with indices less than or equal to \( n \), e.g.,

\[
s_n(z) = \sum_{k=0}^{n} c_k z^k. \tag{5.1}
\]
The series is said to converge (pointwise) to \( s(x) \) if, given any \( \varepsilon > 0 \), there exists an \( N \) such that
\[
|s_n(x) - s(x)| < \varepsilon \quad \text{for all } n \geq N. \tag{5.2}
\]
A series, e.g., \( \sum_k c_k x^k \), is said to converge uniformly for \( x \) in some region \( R \) if the \( N \) in Eq. (5.2) can be chosen independently of \( x \), and to converge absolutely if \( \sum_k |c_k x^k| \) converges. The series is said to satisfy the Cauchy test for convergence, if, given any \( \varepsilon > 0 \), there exists an \( N \) such that
\[
|s_n(x) - s_m(x)| < \varepsilon \quad \text{for all } n \geq N \text{ and } m \geq N. \tag{5.3}
\]
In the case of a power series,
\[
|s_n(x) - s_m(x)| = |c_{m+1} x^{m+1} + c_{m+2} x^{m+2} + \cdots + c_n x^n|, \quad n > m. \tag{5.4}
\]
If Cauchy’s test is satisfied, then the series converges, and conversely. The converse follows from
\[
|s_n - s_m| < |s_n - s| + |s_m - s|. \tag{5.5}
\]

**Proof That Cauchy’s Test Implies Convergence** For fixed \( m \), there are infinitely many \( s_n \) lying within a radius \( \varepsilon \) of \( s_m \). These \( s_n \) possess a point of accumulation \( s \). There can be only one such point, because only a finite number of \( s_n \) can be further apart than any fixed distance.

An absolutely convergent series converges, since, e.g.,
\[
|c_{m+1} x^{m+1} + c_{m+2} x^{m+2} + \cdots + c_n x^n| \leq |c_{m+1} x^{m+1}| + |c_{m+2} x^{m+2}| + \cdots + |c_n x^n|. \tag{5.6}
\]

An extremely useful convergence test is the Weierstrass \( M \) test. Let \( \Sigma b_k \) converge absolutely, let \( \Sigma f_k \) be an infinite series, and let there be an \( M > 0 \) for which
\[
|f_k| \leq M |b_k|, \quad k = 0, 1, 2, \ldots. \tag{5.7}
\]
Then \( \Sigma f_k \) converges absolutely.

**Proof** Use Cauchy’s test and
\[
|f_{m+1}| + \cdots + |f_n| \leq M (|b_{m+1}| + \cdots + |b_n|). \tag{5.8}
\]
The geometric series, $\sum_{k=0}^{\infty} z^k = 1 + z + z^2 + \cdots$, is frequently used as a comparison series. When $|z| < 1$, the geometric series converges to $(1 - z)^{-1}$:

$$s_n(z) - (1 - z)^{-1} = -z^{n+1}(1 - z)^{-1} \to 0 \quad \text{as} \quad n \to \infty, \quad |z| < 1.$$ (5.9)

When $|z| \geq 1$, the series diverges.

**B. BASIC THEOREM ON THE CONVERGENCE OF POWER SERIES**

The convergence properties of complex power series are reasonably neat. A power series converges in the interior of a circle, called the circle of convergence, and it diverges everywhere in the exterior. It may or may not converge at points on the circle. A simple but useful convergence theorem is given first, followed by a sharper result.

**Theorem** If $\sum_{k=0}^{\infty} c_k z^k$ converges, then $\sum_{k=0}^{\infty} c_k z^k$ converges absolutely for all $|z| < |\zeta|$. For fixed $r < |\zeta|$, convergence in $|z| \leq r$ is uniform.

**Proof** $\sum c_k \zeta^k$ converges $\Rightarrow c_k \zeta^k \to 0$ as $k \to \infty \Rightarrow$ there is an $M$ such that $|c_k \zeta^k| \leq M$, for all $k$. Then, since

$$|c_k z^k| = |c_k \zeta^k| |z/\zeta|^k \leq M |z/\zeta|^k,$$ (5.10)

the $\sum c_k z^k$ converges absolutely when $|z/\zeta| < 1$, by the Weierstrass $M$ test. Uniformity follows from

$$|c_{m+1} z^{m+1} + \cdots + c_n z^n| \leq |c_{m+1} z^{m+1}| + \cdots + |c_n z^n|, \quad |z| \leq r.$$ (5.11)

Simple reasoning permits a sharper formulation. Every power series has a radius of convergence $R$ ($0 \leq R \leq \infty$). For $|z| < R$, convergence is absolute. For fixed $r < R$, convergence is uniform in $|z| \leq r$. For $|z| > R$, the series diverges.

**Theorem** $R$ is given by Hadamard's formula

$$\frac{1}{R} = \limsup_{n \to \infty} |c_n|^{1/n}.$$ (5.12)
3. Complex Variable Theory

Proof Define $R$ by Eq. (5.12). We show convergence for $|z| < R$ and divergence for $|z| > R$. Let $\epsilon : 0 < \epsilon < 1$. By definition, lim sup means

$$|c_n|^{1/n} > 1/[R(1 + \epsilon)], \quad \text{for infinitely many } n, \quad (5.13)$$

$$|c_n|^{1/n} > 1/[R(1 - \epsilon)], \quad \text{for at most finitely many } n. \quad (5.14)$$

First let $|z| > R$, and pick $\epsilon$ such that $|z| > R(1 + \epsilon)$. Then

$$|c_nz^n| > |c_nR^n(1 + \epsilon)^n| > 1, \quad \text{for infinitely many } n, \quad (5.15)$$

and the series cannot converge. Second, let $|z| < R$, and pick $\epsilon$ such that $|z| < R(1 - \epsilon)$. By Eq. (5.14), there is an $M$ such that $|c_n|R^n \times (1 - \epsilon)^n \leq M$, for all $n$, and

$$|c_nz^n| = |c_nR^n(1 - \epsilon)^n| |z/[R(1 - \epsilon)]|^n \leq M |z/[R(1 - \epsilon)]|^n. \quad (5.16)$$

Convergence follows from the Weierstrass $M$ test.

Simple Examples The geometric series $\sum z^k$ has $R = 1$. The series $\sum k!z^k$ has $R = 0$, while $\sum (k!)^{-1}z^k$ has $R = \infty$. The series $\sum z^{k+3}/[(k + 1)(k + 2)]$ and the series $\sum (k + 1)(k + 2)z^k$ both have $R = 1$, but the first converges for all $|z| = 1$, whereas the second diverges for all $|z| = 1$.

The complex plane is the natural milieu for power series. The conventional illustration of the complex insight is the power series for $(1 + x^2)^{-1}$. This function is infinitely differentiable for all real $x$, but its power series, $\sum (-x^2)^k$, converges only for $x^2 < 1$. As a function of a complex variable, the divergence of the power series for $(1 + x^2)^{-1}$ when $|z| \geq 1$ is transparently understandable from the convergence theorem and the behavior of $(1 + z^2)^{-1}$ at $z = \pm i$.

C. Integration and Differentiation of Series. Analyticity

We turn now to the analysis of power series. The essential result is that, within their circle of convergence, power series are analytic functions, and they may be integrated and differentiated term by term.
Theorem Let \( \sum c_k x^k \) have radius of convergence \( R > 0 \); let \( |z| < R \); let \( \gamma \) lie in \( |z| < R \); let \( L_\gamma \) be finite; and let \( g(z) \) be continuous for \( z \) on \( \gamma \). Then
\[
\sum_{k=0}^{\infty} c_k x^k \text{ is continuous, } |z| < R \tag{5.17}
\]
\[
\int_\gamma g(z) \sum_{k=0}^{\infty} c_k x^k \, dx = \sum_{k=0}^{\infty} c_k \int_\gamma g(z) x^k \, dz \tag{5.18}
\]
\[
\sum_{k=0}^{\infty} c_k x^k \text{ is analytic, } |z| < R \tag{5.19}
\]
\[
\int_0^z \sum_{k=0}^{\infty} c_k x^k \, dx = \sum_{k=0}^{\infty} c_k x^{k+1}/(k+1) \tag{5.20}
\]
\[
(d/dz) \sum_{k=0}^{\infty} c_k x^k = \sum_{k=0}^{\infty} kc_k x^{k-1}, \tag{5.21}
\]
and the radius of convergence of the integrated and derived series [Eqs. (5.20) and (5.21)] is also \( R \).

Proof Continuity and term by term integrability are direct consequences of uniform convergence on \( |z| \leq r < R \). Assume Eqs. (5.17) and (5.18) to be true. Then for any simple closed curve \( \gamma \) in \( |z| < R \),
\[
\int_\gamma \sum_{k=0}^{\infty} c_k x^k \, dx = \sum_{k=0}^{\infty} c_k \int_\gamma x^k \, dx = 0, \tag{5.22}
\]
so that \( \sum c_k x^k \) is analytic, by Morera's theorem. Equation (5.20) is a trivial consequence of Eq. (5.18), and Eq. (5.21) follows from Eq. (5.18) by choosing \( g(z) \) to be \( (z - z_0)^{-2} \) and \( \gamma \) to be a simple closed curve enclosing \( z_0 \). The statement on radius of convergence is clinched by \( \lim_{n \to \infty} n^{1/n} = 1 \) and Hadamard's formula.

To prove Eq. (5.17), let \( |z - z_0| < \delta \), where \( \delta > 0 \) will be fixed later, let \( r \) satisfy \( |z| < r < R \), \( |z_0| < r < R \), and let \( s_N \) denote the \( N \)th partial sum. Consider
\[
\left| \sum_{k=0}^{\infty} c_k x^k - \sum_{k=0}^{\infty} c_k x_0^k \right| \leq \left| \sum_{k=0}^{\infty} c_k x^k - s_N(x) \right| + \left| s_N(x) - s_N(x_0) \right| + \left| \sum_{k=0}^{\infty} c_k x_0^k - s_N(x_0) \right|. \tag{5.23}
\]

Pick \( \epsilon > 0 \). By uniformity of convergence, \( N \) can be chosen so that
\[
\left| \sum_{k=0}^{\infty} c_k z^k - s_N(\zeta) \right| < \epsilon/3 \quad \text{for all } |\zeta| \leq r. \tag{5.24}
\]
By continuity of the polynomial \( s_N(z) \) at \( z_0 \), \( \delta \) can be chosen so that
\[
| s_N(z) - s_N(z_0) | < \varepsilon/3 \quad \text{whenever} \quad |z - z_0| < \delta. \tag{5.25}
\]

The right-hand side of Eq. (5.23) is thus less than \( \varepsilon \), when \( |z - z_0| < \delta \), and \( \sum c_k z^k \) is continuous.

To prove Eq. (5.18), start with
\[
\left| \int_\gamma g(z) \sum_{k=0}^\infty c_k z^k \, dz - \sum_{k=0}^n c_k \int_\gamma g(z) z^k \, dz \right| = \left| \int_\gamma g(z) \left[ \sum_{k=0}^\infty c_k z^k - s_n(z) \right] \, dz \right|. \tag{5.26}
\]

Fix \( \varepsilon > 0 \). By uniform convergence, \( N \) can be chosen so that
\[
\left| \sum_{k=0}^\infty c_k z^k - s_n(z) \right| < \varepsilon,
\]
for all \( n \geq N \) and all \( |z| \leq r \). Then
\[
\left| \int_\gamma g(z) \sum_{k=0}^\infty c_k z^k \, dz - \sum_{k=0}^n c_k \int_\gamma g(z) z^k \, dz \right| < \max \{|g|\} \varepsilon L_\gamma, \tag{5.27}
\]
which clinches Eq. (5.18).

The preceding theorem depended almost entirely on the uniform convergence of the infinite series. The reader may readily verify a more general result (to be used in the next section).

**Theorem on Continuity and Integrability of Uniformly Convergent Series of Continuous Functions** Let \( f_k(z) \) be continuous for \( z \) in a domain \( D \), let \( \gamma \) be any curve in \( D \) of finite length, and let \( \sum_{k=0}^\infty f_k(z) \) converge uniformly for \( z \) in \( D \). Then \( \sum_{k=0}^\infty f_k(z) \) is continuous in \( D \), and the series may be integrated term by term. If each \( f_k(z) \) is analytic in \( D \), then so is \( \sum_{k=0}^\infty f_k(z) \), and the series may be differentiated term by term.

**D. Representation of Analytic Functions by Power Series**

A convergent power series is an analytic function. The reverse is also true.
Theorem  If \( f(z) \) is analytic in \(| z - z_0 | < r \), then \( f(z) \) can be represented by a Taylor series at \( z_0 \),
\[
f(z) = \sum_{k=0}^{\infty} \frac{f^{(k)}(z_0)}{k!} (z - z_0)^k, \quad |z - z_0| < r.
\] (5.28)

Proof  Given \( z \), choose \( r_1 \) such that \(| z - z_0 | < r_1 < r \). Then substitute into Cauchy’s integral formula
\[
(\zeta - z)^{-1} = [(\zeta - z_0) - (z - z_0)]^{-1} = \sum_{k=0}^{\infty} (z - z_0)^k (\zeta - z_0)^{-k-1},
\] (5.29)
which converges uniformly with respect to \( \zeta \), for \( \zeta \) on the circle \(| \zeta - z_0 | = r_1 \). Term by term integration gives Eq. (5.28).

The radius of convergence of the Taylor series for \( f(z) \) about \( z_0 \) must be at least as large as the distance to the nearest point at which \( f(z) \) is not analytic.

Taylor series are unique: Power series can be differentiated term by term, so that the coefficient of \((z - z_0)^k\) is always \( f^{(k)}(z_0)/k! \).

E. Laurent Series

Consider the simple function \( f(z) = (z - 1)^{-1}(z - 2)^{-1} \). The Taylor series about \( z = 0 \),
\[
(z - 1)^{-1}(z - 2)^{-1} = -(z - 1)^{-1} + (z - 2)^{-1}
\] (5.30)
\[
= \sum_{k=0}^{\infty} (1 - 2^{-k-1})z^k, \quad |z| < 1,
\] (5.31)
diverges when \(| z | > 1 \). In the annulus \( 1 < |z| < 2 \), \((z - 1)^{-1}\) can be expanded in powers of \(z^{-1}\), and \((z - 2)^{-1}\) in powers of \( z/2 \) (both series being just the geometric series):
\[
(z - 1)^{-1}(z - 2)^{-1} = (z - 2)^{-1} - z^{-1}(1 - z^{-1})^{-1}
\] (5.32)
\[
= -\sum_{k=0}^{\infty} z^k/2^{k+1} - \sum_{k=1}^{\infty} z^{-k-1}, \quad 1 < |z| < 2.
\] (5.33)
The net result is a series in positive and negative powers of \( z \) that converges in the annulus \( 1 < |z| < 2 \), but that diverges when \(| z | < 1 \) or \(| z | > 2 \). This behavior is general.
**Theorem**  Let \( f(z) \) be analytic in the annulus \( R_2 < |z - z_0| < R_1 \). Then \( f(z) \) possesses the *Laurent series* about \( z_0 \),

\[
f(z) = \sum_{k=0}^{\infty} c_k (z - z_0)^k + \sum_{k=1}^{\infty} c_{-k} (z - z_0)^{-k},
\]

(5.34)

where

\[
c_k = \frac{1}{2\pi i} \oint_{|\zeta - z_0| = r_1} \frac{f(\zeta)}{(\zeta - z_0)^{k+1}} \, d\zeta, \quad k = 0, 1, 2, \ldots,
\]

(5.35)

\[
c_{-k} = \frac{1}{2\pi i} \oint_{|\zeta - z_0| = r_2} f(\zeta)(\zeta - z_0)^{-k} \, d\zeta, \quad k = 1, 2, 3, \ldots,
\]

(5.36)

and \( R_2 < r_2 < |z - z_0| < r_1 < R_1 \). The series \( \sum c_k (z - z_0)^k \) converges absolutely for \( |z - z_0| < R_1 \) and uniformly for \( |z - z_0| \leq r_1 \), and the series \( \sum c_{-k} (z - z_0)^{-k-1} \) converges absolutely for \( |z - z_0| > R_2 \) and uniformly for \( |z - z_0| \geq r_2 \).

**Proof**  Use Cauchy’s theorem as adapted for multiply connected domains, Eq. (4.63), with \( \gamma_1 \) the circle \( |\zeta - z_0| = r_1 \), \( \gamma_2 \) the circle \( |\zeta - z_0| = r_2 \), \( \gamma_3 \) the circle \( |\zeta - z| = \varepsilon \) (\( \varepsilon \) being small enough not to cause any difficulties), and with \( \zeta \) for \( z \) and \( f(\zeta)/(\zeta - z) \) for \( f(z) \), to obtain

\[
f(z) = \frac{1}{2\pi i} \oint_{|\zeta - z_0| = \varepsilon} \frac{f(\zeta)}{\zeta - z} \, d\zeta - \oint_{|\zeta - z_0| = r_1} \frac{f(\zeta)}{\zeta - z} \, d\zeta - \oint_{|\zeta - z_0| = r_2} \frac{f(\zeta)}{\zeta - z} \, d\zeta.
\]

(5.37)

On \( |\zeta - z_0| = r_1 \), use \((\zeta - z)^{-1} = \sum_{k=0}^{\infty} (z - z_0)^k (\zeta - z_0)^{-k-1}\), and on \( |\zeta - z_0| = r_2 \), use \((\zeta - z)^{-1} = -\sum_{k=1}^{\infty} (\zeta - z_0)^{k-1} (z - z_0)^{-k}\). Term by term integration yields Eqs. (5.34)-(5.36), while the convergence statement is a consequence of the convergence theorem and term by term integrability theorem of Sections V.B and V.C.

**Remarks**  (1) If \( f(z) \) is analytic for \( |z| < R_1 \), then all the \( c_{-k} \) vanish.

(2) Laurent series are unique [substitute the Laurent series about \( z_0 \) for \( f(\zeta) \) into Eqs. (5.35) and (5.36), and integrate term by term].

(3) In practice, Laurent series are seldom obtained by evaluating the integrals in Eqs. (5.35) and (5.36). The use of *ad hoc* methods, as, for example, in Eq. (5.33), is justified by the uniqueness of the result.
F. Analytic Continuation

We conclude the power series section with a discussion of analytic continuation.

In real analysis, a differentiable function defined on a line segment $(a, b)$ can be extended to an adjacent line segment $(b, c)$ in a virtually arbitrary manner. Not so in complex analysis. Analytic extensions are essentially unique. ("Essentially" is explained below.)

**Uniqueness Theorem** Let $f_1(z)$ and $f_2(z)$ both be analytic in the same domain $D$. Further, let $f_1(z) = f_2(z)$ at all points of an arc $\gamma$ in $D$. Then $f_1(z) = f_2(z)$ everywhere in $D$.

**Proof** The proof is a constructive use of power series. Let $z_0$ be on $\gamma$. Derivatives at $z_0$ can be computed using only points on $\gamma$, so that $f_1^{(k)}(z_0) = f_2^{(k)}(z_0)$, for $k = 0, 1, 2, \ldots$. Thus the Taylor series at $z_0$ for $f_1(z)$ and $f_2(z)$ are identical, and $f_1(z) = f_2(z)$ in the largest circle about $z_0$ that fits in $D$. Consider the point $z_1$ in $D$, not inside this circle. Let $z_0$ be connected to $z_1$ by a path $\gamma_{01}$ of finite length $L$ lying entirely in $D$. Let $d$ be the shortest distance from $\gamma_{01}$ to the boundary of $D$. Consider the sequence of open circles of radius $d$, centered at points spaced $d/2$ apart measured along $\gamma_{01}$ from $z_0$. All these circles are contained in $D$. The center of the $n$th circle is contained in the $(n - 1)$st circle on the segment of $\gamma_{01}$ falling in the $(n - 1)$st circle. The point $z_1$ is contained in at least the last circle of this finite sequence (the number of circles is approximately $2L/d$). By induction, $f_1(z) = f_2(z)$ in each circle. Consequently $f_1(z_1) = f_2(z_1)$.

In the next section certain real functions defined on the real axis will be extended to analytic functions defined in domains containing the real axis. By the uniqueness theorem, if such an extension exists, it is unique.

Suppose that $f_1(z)$ is analytic in a domain $D_1$, that $f_2(z)$ is analytic in a domain $D_2$, that the intersection of $D_1$ with $D_2$ is a (nonempty) domain $D$, and that $f_1(z) = f_2(z)$ everywhere in $D$. Then $f_2(z)$ is said to be an analytic continuation of $f_1(z)$ from $D_1$ into $D_2$, and vice versa. (See Fig. 5a.) The construction used in proving the uniqueness theorem clearly can be used to continue analytically a function from one domain into another, or from a smaller domain into a larger domain, to the extent permitted by the function itself.

Let $f_1(z)$ be analytic in a domain $D_1$, and let the domains $D_2$ and $D_3$ intersect $D_1$ and each other as illustrated in Fig. 5b. Let $z_0$ be in both
3. Complex Variable Theory

Fig. 5. Intersecting domains for analytic continuation.

$D_2$ and $D_3$ but not in $D_1$. Let there be analytic continuations $f_2(z)$ and $f_3(z)$ of $f_1(z)$ from $D_1$ into $D_2$ and $D_3$, respectively. Both $f_2(z)$ and $f_3(z)$ are uniquely determined, but it is not necessarily true that $f_2(z_0) = f_3(z_0)$. Stated alternatively, $f_2(z)$ is not necessarily a direct analytic continuation of $f_3(z)$ from $D_2$ into $D_3$, even though both are direct analytic continuations of $f_1(z)$. Specific examples in the next section illustrate this situation.

Finally, we contrast a property of power series with a property of Cauchy’s integral formula: The former permits values of $f(z)$ to be determined in an outer region from values in an inner region, whereas the latter permits values of $f(z)$ to be determined in an inner region from values in an outer region.

VI. Elementary Functions

We have already encountered the simplest elementary functions: polynomials, rational functions, and $n$th roots. In this section, properties of these and other elementary functions, including the exponential and logarithm, are developed in some detail.

A. SINGULARITIES. ZEROS. THE POINT AT INFINITY

Some terminology facilitating the description of functions is given first.

A function analytic in the entire $z$ plane is called an entire function. Examples: polynomials; $\sum_{k=0}^{\infty} a_k z^k/k!$.

A point $z_0$ at which $f(z)$ is not analytic is called a singularity of $f$. Example: $(z - z_0)^{-1}$.

A point $z_0$ is called an isolated singularity of $f(z)$ if $f(z)$ is analytic everywhere in some neighborhood of $z_0$, except at the point $z_0$ itself. Example: same as preceding example.

Let $z_0$ be an isolated singularity of $f(z)$, and let $f(z)$ have the Laurent series

$$f(z) = \sum_{k=0}^{\infty} c_k (z - z_0)^k + \sum_{k=1}^{\infty} c_{-k} (z - z_0)^{-k}, \quad 0 < |z - z_0| < \varepsilon.$$ (6.1)
1. If \( c_{-k} = 0 \) for all \( k \geq 1 \), then \( f \) is said to have a removable singularity at \( z_0 \) [removed by defining \( f(z_0) \) to be \( c_0 \)]. A removable singularity is an unnatural, correctable singularity.

2. If \( c_{-n} \neq 0, c_{-m} = 0 \) for all \( m > n \), then \( f \) is said to have a pole of order \( n \) at \( z_0 \).

3. If \( c_{-n} \neq 0 \) for infinitely many \( n > 0 \), then \( f \) is said to have an essential singularity at \( z_0 \). Example: \( \sum_{k=0}^{\infty} (z - z_0)^{-k}/k! \).

4. The \( \sum_{k=1}^{\infty} c_{-k}(z - z_0)^{-k} \) in Eq. (6.1) where \( z_0 \) is an isolated singularity of \( f(z) \), is called the principal part of \( f \) at \( z_0 \).

**Note:** If \( f \) has a pole of order \( n \) at \( z_0 \), then
\[
g(z) = \begin{cases} (z - z_0)^n f(z), & z \neq z_0 \\ c_{-n}, & z = z_0 \end{cases} \quad (6.2)
\]

\[
g(z) = \sum_{k=0}^{\infty} c_{k-n}(z - z_0)^k \quad (6.3)
\]

is analytic and nonvanishing at \( z_0 \).

If the first \( n \) terms of the Taylor series for \( f(z) \) at \( z_0 \) vanish,
\[
f(z) = \sum_{k=n}^{\infty} c_k(z - z_0)^k, \quad n \geq 1, \quad c_n \neq 0, \quad (6.5)
\]
then \( f \) is said to have a zero of order \( n \) at \( z_0 \).

**Simple pole** and **simple zero** are synonymous with first-order pole and first-order zero.

**Note:** \( f(z) \) has a pole of order \( n \) at \( z_0 \) if and only if \( 1/f(z) \) has a zero of order \( n \) at \( z_0 \).

If \( f(1/\zeta) \) has a pole or zero at \( \zeta = 0 \), we say that \( f(z) \) has a pole or zero at \( z = \infty \).

By the behavior of \( f(z) \) at the point at infinity, we mean the behavior of \( f(1/\zeta) \) at the point \( \zeta = 0 \).

By **extended complex plane**, we mean the complex plane plus the point at infinity.

**B. Algebraic Functions**

Let \( w = w(z) \) and let \( p(w, z) \) be a polynomial in \( w \) and \( z \) for which \( p(w(z), z) = 0 \). Then \( w(z) \) is said to be an algebraic function of \( z \). Polynomials, rational functions, and \( n \)th roots are examples of algebraic functions that we discuss below. For a discussion of more general algebraic functions, the reader is referred to other texts (e.g., Ahlfors, 1966).
1. Polynomials and Rational Functions

Polynomials are entire functions. We add here one more fact: If \( p_n(z) \) is a polynomial of degree \( n \),

\[
p_n(z) = \sum_{k=0}^{n} c_k z^k, \quad c_n \neq 0, \tag{6.6}
\]

then by the fundamental theorem of algebra and the division algorithm [in this case, \( p_n(z) = (z - a)p_{n-1}(z) + b \) where \( p_{n-1} \) is a polynomial of degree \( n - 1 \), and \( b \) is a constant], \( p_n(z) \) has precisely \( n \) (not necessarily distinct) roots, \( z_1, z_2, \ldots, z_n \), and the unique factorization

\[
p_n(z) = c_n(z - z_1)(z - z_2) \cdots (z - z_n). \tag{6.7}
\]

The additional features of rational functions are essentially those of the reciprocal of a polynomial. From Eq. (6.7), the singularities of the reciprocal of a polynomial are poles at the zeros of the polynomial. A useful fact is that the reciprocal of a polynomial can be resolved into partial fractions. Let \( z_1, z_2, \ldots, z_m \) all be distinct. Then

\[
(z - z_1)^{-n_1}(z - z_2)^{-n_2} \cdots (z - z_m)^{-n_m} = \sum_{j=1}^{m} \sum_{k=0}^{n_{j}-1} c_{jk}(z - z_j)^{-n_{j}+k} \tag{6.8}
\]

where the constants \( c_{jk} \) are given explicitly by

\[
c_{jk} = (1/k!)(d/dz_1)^k \prod_{j \neq l}^{m} (z_1 - z_j)^{-n_j}. \tag{6.9}
\]

That Eq. (6.8) exists in principle follows inductively from

\[
(z - z_1)^{-1}(z - z_2)^{-1} = [(z - z_1)^{-1} - (z - z_2)^{-1}](z_1 - z_2)^{-1}. \tag{6.10}
\]

The explicit formula for \( c_{jk} \) is derived in Section VII.D.

In many texts, the special rational function

\[
w(z) = c[(z - z_1)/(z - z_2)], \quad z_1 \neq z_2, \tag{6.11}
\]

is discussed in detail. Various known as a linear transformation, bilinear transformation, linear fractional transformation, and Möbius transformation, its importance is that it maps the extended \( z \) plane one to one onto the extended \( w \) plane, and that it maps circles into circles (with straight lines regarded as limiting cases of circles).
2. *nth Roots. Multiple-Valued Functions*

The singularities of the *nth* roots of *z*, called *branch points* and *branch cuts*, are not isolated; *nth* roots lead naturally to the concepts *multiple-valued function* and *Riemann surface*.

We proceed heuristically. Equations (2.52)–(2.54) define *n* *nth* roots of *z*, which we denote by *w*<sub>*</sub>*k*(*z*),

\[
w_k(z) = |z|^{1/n} \left( \cos \frac{\text{arg } z}{n} + i \sin \frac{\text{arg } z}{n} \right),
\]

\[(2k - 1)\pi < \text{arg } z \leq (2k + 1)\pi, \quad k = 0, 1, 2, \ldots, n - 1,
\]

\[= \omega_n^kw_0(z). \quad (6.12)
\]

Each *w*<sub>k</sub>(*z*) satisfies the Cauchy–Riemann equations in \((2k - 1)\pi < \text{arg } z < (2k + 1)\pi\), and has the derivative

\[
\frac{dw_k(z)}{dz} = \frac{1}{n} \frac{1}{z} w_k(z), \quad \text{i.e.,} \quad \frac{1}{n} z^{(1/n) - 1}. \quad (6.14)
\]

Each *n*th root is analytic in the domain consisting of the entire complex plane with the origin and negative real axis removed. Figure 6 illustrates the domain and range of each *w*<sub>k</sub> for *n* = 6.

We examine in detail the nature of the singularities of *w*<sub>k</sub>(*z*).

a. \(dw_k/dz\) does not exist at \(z = 0\). There is a singularity at the origin.
b. The origin is not an isolated singularity. For \(x > 0, \varepsilon > 0\), then

\[
\lim_{\varepsilon \to 0} [\text{Arg}(−x + i\varepsilon) − \text{Arg}(−x − i\varepsilon)] = 2\pi,
\]
and
\[
\lim_{\varepsilon \to 0} [w_0(-x + i\varepsilon) - w_0(-x - i\varepsilon)] = (1 - \omega_n^{-1})w_0(-x) \neq 0.
\]

Thus the domain of analyticity can contain no circle or other simple closed curve that encloses the origin.

c. Any simple curve running from the origin to infinity defines a domain in which \( \arg z \) can be both single valued and continuous and in which analytic \( n \)th roots can be defined (see Fig. 6).

d. The "domain" is as much a part of the definition of a function as the "rule." Thus there can be as many sets of analytic \( n \)th root functions as there are simple curves drawn from the origin to infinity. Nevertheless, the totality of values taken on remains the same.

e. The simple curve that runs from 0 to \( \infty \) is called a branch cut. The two endpoints, 0 and \( \infty \), are called branch points. The functions \( w_k(z) \) are called branches of \( z^{1/n} \). For definiteness,
\[
|z|^{1/n} \left( \cos \frac{\text{Arg} z}{n} + i \sin \frac{\text{Arg} z}{n} \right), \quad -\pi < \text{Arg} z \leq \pi,
\]
with domain of analyticity \( |\text{Arg} z| < \pi \), is called the principal value or principal branch of \( z^{1/n} \).

The branches of \( z^{1/n} \) are even more intimately connected than by the simple relation, Eq. (6.13), or by the fact that they all satisfy \( w^n = z \). Let \( D_1 \) denote the second quadrant and \( D_2 \) the left half-plane. Let \( \pi/2 < \arg z < \pi \) in \( D_1 \), and \( \pi/2 < \arg z < 3\pi/2 \) in \( D_2 \). In the sense of Section V.F, \( w_1(z) \) is the analytic continuation of \( w_0(z) \) across the negative real axis from the second quadrant into the third quadrant. Indeed, examination of Eq. (6.12) and Fig. 6 shows that each \( w_k(z) \) is the analytic continuation of \( w_{k-1}(z) \) from the second quadrant across the branch cut to the third, with \( w_{n-1} \) leading to \( w_0 \).

This situation is unified by the concept of multiple-valued function. One says that \( z^{1/n} \) is a multiple-valued function. When a suitable branch cut is specified, the resulting \( w_k(z) \) are said to be the single-valued branches of the multiple-valued function \( z^{1/n} \). It is to be emphasized that "multiple-valued function" means not a function in the sense of Section III.A, but a "collection of functions related by analytic continuation."

More precisely, we say that \( f_1(z) \) and \( f_2(z) \), both analytic in the same simply connected domain \( D \), are branches of the same multiple-valued analytic function \( f(z) \) if there is a finite sequence of functions, \( g_1(z), g_2(z), \ldots, g_n(z) \), analytic in the simply connected domains \( D_1, D_2, \ldots, D_n \), such
that $D \cap D_1, D_1 \cap D_2, \ldots, D_n \cap D$ are all nonempty simply connected domains, and such that $g_1$ is the analytic continuation of $f_1$, $g_2$ is the analytic continuation of $g_1$, \ldots, $g_n$ is the analytic continuation of $g_{n-1}$, and $f_2$ is the analytic continuation of $g_n$.

3. Riemann Surface

Further insight into multiple-valued functions is provided by the notion Riemann surface, which we discuss for $z^{1/n}$.

Imagine taking $n$ sheets of paper, infinite in extent, and slicing each from 0 to $-\infty$ on the real axis. Number the sheets from 0 to $n-1$. Join the second quadrant of each sheet to the third quadrant of the next sheet at the cut. Imagine also connecting sheet $n-1$ back to sheet 0. Assign $w_k(z)$ to sheet $k$. Follow a path that winds around the origin $n$ times, from sheet 0 onto sheet 1, from sheet 1 onto sheet 2, \ldots, from sheet $n-2$ to sheet $n-1$, from sheet $n-1$ to sheet 0, back to the starting point. The value of $z^{1/n}$ varies continuously along this path. The hypothetical construction is called the Riemann surface for $z^{1/n}$. The individual cut planes are called Riemann sheets. One crosses from one Riemann sheet to the next when crossing a branch cut. We may regard $z^{1/n}$ as a single-valued analytic function of $z$, where $z$ varies continuously on the Riemann surface for $z^{1/n}$.

C. THE EXPONENTIAL AND RELATED FUNCTIONS

Nonalgebraic functions are called transcendental. The exponential, logarithmic, trigonometric, and hyperbolic functions are the elementary transcendental functions of real analysis. In complex analysis, these different functions all turn out to be aspects of a single analytic function, the exponential.

1. Definition and Properties of the Exponential Function

Four equations are basic to the exponential function, denoted by $\exp(z)$ or just $e^z$:

\begin{equation}
\exp(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!}
\end{equation}

\begin{equation}
(d/dz)e^z = e^z, \quad e^0 = 1
\end{equation}

\begin{equation}
\exp(x_1) \exp(x_2) = \exp(x_1 + x_2)
\end{equation}

\begin{equation}
e^{z+i\nu} = e^z(\cos \nu + i \sin \nu).
\end{equation}
Any one of Eqs. (6.16) to (6.19) can be chosen as fundamental. The other three then follow. (Here $e^x$ means the known real exponential function of a real variable $x$.) We adopt the power series (6.16) as the definition of $e^z$. Then the following comments pertain:

(a) The exponential function is an entire function of $z$.

(b) Since $\sum_{k=0}^{\infty} \frac{x^k}{k!}$ is the known power series for the real exponential, $e^z$ is the unique analytic extension of $e^x$.

(c) Differentiation of Eq. (6.16) term by term gives Eq. (6.17).

(d) Equation (6.18) follows from Eq. (6.17) and from

$$(d/dz)(e^{z^2 e^{a-x}}) = 0.$$ 

(e) Equation (6.19) follows from Eqs. (6.18) and (6.16) and from the known power series for the real functions $\cos y$ and $\sin y$.

(f) If $|z| = r$, and $\arg z = \theta$, then

$$z = |z| [\cos(\arg z) + i \sin(\arg z)] = |z| \exp(i \arg z) = re^{i\theta}. \quad (6.20)$$

(g) Modulus of $e^z$:

$$|e^z| = e^{\Re z}; \quad |e^{i\theta}| = 1, \quad \theta \text{ real.} \quad (6.21)$$

(h) $e^z$ is never zero or infinity ($z$ finite).

(i) $e^z$ is periodic with period $2\pi i$. The only period for $e^z$ is $2\pi i$:

$$\exp(z + 2\pi i) = e^z \quad (6.22)$$

$$e^{2\pi i} = 1 \quad (6.23)$$

$$e^{\pi i} = -1. \quad (6.24)$$

(j) Complex conjugate:

$$\overline{e^z} = e^{\overline{z}}. \quad (6.25)$$

(k) In general, if $f(z)$ is analytic and $f(x)$ is real, then $\overline{f(z)} = f(\bar{z})$. This is easy to see if $f(z)$ is analytic in a circle centered on $\Re z$ with radius greater than $\Im z$.

(l) $w = e^z$ maps lines of constant $x$ into circles $|w| = e^x$, and lines of constant $y$ into rays $\arg w = y$. The domain \{ $x < 0, |y| < \pi$ \} is mapped into \{ $|w| < 1$ \}, and \{ $x > 0, |y| < \pi$ \} is mapped into \{ $|w| > 1$ \}, as in Fig. 7.
2. The Trigonometric and Hyperbolic Functions

For complex $z$, the functions $\sin z$, $\cos z$, $\sinh z$, and $\cosh z$ are defined by

$$\sin z = (e^{iz} - e^{-iz})/2i$$  \hspace{1cm} (6.26)

$$\cos z = (e^{iz} + e^{-iz})/2$$  \hspace{1cm} (6.27)

$$\sinh z = (e^z - e^{-z})/2 = -i \sin iz$$  \hspace{1cm} (6.28)

$$\cosh z = (e^z + e^{-z})/2 = \cos iz.$$  \hspace{1cm} (6.29)

The trigonometric and hyperbolic sines and cosines are entire functions. They satisfy a number of simple relations that are immediate consequences of their definitions via exponentials:

$$\sin z = \sum_{k=0}^{\infty} \frac{(-1)^k z^{2k+1}}{(2k + 1)!}$$  \hspace{1cm} (6.30)

$$\cos z = \sum_{k=0}^{\infty} \frac{(-1)^k z^{2k}}{(2k)!}$$  \hspace{1cm} (6.31)

$$\sinh z = \sum_{k=0}^{\infty} \frac{z^{2k+1}}{(2k + 1)!}$$  \hspace{1cm} (6.32)

$$\cosh z = \sum_{k=0}^{\infty} \frac{z^{2k}}{(2k)!}.$$  \hspace{1cm} (6.33)

$$e^{iz} = \cos z + i \sin z, \quad z \text{ complex},$$  \hspace{1cm} (6.34)

$$(d/dz) \sin z = \cos z, \quad (d/dz) \sinh z = \cosh z$$  \hspace{1cm} (6.35)

$$(d/dz) \cos z = -\sin z, \quad (d/dz) \cosh z = \sinh z,$$  \hspace{1cm} (6.36)

$$\sin^2 z + \cos^2 z = 1 = \cosh^2 z - \sinh^2 z,$$  \hspace{1cm} (6.37)

$$\overline{\sin z} = \sin \bar{z}, \quad \overline{\cos z} = \cos \bar{z}$$  \hspace{1cm} (6.38)

$$\overline{\sinh z} = \sinh \bar{z}, \quad \overline{\cosh z} = \cosh \bar{z},$$  \hspace{1cm} (6.39)
3. Complex Variable Theory

\[ 2 | \sin z |^2 = \cosh 2y - \cos 2x \]  
\[ 2 | \sinh z |^2 = \cosh 2x - \cos 2y \]  
\[ 2 | \cos z |^2 = \cosh 2y + \cos 2x \]  
\[ 2 | \cosh z |^2 = \cosh 2x + \cos 2y, \]  
\[ \sin(z_1 + z_2) = \sin z_1 \cos z_2 + \cos z_1 \sin z_2 \]  
\[ \sinh(z_1 + z_2) = \sinh z_1 \cosh z_2 + \cosh z_1 \sinh z_2 \]  
\[ \cos(z_1 + z_2) = \cos z_1 \cos z_2 - \sin z_1 \sin z_2 \]  
\[ \cosh(z_1 + z_2) = \cosh z_1 \cosh z_2 + \sinh z_1 \sinh z_2, \]
\[ \sin(z + z_0) = \sin z \quad \text{(all } z \text{)} \iff z_0 = \pm 2\pi n, \quad n = 0, 1, 2, \ldots \]  
\[ \cos(z + z_0) = \cos z \quad \text{(all } z \text{)} \iff z_0 = \pm 2\pi n, \quad n = 0, 1, 2, \ldots. \]
\[ \sin z = 0 \iff z = \pm n, \quad n = 0, 1, 2, \ldots \]  
\[ \cos z = 0 \iff z = (\pm n + \frac{1}{2})\pi, \quad n = 0, 1, 2, \ldots, \]
\[ \sin z = \sin(\pi - z) = -\sin(\pi + z) = -\sin(-z) \]  
\[ \cos z = -\cos(\pi - z) = -\cos(\pi + z) = \cos(-z), \]  
\[ \sin(\frac{\pi}{2} - z) = \cos z, \quad \cos(\frac{\pi}{2} - z) = \sin z. \]

By Eqs. (6.30)–(6.33) and the known power series for the real functions, \( \sin z, \cos z, \sinh z, \) and \( \cosh z \) are the unique analytic extensions of the corresponding real functions. All the identities for the real functions carry over to the complex functions. Note also Eq. (6.34) for \( e^{iz}. \) Note especially the location of the zeros of \( \sin z \) and \( \cos z. \) The zeros are all simple zeros.

The derivations of most of Eqs. (6.30)–(6.54) are fairly simple. We single out only Eq. (6.50):

\[ \sin z = 0, \quad \Rightarrow e^{iz} - e^{-iz} = 0, \quad \Rightarrow e^{2iz} = 1, \quad \Rightarrow 2iz = \pm 2\pi n. \]

The other trigonometric and hyperbolic functions are defined in terms of \( \sin z, \cos z, \) \( \sinh z, \) and \( \cosh z, \) as in the real case.

\[ \tan z = \sin z / \cos z, \quad \tanh z = \sinh z / \cosh z, \]
\[ \cot z = 1 / \tan z, \quad \coth z = 1 / \tanh z, \]
\[ \sec z = 1 / \cos z, \quad \sech z = 1 / \cosh z, \]
\[ \csc z = 1 / \sin z, \quad \csch z = 1 / \sinh z. \]
The usual addition and differentiation formulas hold. For example,

\[(d/dz) \tan z = 1/\cos^2 z.\] (6.60)

Note that \(\tan z\) has period \(\pi\), simple poles at \((n + \frac{1}{2})\pi\) \((n = 0, \pm 1, \pm 2, \ldots)\), and simple zeros at \(n\pi\) \((n = 0, \pm 1, \pm 2, \ldots)\).

3. The Logarithm. Principal Branch, \(\text{Log} z\)

The logarithm is the inverse of the exponential; \(\text{log} z\) is a multiple-valued function. We first discuss the principal value or principal branch of \(\text{log} z\), whose domain of analyticity is the plane cut from 0 to \(-\infty\) along the negative real axis. The equations basic to the logarithm are

\[\text{Log } z = \int_{1}^{z} \frac{1}{\zeta} d\zeta, \quad z \neq 0 \neq \zeta, \quad -\pi < \text{Arg } z \leq \pi\]
\[-\pi < \text{Arg } \zeta \leq \pi \] (6.61)

\[\text{Log } z = \text{Log } |z| + i \text{ Arg } z, \quad -\pi < \text{Arg } z \leq \pi, \] (6.62)

\[(d/dz) \text{Log } z = z^{-1}, \quad \text{Log } 1 = 0, \quad z \neq 0, \quad |\text{Arg } z| < \pi \] (6.63)

\[e^{\text{Log } z} = z, \quad z \neq 0; \quad \text{Log } e^z = z, \quad -\pi < \text{Im } z \leq \pi, \] (6.64)

\[\text{Log } z = -\sum_{k=0}^{\infty} \frac{(1 - z)^{k+1}}{(k + 1)}, \quad |1 - z| < 1 \] (6.65)

\[\text{Log}(1 - z) = -\sum_{k=0}^{\infty} \frac{z^{k+1}}{(k + 1)}, \quad |z| < 1, \] (6.66)

\[\text{Log}(z_1 z_2) = \text{Log } z_1 + \text{Log } z_2, \quad -\pi < \text{Arg } z_1 + \text{Arg } z_2 \leq \pi \] (6.67)

\[= \text{Log } z_1 + \text{Log } z_2 - 2\pi i, \quad \pi < \text{Arg } z_1 + \text{Arg } z_2 \leq 2\pi \] (6.68)

\[= \text{Log } z_1 + \text{Log } z_2 + 2\pi i, \quad -2\pi < \text{Arg } z_1 + \text{Arg } z_2 \leq -\pi. \] (6.69)
3. Complex Variable Theory

One could start with any one of Eqs. (6.61) to (6.69) and obtain the others as consequences. We choose Eq. (6.61) to define \( \log z \). Then the following remarks are pertinent:

(a) Since \( z^{-1} \) is analytic in the cut plane \( |\arg z| < \pi \), and the cut plane is a simply connected domain, by Cauchy's theorem and the converse of the fundamental theorem (Section IV.D.3), \( \int_1^2 z^{-1} d\zeta \) defines a function, analytic in the cut plane, with derivative given by Eq. (6.63). The values of \( \log z \) on \( \arg z = \pi \) are obtained by continuity from above.

(b) \( \log |z| + i \arg z \) [Eq. (6.62)] corresponds to the path, \( 1 \leq \zeta \leq |z| \), then \( |\zeta| = |z| \). When \( z \) is real and positive, \( \log z \) is \( \log |z| \), the real, natural logarithm, so that \( \log z \) is the unique analytic extension of \( \log x \).

(c) \( \log(0) \) is not defined.

(d) The range of \( \log z \) is the infinite strip, \( -\pi < \im z \leq \pi \). (See Fig. 7.)

(e) Equations (6.64) may be regarded as the consequence either of the formula for the real logarithm or of \( (d/dz) \log e^z = 1 \) (use chain rule).

(f) The power series is the term by term integral of the geometric series.

(g) The addition formula follows from Eq. (6.64).

(h) Note that

\[
\log(1/z) = -\log z, \quad |\arg z| < \pi.
\]  

(6.70)

4. Logarithmic Branch Point. \( \log z \)

By remark (a) just given, any cut from 0 to \( \infty \) by a simple curve makes \( \int_1^2 z^{-1} d\zeta \) an analytic logarithm. The situation is analogous to the \( z^{1/n} \) discussed in Sections VI.B.2 and VI.B.3. \( \log z \) is one branch of a multiple-valued function, \( \log z \). The values of \( \log z \) are

\[
\log z = \log z + 2\pi in, \quad n = 0, \pm 1, \pm 2, \ldots
\]  

(6.71)

One uses \( \log z \) to denote both the multiple-valued function and any particular single-valued branch. The Riemann surface for \( \log z \) is analogous to that for \( z^{1/n} \), except that the sheets form an infinite spiral. There is no first sheet or last sheet. Equations (6.61)–(6.69) may be rewritten with \( \log z \), provided one qualifies each by the phrase, "for a suitable branch of \( \log z \)." Equations (6.74) and (6.75) below, however, hold for
all branches.

\[ \log z = \int_1^z \frac{1}{\xi} \, d\xi, \quad z \neq 0 \neq \xi \]  \hspace{1cm} (6.72)

\[ \log z = \log |z| + i \arg z, \] \hspace{1cm} (6.73)

\[ (d/dz) \log z = z^{-1} \] \hspace{1cm} (all branches) \hspace{1cm} (6.74)

\[ e^{\log z} = z \] \hspace{1cm} (all branches) \hspace{1cm} (6.75)

\[ \log e^z = z, \] \hspace{1cm} (6.76)

\[ \log z = 2\pi i n - \sum_{k=0}^{\infty} \frac{(1 - z)^{k+1}}{(k+1)}, \quad |1 - z| < 1 \] \hspace{1cm} (6.77)

\[ \log(1 - z) = 2\pi i n - \sum_{k=0}^{\infty} \frac{z^{k+1}}{(k+1)}, \quad |z| < 1 \] \hspace{1cm} (6.78)

\[ \log(z_1 z_2) = \log z_1 + \log z_2. \] \hspace{1cm} (6.79)

5. **Inverse Trigonometric and Hyperbolic Functions**

Since the trigonometric and hyperbolic functions are periodic, the inverse functions are multiple valued. Indeed, they can be explicitly expressed in terms of the logarithm. We discuss only \( \text{arc sin } z \), which is typical. In every equation immediately below containing \( \text{arc sin } z \) and \( \log \), the words “for a suitable branch” are understood.

\[ z = \sin w = (e^{iw} - e^{-iw})/2i \] \hspace{1cm} (6.80)

can be inverted to give

\[ w = \text{arc sin } z = -i \log(iz + (1 - z^2)^{1/2}). \] \hspace{1cm} (6.81)

The multiple valuedness arises from both the log and the \((1 - z^2)^{1/2}\). From the log, one set of branches is characterized by values differing by \(2\pi n\), whereas the second set reflects the identity \(\sin(\pi - w) = \sin w\), in that

\[ -i \log(iz + (1 - z^2)^{1/2}) - i \log(iz - (1 - z^2)^{1/2}) = -i \log(-1) \]

\[ = (2n + 1)i\pi. \] \hspace{1cm} (6.82)

One can easily compute

\[ (d/dz) \text{arc sin } z = (1 - z^2)^{-1/2}. \] \hspace{1cm} (6.83)

The other inverse functions behave similarly, with identities and differentiation formulas being the same as their real counterparts.
6. The Functions $z^\alpha$ and $\alpha^z$

Define $z^\alpha$ and $\alpha^z$ by

$$z^\alpha = \exp(\alpha \log z) \quad (6.84)$$
$$\alpha^z = \exp(z \log \alpha). \quad (6.85)$$

Some remarks follow:

(a) When $\alpha$ is not an integer, $z^\alpha$ is multiple valued, with a branch cut from 0 to $\infty$ required to specify single-valued branches. On any branch

$$(d/dz)z^\alpha = \alpha z^{\alpha-1}.$$

(6.86)

When $\alpha$ is a negative integer, there is a pole at $z = 0$.

(b) The values of $z^\alpha$ on two contiguous branches differ by a factor $e^{2\pi i n\alpha}$. The number of branches is infinite, unless $\alpha$ is rational.

(c) When $\alpha$ is rational, the definition above agrees with Eq. (2.55) $[z^{m/n} = (z^m)^{1/n}]$.

(d) Given $\alpha$, there are an infinite number of such functions $\alpha^z$, differing by factors $e^{2\pi in\alpha}$. When a particular value of $\log \alpha$ is fixed, $\alpha^z$ is an entire function, and

$$(d/dz)\alpha^z = \alpha^z \log \alpha. \quad (6.87)$$

(e) The exponential $e^z$ agrees with Eq. (6.85) in the sense $\alpha = e$, provided that one uses $\log e = 1$ in Eq. (6.85), and not $1 + 2\pi i n \quad (n \neq 0)$.

VII. Evaluation of Real Definite Integrals

Some classes of real definite integrals can be recast as integrals around simple closed curves in the complex plane, $\oint_\gamma f(z) \, dz$. If $f(z)$ is analytic on and within $\gamma$, the integral vanishes. If $f(z)$ has a single isolated singularity inside $\gamma$ at $z_0$, then the integral is $2\pi i$ times the coefficient of $(z - z_0)^{-1}$ in the Laurent series for $f(z)$ about $z_0$. This seemingly trivial observation is the basis for a powerful technique for evaluating integrals and is stated more precisely below.

A. Residue Theorem

Let $f(z)$ have an isolated singularity at $z_0$. Then the residue of $f(z)$ at $z_0$ is defined as the coefficient of $(z - z_0)^{-1}$ in the Laurent series for $f(z)$ about $z_0$. 

Residue Theorem Let \( f(z) \) be analytic on and within a simple closed curve \( \gamma \), except at a finite number of points \( z_1, z_2, \ldots, z_n \), which do not lie on \( \gamma \). Then

\[
\oint_{\gamma} f(z) \, dz = 2\pi i \sum_{k=1}^{n} \{ \text{residue of } f(z) \text{ at } z_k \}.
\]

Equation (7.1) is an immediate consequence of Cauchy's theorem [Eq. (4.63)] and Eq. (5.36).

B. Five Classes of Integrals Amenable to the Residue Theorem

As examples of applications of the residue theorem, we evaluate integrals of five different classes. In what follows, \( p_m(z) \) and \( q_n(z) \) denote polynomials of degrees \( m \) and \( n \), \( r(\cos \theta, \sin \theta) \) denotes a rational function of \( \cos \theta \) and \( \sin \theta \) with no poles on \( 0 \leq \theta \leq 2\pi \), and \( \alpha \) and \( k \) are real numbers.

First the integrals, and the results:

\[
\int_{-\infty}^{\infty} \frac{}{q_n(x)} \, dx = 2\pi i \times \sum \{ \text{residues of } \frac{p_m}{q_n} \text{ in upper half plane} \},
\]

\[
\begin{align*}
q_n(x) & \neq 0, \quad -\infty < x < \infty; \quad n \geq m + 2, \\
\end{align*}
\]

\[
\int_{-\infty}^{\infty} e^{ikx} \frac{p_m(x)}{q_n(x)} \, dx = 2\pi i \times \sum \{ \text{residues of } e^{ikx} \frac{p_m}{q_n} \text{ in upper half plane} \},
\]

\[
\begin{align*}
q_n(x) & \neq 0, \quad -\infty < x < \infty; \quad n \geq m + 1; \quad k > 0, \\
\end{align*}
\]

\[
\int_{-\infty}^{\infty} \frac{x^\alpha p_m(x)}{q_n(x)} \, dx = 2\pi i \times \sum \{ \text{residues of } x^\alpha \frac{p_m}{q_n} \text{ in lower half plane} \},
\]

\[
\begin{align*}
q_n(x) & \neq 0, \quad -\infty < x < \infty; \quad n \geq m + 1; \quad k < 0, \\
\end{align*}
\]

\[
\int_{0}^{\infty} \frac{x^\alpha p_m(x)}{q_n(x)} \, dx = \frac{2\pi i}{1 - e^{\alpha \pi i}} \times \sum \{ \text{residues of } x^\alpha \frac{p_m}{q_n} \text{ in cut plane} \},
\]

\[
\begin{align*}
q_n(x) & \neq 0, \quad 0 \leq x < \infty; \quad -1 < \alpha < 1; \quad \alpha \neq 0; \\
n & > m + \alpha + 1; \quad 0 < \arg z < 2\pi,
\end{align*}
\]

(7.5)
\[
\int_0^\infty \frac{p_m(x)}{q_n(x)} \, dx = -\sum \{\text{residues of } \log z \frac{p_m}{q_n} \text{ in cut plane}\},
\]
\[q_n(x) \neq 0, \quad 0 \leq x < \infty; \quad n \geq m + 2; \quad 0 < \arg z < 2\pi, \quad (7.6)\]
\[
\int_0^{2\pi} r(\cos \theta, \sin \theta) \, d\theta = 2\pi \sum \{\text{residues of } \left[ z^{-1} r \left( \frac{z + z^{-1}}{2}, \frac{z - z^{-1}}{2i} \right) \right] \text{ inside } |z| = 1\}.
\]
\[(7.7)\]

**The Derivations** Equation (7.7) is obtained by a transformation to an integral around the unit circle. Substitute \(z = e^{i\theta}, \cos \theta = (z + z^{-1})/2, \sin \theta = (z - z^{-1})/2i, \text{ and } d\theta = -i z^{-1} \, dx\). Then
\[
\int_0^{2\pi} r(\cos \theta, \sin \theta) \, d\theta = -i \oint_{|z|=1} z^{-1} r \left( \frac{z + z^{-1}}{2}, \frac{z - z^{-1}}{2i} \right) \, dz, \quad (7.8)
\]
and Eq. (7.7) follows by the residue theorem.

Equation (7.2) is *in essence* derived by shortening the integration path to \([-R, R]\) and then by closing the integration path by a large semicircle. Since \(p_m/q_n\) vanishes like \(R^{-(n-m)} \leq R^{-2}\) for large \(|z| = R\), the integral around the semicircle vanishes at least as fast as \(R^{-1}\):
\[
\lim_{R \to \infty} \int_0^\pi \frac{p_m(Re^{i\theta})}{q_n(Re^{i\theta})} iRe^{i\theta} \, d\theta = 0, \quad n \geq m + 2.
\]
\[(7.9)\]
(The semicircle \(|z| = R, \quad 0 \leq \arg z \leq \pi\), has the parametric representation \(z = Re^{i\theta}, \quad 0 \leq \theta \leq \pi\).) Then
\[
\int_{-\infty}^\infty \frac{p_m(x)}{q_n(x)} \, dx = \lim_{R \to \infty} \int_{-R}^R \frac{p_m(x)}{q_n(x)} \, dx \quad (7.10)
\]
\[
= \lim_{R \to \infty} \left\{ \int_{-R}^R \frac{p_m(x)}{q_n(x)} \, dx + \int_0^\pi \frac{p_m(Re^{i\theta})}{q_n(Re^{i\theta})} iRe^{i\theta} \, d\theta \right\} \quad (7.11)
\]
\[
= \lim_{R \to \infty} \int_{\gamma_R} \frac{p_m(z)}{q_n(z)} \, dz. \quad (7.12)
\]
In Eq. (7.12), \(\gamma_R\) denotes the path from \(-R\) to \(R\) along the real axis, then from \(R\) to \(-R\) along the semicircle \(z = Re^{i\theta}, \quad 0 \leq \theta \leq \pi\). Figure 8a shows \(\gamma_R\). Equation (7.2) follows by the residue theorem.
A picturesque description of the procedure just given is that the contour is closed at infinity by a semicircle in the upper half-plane, where the integrand vanishes sufficiently fast, and then the integral is evaluated by the residue theorem.

For Eq. (7.3), note that $|e^{ikz}| = e^{-ky}$. When $k > 0$, $e^{ikz}$ is bounded in the upper half-plane, and when $k < 0$, in the lower half-plane. When $n \geq m + 2$ and $k > 0$, the contour can be closed at infinity in the upper half-plane, as for Eq. (7.2), and Eq. (7.3) results. When $k < 0$, the same argument is valid for the lower half-plane, and Eq. (7.4) results. The minus sign results from the clockwise sense of the closed contour.

That Eqs. (7.3) and (7.4) hold when $n = m + 1$ is known as Jordan's lemma. The exponential factor helps make the integral over the semicircle vanish as $R \to \infty$. Care is required, however, because $|e^{ikz}| = 1$ when $z$ is on the real axis. We use the estimates

$$\sin \theta \geq 2\theta/\pi, \quad 0 \leq \theta \leq \frac{1}{2}\pi \quad (7.13)$$

$$\sin \theta \geq 2 - 2\theta/\pi, \quad \frac{1}{2}\pi \leq \theta \leq \pi, \quad (7.14)$$

and that $zp_m/q_{m+1}$ is bounded as $z \to \infty$,

$$\left| \frac{zp_m(z)}{q_{m+1}(z)} \right| \leq M \quad \text{as} \quad |z| \to \infty. \quad (7.15)$$
3. Complex Variable Theory

Then Jordan's lemma is clinched by (when \( k > 0 \))

\[
\left| \int_{|z| = R, \Im z \geq 0} e^{ikz} \frac{P_m(z)}{q_n(z)} \, dz \right| \leq M \int_{|z| = R, \Im z \geq 0} |e^{ikz}| \cdot |x^{-1}| \, dz \quad \text{as} \quad R \to \infty
\]  
\[ (7.16) \]

\[ = M \int_0^\pi \exp(-kR \sin \theta) \, d\theta \]  
\[ (7.17) \]

\[ \leq M \left( \int_0^{\pi/2} \exp(-kR \theta / \pi) \, d\theta + \int_{\pi/2}^{\pi} \exp(-kR(2 - 2\theta / \pi)) \, d\theta \right) \]  
\[ (7.18) \]

\[ = M \frac{\pi}{kR} \left( 1 - e^{-kR} \right). \]  
\[ (7.19) \]

A more elaborate manipulation of contours leads to Eqs. (7.5) and (7.6). In preview, the path from 0 to \( \infty \) is first replaced by the contour \( \gamma_{8(b)} \) of Fig. 8b, which is essentially \( \infty \) to 0, then around the origin so that \( z^a \) becomes \( e^{2\pi i a} z^a \), followed by 0 to \( \infty \). Then \( \gamma_{8(b)} \) is "closed at \( \infty \)" by a large circle (Fig. 8c). The residue theorem applies to the closed contour.

The first detail of the derivation is a slight extension of Cauchy's theorem when one endpoint is at \( \infty \). Let \( D_1 \) denote the domain \{ \( |z| > r \), \( \theta_1 < \arg z < \theta_2 \} \}; let \( f(z) \) be analytic in a simply connected domain \( D \) that contains \( D_1 \); and let \( |f(z)| \leq M |z|^{-1-\sigma} \) (\( \sigma > 0 \)) for all \( z \) in \( D_1 \). Let both \( \gamma_1 \) and \( \gamma_2 \) extend to \( \infty \) in \( D_1 \) from the same initial point \( a \) in \( D \), and let all points on \( \gamma_1 \) and \( \gamma_2 \) with \( |z| > r \) lie in \( D_1 \). Then

\[
\int_{\gamma_1} f(z) \, dz = \int_{\gamma_2} f(z) \, dz = \int_{a}^{\infty} f(z) \, dz. \]  
\[ (7.20) \]

The proof is obtained by cutting both \( \gamma_1 \) and \( \gamma_2 \) by the circle \( |z| = R > r \) at the points \( b_1 \) and \( b_2 \) (Fig. 8d). Then, using Cauchy's theorem,

\[
\int_{\gamma_1} f(z) \, dz = \lim_{b_1 \to \infty \text{ on } \gamma_1} \int_{a}^{b_1} f(z) \, dz = \lim_{R \to \infty} \int_{a}^{b_1} f(z) \, dz \]  
\[ (7.21) \]

\[ = \lim_{R \to \infty} \int_{a}^{b_2} f(z) \, dz + \lim_{R \to \infty} \int_{b_1}^{b_2} f(z) \, dz \]  
\[ (7.22) \]

\[ = \int_{\gamma_2} f(z) \, dz + \lim_{R \to \infty} \int_{b_1}^{b_2} f(z) \, dz. \]  
\[ (7.23) \]

But, \( |\int_{b_1}^{b_2} f(z) \, dz| \leq 2\pi M R^{-\sigma}. \)
The second detail is that for $\varepsilon > 0$,
\[
\int_{\varepsilon}^{\infty} x^\alpha \frac{p_m(x)}{q_n(x)} \, dx = \left( \int_{\varepsilon}^{\varepsilon e^{i\theta}} + \int_{\varepsilon e^{i\theta}}^{\infty} \right) x^\alpha \frac{p_m(x)}{q_n(x)} \, dx \\
= \left( \int_{\varepsilon}^{\varepsilon e^{-i\theta}} + \int_{\varepsilon e^{-i\theta}}^{\infty} \right) x^\alpha \frac{p_m(x)}{q_n(x)} \, dx. \tag{7.25}
\]
See Fig. 8e. If in Eq. (7.25), Arg $z + 2\pi$ is used for Arg $x$, one obtains
\[
\int_{\varepsilon}^{\infty} x^\alpha \frac{p_m(x)}{q_n(x)} \, dx = e^{-2\pi i \alpha} \left( \int_{\varepsilon e^{i\theta}}^{\varepsilon e^{i(2\pi - \theta)}} + \int_{\varepsilon e^{i(2\pi - \theta)}}^{\infty} \right) x^\alpha \frac{p_m(x)}{q_n(x)} \, dx. \tag{7.26}
\]

The third detail is to add $\int_{\varepsilon e^{i\theta}}^{\infty}$, $\int_{\varepsilon e^{i(2\pi - \theta)}}^{\infty}$, $\int_{\varepsilon}^{\varepsilon e^{i\theta} + \varepsilon e^{i(2\pi - \theta)}}$ (Fig. 8f) to obtain an integral over $\gamma_{8(\theta)}$ (Fig. 8g),
\[
(e^{2\pi i \alpha} - 1) \int_{\varepsilon}^{\infty} x^\alpha \frac{p_m(x)}{q_n(x)} \, dx + \int_{\varepsilon}^{e^{2\pi i \alpha} - 1} x^\alpha \frac{p_m(x)}{q_n(x)} \, dx \\
= \left( \int_{\varepsilon e^{i\theta}}^{\varepsilon e^{i(2\pi - \theta)}} + \int_{\varepsilon e^{i(2\pi - \theta)}}^{\infty} \right) x^\alpha \frac{p_m(x)}{q_n(x)} \, dx \tag{7.27}
\]
\[
= \int_{\gamma_{8(\theta)}} x^\alpha \frac{p_m(x)}{q_n(x)} \, dx. \tag{7.28}
\]

Note the location of the branch cut in Fig. 8g. Note also that by the extension of Cauchy's theorem applied separately to each endpoint, $\int_{\gamma_{8(\theta)}}$ is independent of $\varepsilon$ and $\theta$—indeed, $\int_{\gamma_{8(b)}} = \int_{\gamma_{8(b)}}$—provided that $q_n(z)$ has no zeros on or "inside" $\gamma_{8(\theta)}$ or $\gamma_{8(b)}$.

The fourth detail is to evaluate the left-hand side of Eq. (7.27) at a convenient value of $\varepsilon$: $\varepsilon = 0$. Since
\[
\left| \int_{\varepsilon}^{e^{2\pi i} \varepsilon} x^\alpha \frac{p_m(x)}{q_n(x)} \, dx \right| \leq 2\pi |e|^{\alpha+1} p_m(0)/q_n(0), \tag{7.29}
\]
and since $(\alpha + 1) > 0$,
\[
\lim_{\varepsilon \to 0} \left[ (e^{2\pi i \alpha} - 1) \int_{\varepsilon}^{\infty} \cdots \right. \left. dx + \int_{\varepsilon}^{e^{2\pi i} \varepsilon} \cdots dx \right] = (e^{2\pi i \alpha} - 1) \int_{0}^{\infty} \cdots dx.
\]

By assumption, $e^{2\pi i \alpha} \neq 1$, so that
\[
\int_{0}^{\infty} x^\alpha \frac{p_m(x)}{q_n(x)} \, dx = (e^{2\pi i \alpha} - 1)^{-1} \int_{\gamma_{8(b)}} x^\alpha \frac{p_m(x)}{q_n(x)} \, dx. \tag{7.30}
\]

The fifth detail is to "close the contour at $\infty$" (Fig. 8c). The justification is virtually the same as in the derivation of Eq. (7.2). The residue theorem then applies to the integral over the closed contour $\gamma_{8(\theta)}$.\]
The derivation of Eq. (7.6) is based on the relation
\[ \log(xe^{2\pi i}) = \log x + 2\pi i, \]  
(7.31)
rather than \((xe^{2\pi i})^x = e^{2\pi ix}x^x\). The analog of Eq. (7.26) is
\[ \left( \int_{e^{2\pi i}}^{e^{2(\pi - \theta)i}} + \int_{-e^{(2\pi - \theta)i}}^{-e^{2\pi i}} \right) \log z \frac{p_m(z)}{q_n(z)} \, dz 
= \int_{e^{2\pi i}}^{e^{2\pi i}} \log z \frac{p_m(z)}{q_n(z)} \, dz 
= \int_{\epsilon}^{\infty} \log x \frac{p_m(x)}{q_n(x)} \, dx + 2\pi i \int_{\epsilon}^{\infty} \frac{p_m(x)}{q_n(x)} \, dx. \]  
(7.32)
(7.33)

Otherwise the considerations are very similar to those leading to Eq. (7.5). As an exercise, the reader might obtain Eq. (7.6) from Eq. (7.5) by letting \( \alpha \to 0 \).

**Notation** Contours similar to \( \gamma_{(0)} \) appear so frequently that it is convenient to have a more suggestive notation. The symbols \( _{\gamma_{(0)}}^\infty \) and \( \int_{\gamma_{(0)}}^{(0+)} \) are equivalent. \( \int_{\gamma_{(0)}}^{(0+)} \) is read, “the integral about a path that starts at the ‘point’ \( +\infty \), circles the origin counterclockwise, and returns to \( +\infty \).”

### C. Examples

Some examples of Eqs. (7.2)–(7.6) are
\[ \int_{-\infty}^{\infty} \left( 1 + x^2 \right)^{-1} \, dx = \pi \]  
(7.34)
\[ \int_{-\infty}^{\infty} \frac{\cos kx}{1 + x^2} \, dx = \int_{-\infty}^{\infty} \frac{e^{ikx}}{1 + x^2} \, dx = \pi e^{-|k|}, \quad k \text{ real} \]  
(7.35)
\[ \int_{0}^{\infty} x^\alpha(1 + x^2)^{-1} \, dx = \pi \frac{\sin(\frac{1}{2}\pi \alpha)}{\sin(\pi \alpha)} \]  
(7.36)
\[ \int_{0}^{\infty} (x + 1)^{-2}(x + 2)^{-1} \, dx = 1 - \log 2 \]  
(7.37)
\[ \int_{0}^{2\pi} (a + \cos \theta)^{-1} \, d\theta = -2i \int_{|z| = 1} \frac{(z^2 + 2az + 1)^{-1}}{z^2 + 2az + 1} \, dz 
= 2\pi(a^2 - 1)^{-1/2}, \quad a > 1. \]  
(7.38)

Another example, \( \int_{-\infty}^{\infty} x^{-1} \sin x \, dx \), is slightly outside the framework of Eq. (7.3), although not the spirit, since \( x^{-1} e^{\pm ix} \) has a pole at \( x = 0 \).
Since \( z^{-1} \sin z \) is analytic at \( z = 0 \) (\( z^{-1} \sin z \equiv 1 \) at \( z = 0 \)), the contour can be deformed to avoid the origin, as in Fig. 8h. Then

\[
\int_{-\infty}^{\infty} x^{-1} \sin x \, dx = \int_{\gamma_{b(h)}} z^{-1} \sin z \, dz \\
= (2i)^{-1} \int_{\gamma_{b(h)}} z^{-1} e^{iz} \, dz - (2i)^{-1} \int_{\gamma_{b(h)}} z^{-1} e^{-iz} \, dz. \tag{7.39}
\]

The contour for the \( e^{iz} \) term can be closed at \( \infty \) in the upper half-plane, enclosing the pole at \( z = 0 \); the contour for the \( e^{-iz} \) can be closed at \( \infty \) in the lower half-plane, in which there is no singularity. The result is

\[
\int_{-\infty}^{\infty} x^{-1} \sin x \, dx = \pi. \tag{7.40}
\]

D. On Computing Residues

There is one standard situation whereby computing a residue is equivalent to taking a derivative. Let \( f(z) \) be analytic at \( z_0 \), so that

\[
f(z) = \sum_{k=0}^{\infty} f^{(k)}(z_0)(z - z_0)^k/k!
\]

converges in a neighborhood of \( z_0 \). The residue of \( (z - z_0)^{-n}f(z) \) at \( z_0 \) is \( f^{(n-1)}(z_0)/(n - 1)! \):

\[
\text{residue at } z_0 \text{ of } \frac{f(z)}{(z - z_0)^n} = \frac{1}{(n - 1)!} \left( \frac{d}{dz_0} \right)^{n-1} f(z_0). \tag{7.42}
\]

As an example, the coefficient \( c_{l_k} \) of Eq. (6.8) is \( (2\pi i)^{-1} \oint_{|z-z_l| = \alpha} dz \) of \( (z - z_l)^{n_l-k-1} \times \) the right side of Eq. (6.8). Equation (6.9) is just the residue at \( z_l \), by Eq. (7.42).

E. Cauchy Principal Value

Let \( f(z) \) be analytic at \( z = 0 \), and let \( f(0) \neq 0 \). In applications one sometimes encounters expressions like \( \int_a^b x^{-1} f(x) \, dx \), where \( a > 0 \) and \( b > 0 \), which are superficially meaningless. More properly, one encounters limits of related expression which are discussed here.

Since \( x^{-1}[f(x) - f(0)] \) is analytic at the origin [the value at zero being \( f'(0) \)], it is sufficient to consider integrals of \( x^{-1} \).
Consider
\[
\int_{-\varepsilon}^{\varepsilon} x^{-1} \, dx = \log (\varepsilon/a) \quad (7.43)
\]
\[
\int_{\varepsilon}^{b} x^{-1} \, dx = \log (b/\varepsilon). \quad (7.44)
\]

The symmetric limit, called the Cauchy principal value and indicated by \( \mathcal{P} \), exists and is given by
\[
\mathcal{P} \int_{-a}^{b} x^{-1} \, dx = \lim_{\varepsilon \to 0} \left( \int_{-a}^{-\varepsilon} + \int_{\varepsilon}^{b} \right) x^{-1} \, dx = \log (b/a) \quad (7.45)
\]
\[
\mathcal{P} \int_{-a}^{b} x^{-1} f(x) \, dx = \lim_{\varepsilon \to 0} \left( \int_{-a}^{-\varepsilon} + \int_{\varepsilon}^{b} \right) x^{-1} f(x) \, dx
\]
\[
= \int_{-a}^{b} x^{-1} [f(x) - f(0)] \, dx + f(0) \log (b/a). \quad (7.47)
\]

Another situation is represented by
\[
\lim_{\varepsilon \to 0} \int_{-a}^{b} (x + i\varepsilon)^{-1} f(x) \, dx, \quad \varepsilon > 0. \quad (7.48)
\]

For nonzero \( \varepsilon \), there is no singularity on the real axis. Indeed,
\[
\int_{-a}^{b} (x + i\varepsilon)^{-1} f(x) \, dx = \int_{-a}^{b} (x + i\varepsilon)^{-1} [f(x) - f(-i\varepsilon)] \, dx
\]
\[
+ \int_{-a}^{b} (x + i\varepsilon)^{-1} f(-i\varepsilon) \, dx, \quad (7.49)
\]
\[
= \int_{-a}^{b} (x + i\varepsilon)^{-1} [f(x) - f(-i\varepsilon)] \, dx
\]
\[
+ f(-i\varepsilon) \left( \log \frac{b + i\varepsilon}{a - i\varepsilon} - i\pi \right). \quad (7.50)
\]

Taking the limit \( \varepsilon \to 0 \), and using Eq. (7.47), one obtains
\[
\lim_{\varepsilon \to 0} \int_{-a}^{b} (x + i\varepsilon)^{-1} f(x) \, dx = \mathcal{P} \int_{-a}^{b} x^{-1} f(x) \, dx - i\pi f(0). \quad (7.51)
\]

Similarly,
\[
\lim_{\varepsilon \to 0} \int_{-a}^{b} (x - i\varepsilon)^{-1} f(x) \, dx = \mathcal{P} \int_{-a}^{b} x^{-1} f(x) \, dx + i\pi f(0). \quad (7.52)
\]

Equations (7.51) and (7.52) are sometimes referred to by the notation
\[(x \pm i\varepsilon)^{-1} = \mathcal{P} x^{-1} \mp i\pi \delta(x) \quad (7.53)\]
where \( \delta(x) \) denotes the Dirac delta function [Chapter 2 of this volume, or Lighthill (1958)].

An alternative but equivalent situation to \( \lim (x \pm ie)^{-1} \) is where the contour is indented to avoid the singularity. Thus (cf. Fig. 8h),

\[
\left( \int_{-\infty}^{-\epsilon} + \int_{\epsilon}^{\epsilon e^{2\pi i}} + \int_{\epsilon e^{2\pi i}}^{b} \right) x^{-1}f(x) \, dx = \lim_{\epsilon \to 0} \int_{-a}^{b} (x - i\epsilon)^{-1} f(x) \, dx. \tag{7.54}
\]

Note that in the sense of Eqs. (7.51)–(7.53)

\[
\mathcal{P} x^{-1} = \frac{1}{2i} [(x + i\epsilon)^{-1} + (x - i\epsilon)^{-1}], \tag{7.55}
\]

i.e., \( \mathcal{P} \int_{-a}^{b} x^{-1}f(x) \, dx \) is the average of avoiding \( x = 0 \) by indenting both above and below the origin. For example,

\[
\mathcal{P} \int_{-\infty}^{\infty} x^{-1} e^{ix} \, dx = \pi i. \tag{7.56}
\]

VIII. Higher Transcendental Functions

Functions that are not algebraic are called transcendental. Several transcendental functions appear frequently in applications: The gamma function, the hypergeometric function, and the confluent hypergeometric function are the most important. These functions can be defined by contour integrals, which provide an excellent vehicle for both developing the properties of these functions and for developing further techniques in contour integration.

A. The Gamma Function

1. Euler’s Integral

The gamma function is defined, for \( \text{Re} \, z > 0 \), by

\[
\Gamma(z) = \int_{0}^{\infty} t^{z-1} e^{-t} \, dt, \quad \text{Re} \, z > 0. \tag{8.1}
\]

\( \Gamma(z) \) is a natural generalization of the factorial

\[
\Gamma(n + 1) = n! \tag{8.2}
\]

and it coincides with \( \int_{-\infty}^{\infty} \tau^{2n} e^{-\tau^2} \, d\tau \), when \( z = n + \frac{1}{2} \) (substitute \( t = \tau^2 \)).
For example,
\[ \Gamma(\frac{1}{2}) = \pi^{1/2}. \]  
(8.3)

Since \( |t^z| = t^x \) \((t \geq 0)\), the condition for convergence of Euler's integral is \( x > 0 \).

2. Recurrence and Reflection Formulas

Integration by parts yields the recurrence formula. The reflection formula is derived in Section VIII.B.3.

\[ z\Gamma(z) = \Gamma(z + 1) \quad \text{(recurrence formula)} \]  
(8.4)

\[ \Gamma(z) = [z(z + 1) \cdots (z + n - 1)]^{-1}\Gamma(z + n) \quad \text{(iterated recurrence formula)} \]  
(8.5)

\[ \Gamma(z)\Gamma(1 - z) = \pi/\sin \pi z \quad \text{(reflection formula)}. \]  
(8.6)

3. Analyticity

Differentiating Euler's integral under the integral sign, one obtains heuristically
\[ (d/dz)\Gamma(z) = \int_0^\infty t^{z-1}e^{-t} \log t \, dt, \quad \text{Re } z > 0, \]  
(8.7)

which also converges in \( \text{Re } z > 0 \). More rigorously,
\[ \left| \frac{\Gamma(z + h) - \Gamma(z)}{h} \right| = \left| \int_0^\infty t^{z-1}e^{-t}\left( \frac{h}{h} - \log t \right) \, dt \right| \]  
(8.8)

\[ \leq \left| \int_0^1 t^{z-1}e^{-t}\left( \frac{h}{h} - \log t \right) \, dt \right| \]  

\[ + \left| \int_1^\infty t^{z-1}e^{-t}\left( \frac{h}{h} - \log t \right) \, dt \right| \]  
(8.9)

\[ \leq |h| \left| \int_0^1 t^{h-1} \left[ \int_0^t (1/\tau') \left( \int_0^{\tau'} \tau^{z-1}e^{-\tau} \, d\tau' \right) \, d\tau' \right] \, dt \right| \]  

\[ + |h| \left| \int_1^\infty t^{z-1}e^{-t} \, dt \right| \]  
(8.10)

\[ \leq |h| \left[ x^{-2}(\text{Re } h + x)^{-1} + e^{-1} \right]. \]  
(8.11)
For the first terms in Eqs. (8.10) and (8.11), one integrates by parts twice and uses

\[
\left| \int_0^1 t^{h-1} \left[ \int_0^t (1/\tau') \left( \int_0^\tau \tau^{x-1} e^{-\tau} \, d\tau \right) \, d\tau' \right] \, dt \right| \\
\leq \int_0^1 t^{Re h-1} \left[ \int_0^t (1/\tau') \left( \int_0^\tau \tau^{x-1} \, d\tau \right) \, d\tau' \right] \, dt = x^{-x} (Re h + x)^{-1}.
\tag{8.12}
\]

For the second term, one uses

\[
\left| \frac{t^h - 1}{h} - \log t \right| = \left| \sum_{k=2}^{\infty} \frac{h^{k-1} (\log t)^k}{k!} \right| \leq |h| \sum_{k=0}^{\infty} \frac{|\log t|^k}{k!} = |h| |t|, \quad |h| \leq 1, \quad t > 1
\tag{8.13}
\]

\[
\left| \int_1^\infty t^x e^{-t} \, dt \right| \leq \int_1^\infty t^x e^{-t} \, dt \leq \int_1^\infty e^{-t} \, dt = e^{-1}.
\tag{8.14}
\]

Euler's formula defines an analytic function of \( z \) in the half-plane \( Re z > 0 \).

The right side of Eq. (8.5) is analytic for \( Re z > -n, z \neq 0, -1, -2, \ldots, -n + 1 \), and it coincides with \( I'(z) \) when \( Re z > 0 \). It thus provides the analytic continuation of \( I'(z) \) to \( Re z \leq 0 \).

The only singularities of \( I'(z) \) in the finite plane are simple poles at \( z = 0, -1, -2, \ldots \).

4. Hankel's Formula

In the derivation of Eq. (7.5) of Section VII.B, the \( \int_0^\infty \) was replaced by \( \int_0^{(+)} \). The motivation was to be able to close the contour at \( \infty \). The same manipulation is invoked here for Euler's formula. The detailed justification is virtually the same and is not repeated, but the motivation is different: to obtain a formula, analytic for a wider range of \( z \). Since the integration contour no longer passes through the singularity of the integrand at \( z = 0 \), only the equivalent of Eq. (8.13) for complex \( t \) is needed to clinch the existence of \( I''(z) \). The resulting formulas are all referred to as Hankel’s formula. In the three versions given below, the first two reflect alternate ways of indicating \( \arg t \), while the third is a combination
of the first with the reflection formula, followed by $z \to 1 - z$.

$$I(z) = (e^{2\pi iz} - 1)^{-1} \int_{\infty}^{(0+)} t^{z-1} e^{-t} \, dt,$$

$$\arg t = 0 \text{ at "beginning"}, \quad z \neq \text{integer} \quad (8.15)$$

$$= -(2i \sin \pi z)^{-1} \int_{\infty}^{(0+)} (-t)^{z-1} e^{-t} \, dt,$$

$$\arg(-t) = -\pi i \text{ at "beginning"}, \quad z \neq \text{integer} \quad (8.16)$$

$$\frac{1}{I(z)} = -e^{\pi iz}(2\pi i)^{-1} \int_{\infty}^{(0+)} t^{-z} e^{-t} \, dt,$$

$$\arg t = 0 \text{ at "beginning"}, \quad \text{valid for all } z. \quad (8.17)$$

Hankel’s formula is equivalent to Euler’s integral when $\Re z > 0$, but it represents an analytic function in a much larger domain. It therefore represents the analytic continuation of $I(z)$ to the larger domain.

5. Zeros of $I(z)$

A direct consequence of the reflection formula (8.6) is that $I(z)$ has no zeros for finite $z$.

B. The Beta Function

The integral

$$B(p, q) = \int_{0}^{1} t^{p-1}(1 - t)^{q-1} \, dt, \quad \Re p > 0, \quad \Re q > 0, \quad (8.18)$$

defines the beta function when $\Re p > 0$ and $\Re q > 0$. The beta function is closely related to the gamma function, but more important, the extensions of the integral representation involve manipulations that are among the most intricate encountered in elementary complex analysis.
1. Relation to Gamma Function

The beta function is computed from the gamma function by

$$B(p, q) = \Gamma(p)\Gamma(q)/\Gamma(p + q), \quad (8.19)$$

an equation that also provides an analytic continuation with respect to both $p$ and $q$ to $\text{Re } p \leq 0$ and $\text{Re } q \leq 0$, and shows that

$$B(p, q) = B(q, p). \quad (8.20)$$

Equation (8.19) is derived as follows:

$$\Gamma(p)\Gamma(q) = \int_0^\infty s^{p-1}e^{-s} \, ds \int_0^\infty t^{q-1} e^{-t} \, dt \quad (8.21)$$

$$= 4 \int_0^\infty \int_0^\infty x^{2p-1}y^{2q-1} \exp[-(x^2 + y^2)] \, dx \, dy,$$

$$s = x^2, \quad t = y^2 \quad (8.22)$$

$$= \left(2 \int_0^\infty r^{2p+2q-1} \exp(-r^2) \, dr\right) \left(2 \int_0^{\pi/2} \cos^{2p-1} \theta \sin^{2q-1} \theta \, d\theta \right)$$

(polar coordinates) \quad (8.23)

$$= \int_0^\infty q^{p+q-1}e^{-q} \, dq \int_0^1 \tau^{p-1}(1 - \tau)^{q-1} \, d\tau,$$

$$q = r^2, \quad \tau = \cos^2 \theta \quad (8.24)$$

$$= \Gamma(p + q)B(p, q). \quad (8.25)$$

2. Other Integral Representations

As for $\Gamma(x)$, the multiple-valuedness of $\tau^{p-1}$ and $(1 - \tau)^{q-1}$ can be exploited to obtain integral representations that both avoid the branch points at $t = 0$ and $t = 1$, and are valid when $\text{Re } p \leq 0$ and $\text{Re } q \leq 0$. 

![Figure 9](image_url)

**Fig. 9.** Contours for Eqs. (8.26)–(8.32): (a) Eq. (8.26); (b) Eq. (8.27); (c) Eqs. (8.28) and (8.29); (d) Pochhammer's contour, for Eq. (8.30); (e) Eq. (8.32).
The contours are illustrated in Fig. 9. The integrals are

\[
B(p, q) = e^{-\pi ip} (2i \sin \pi p)^{-1} \int_{1}^{0+} t^{p-1} (1 - t)^{q-1} dt, \\
\quad \text{Re } q > 0, \quad p \neq \text{integer} \quad (8.26)
\]

\[
= -e^{-\pi iq} (2i \sin \pi q)^{-1} \int_{0}^{1+} t^{p-1} (1 - t)^{q-1} dt, \\
\quad \text{Re } p > 0, \quad q \neq \text{integer} \quad (8.27)
\]

\[
B(p, 1-p) = e^{\pi ip} (2i \sin \pi p)^{-1} \int_{\pi}^{(1+,0+)} t^{p-1} (1 - t)^{-p} dt, \\
\quad 0 < x < 1, \quad \arg x = \arg(1 - x) = 0; \quad p \neq \text{integer} \quad (8.28)
\]

\[
= (2i \sin \pi p)^{-1} \int_{1}^{r \to 1} t^{p-1} (t - 1)^{-p} dt, \\
\quad \arg t = 0 \quad \text{when } t = r; \quad p \neq \text{integer.} \quad (8.29)
\]

\[
B(p, q) = -\exp(-\pi i(p + q))(4 \sin \pi p \sin \pi q)^{-1} \\
\times \int_{\pi}^{(1+,0+,-1,-0-)} t^{p-1} (1 - t)^{q-1} dt, \\
\quad p \neq \text{integer}, \quad q \neq \text{integer} \quad (8.30)
\]

\[
B(p, q) = \int_{1}^{t=1/s} s^{-p-1}(s - 1)^{q-1} ds, \\
\quad \text{Re } q > 0, \quad \text{Re } p > 0 \quad (t = 1/s) \quad (8.31)
\]

\[
= e^{-\pi iq} (2i \sin \pi q)^{-1} \int_{\infty}^{0+} (1 + t)^{-p} q^{q-1} dt, \\
\quad \text{Re } p > 0, \quad q \neq \text{integer.} \quad (8.32)
\]

Apart from Eq. (8.31), the detailed derivation of each parallels the first part of the derivation of Eq. (7.5) in which \(\int_{0}^{\infty} \) is replaced by \((e^{2\pi i a} - 1)^{-1} \int_{0}^{(0+)}\), except that the upper limit in Eq. (8.18) is 1, not \(\infty\). By Cauchy's theorem, the contour for each case can be deformed to consist of straight line segments along the real axis and infinitesimal circles about \(z = 0\) and \(z = 1\), as indicated by the right-hand member of each pair in Fig. 9. When \(\text{Re } p > 0\) and \(\text{Re } q > 0\), the infinitesimal circles contribute infinitesimally, and the straight line paths are essentially the original integration path. The various integrals provide analytic continuations of \(B(p, q)\) to \(\text{Re } p \leq 0\), or \(\text{Re } q \leq 0\), or both, depending on which singularity of the integrand has been avoided.

The integrand of Eqs. (8.28) and (8.29) is essentially different from the others. The function \(t^{p-1}(1 - t)^{-p}\) changes by a factor \(e^{2\pi ip} \) or \(e^{-2\pi ip}\)
when \( \arg t \) or \( \arg(1 - t) \) is increased by \( 2\pi \). If both increase by \( 2\pi \), the function is unchanged. Thus, a satisfactory branch cut for \( t^{p-1}(1 - t)^{q-1} \) runs from \( t = 0 \) to \( t = 1 \), as shown in Fig. 9c.

The \( \int_{x}^{1,0+1,0-} dt \ (0 < x < 1) \) in Eq. (8.30) is read: the integral from \( t = x \) (on the real axis between 0 and 1), counterclockwise around \( t = 1 \), counterclockwise around \( t = 0 \), then clockwise around \( t = 1 \), clockwise around \( t = 0 \), and back to \( t = x \), as illustrated in Fig. 9d. This contour is called Pochhammer’s contour. So far we have only considered integrands that have been analytic, and ipso facto single valued, in the domain in which the integration path lay (except perhaps for the endpoints). If necessary, branch cuts specified single-valued branches of multiple-valued functions, and integration contours were kept in the corresponding domains of analyticity. In Eq. (8.30) the integration contour does not stay in a domain in which a single-valued branch of the integrand can be defined. Moreover, the integrand is taken to vary continuously on the contour (if branch cuts were drawn, then a change of \( \pm 2\pi \) in \( \arg t \) or \( \arg(1 - t) \) would be indicated when the path crossed a branch cut). Since the branch points at \( t = 0 \) and \( t = 1 \) are each circled twice, once counterclockwise and once clockwise, both \( \arg t \) and \( \arg(1 - t) \) return to the same value (0) at the endpoint \( t = x \), as at the initial point \( t = x \), so that \( t^{p-1}(1 - t)^{q-1} \) is continuous at all points of the contour.

To what extent can Pochhammer’s contour be deformed without changing the value of the integral? Cauchy’s theorem can be applied to any segment that lies in a domain in which \( t^{p-1}(1 - t)^{q-1} \) is single valued. Consequently any deformation in the domain \( \{z \mid z \neq 0, \ z \neq 1\} \), that is, any deformation that does not change how the contour loops around \( z = 0 \) and \( z = 1 \), does not change the value of the integral.

We follow the phase of the integrand; i.e.,

\[
t^{p-1}(1 - t)^{q-1}/[ |t|^{p-1} |1 - t|^{q-1}]
\]

on the right-hand contour of Fig. 9d. On the first horizontal segment, it is 1; on the second, \( e^{2\pi i q} \); on the third, \( \exp(2\pi i (p + q)) \); and on the fourth, \( e^{2\pi ip} \). When direction is taken into account,

\[
\int_{x}^{1,0+1,0-} t^{p-1}(1 - t)^{q-1} \ dt
\]

\[
= (1 - e^{2\pi i q} + e^{2\pi i (p + q)} - e^{2\pi i p}) \int_{0}^{1} t^{p-1}(1 - t)^{q-1} \ dt,
\]

\[
\text{Re } p > 0, \quad \text{Re } q > 0 \quad (8.33)
\]

\[
= -4 \ e^{\pi i (p + q)} \sin \pi p \sin \pi q \ B(p, q). \quad (8.34)
\]
The discussion above gives the essence of the justification of Eqs. (8.26)–(8.32). The fine details are left to the reader.

3. Gamma Function Reflection Formula

Equations (8.29) and (8.25), with a Laurent series expansion, give an immediate proof of Eq. (8.6):

\[
\Gamma(z)\Gamma(1 - z) = B(z, 1 - z)
\]

\[
= (2i \sin \pi z)^{-1} \int_{|t| = \tau > 1} t^{-1}(t - 1)^{-z} \, dt
\]

\[
= (2i \sin \pi z)^{-1} \int_{|t| = \tau > 1} t^{-1}(1 - t^{-1})^{-z} \, dt
\]

\[
= (2i \sin \pi z)^{-1} \times \int_{|t| = \tau > 1} \sum_{k=0}^{\infty} t^{-k-1} \frac{1 \cdot z(z + 1) \cdots (z + k - 1)}{k!} \, dt
\]

\[
= \frac{\pi}{\sin \pi z},
\]

since only the \( k = 0 \) term has a nonzero integral. We note in passing that the Taylor series for \((1 + z)^n\) is

\[
(1 + z)^n = \sum_{k=0}^{\infty} \frac{\Gamma(n + 1)}{\Gamma(n + 1 - k)k!} z^k, \quad |z| < 1,
\]

and that when \( n \) is a positive integer, the summation is finite (binomial theorem). The expansion holds when \( n \) is a negative integer via

\[
\frac{\Gamma(n + 1)}{\Gamma(n + 1 - k)} = \frac{\sin(n + 1 - k)\pi}{\sin(n + 1)\pi} \frac{\Gamma(k - n)}{\Gamma(-n)} = \frac{(-1)^k \Gamma(k - n)}{\Gamma(-n)}.
\]

C. The Hypergeometric Function

1. Definition

The hypergeometric function is defined by

\[
F(a, b ; c ; z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c - b)} \int_0^1 t^{b-1}(1 - t)^{c-b-1}(1 - zt)^{-a} \, dt,
\]

\[ \text{Re } c > \text{Re } b > 0, \quad z \text{ not real and } \geq 1. \]
Several important "special functions" are special cases of \( F(a, b; c; z) \), a notable example being the Legendre polynomials. The intention of this section is to show how the integral representation leads naturally to some of the important properties of \( F(a, b; c; z) \). More complete treatments of the hypergeometric function can be found in Abramowitz and Stegun (1964), Erdélyi (1953), and Whittaker and Watson (1927).

2. Analyticity

The locations of the branch points, branch cuts, and integration path for Eq. (8.42) are illustrated in Fig. 10. From Eq. (8.42) and from the discussion of the beta function, it is apparent that \( F(a, b; c; z) \) is an analytic function of each parameter \( a, b \) and \( c \), and it is an analytic function of \( z \) with a branch cut running from \( z = 1 \) to \( \infty \). For specific values of the parameters, the branch point at \( z = 1 \) may become a pole or even no singularity at all. For example, if \( a \) is a negative integer, \( F(a, b; c; z) \) is a polynomial of degree \(-a\) in \( z \).

![Fig. 10. Branch points, branch cuts, and integration path for \( F(a, b; c; z) \), Eq. (8.42).](image)

More general versions of Eq. (8.42) can be obtained with any of the contours of Fig. 9 [cf. Eqs. (8.26)–(8.32)]. With Pochhammer's contour,

\[
F(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c - b)} \frac{-e^{-\pi i\sigma}}{4 \sin \pi b \sin \pi(c - b)} \times \int_{\gamma(\sigma)}^{(1+0+1-0-)} \frac{t^{b-1}(1 - t)^{c-b-1}(1 - zt)^{-a}}{\Gamma(1 - b)\Gamma(1 + b - c)} e^{-\pi i\sigma} \, dt \tag{8.43}
\]

\[
= \frac{\Gamma(1 - b)\Gamma(1 + b - c)\Gamma(c)e^{-\pi i\sigma}}{4\pi^2} \times \int_{0}^{1} t^{b-1}(1 - t)^{c-b-1}(1 - zt)^{-a} \, dt, \tag{8.44}
\]

valid when \( b \) is not a positive integer, \( c - b \) is not a positive integer, and the contour does not intersect the branch cut from \( t = 1/z \) to \( \infty \).
3. Important Formulas

We discuss the derivation of the following formulas from Eqs. (8.42)-(8.44):

\[ F(a, b; c; z) = 1 + \frac{ab}{c} z + \frac{a(a + 1)b(b + 1)}{c(c + 1)} \frac{z^2}{2!} + \cdots \]

\[ = \sum_{k=0}^{\infty} \frac{(a)_k(b)_k}{(c)_k} \frac{z^k}{k!} \quad \text{(|z| < 1; Gauss's hypergeometric series)} \]  

\[ (a)_k = \Gamma(a + k)/\Gamma(a) \quad \text{(Pochhammer's symbol)} \]

\[ F(a, b; c; z) = F(b, a; c; z) \quad \text{(symmetry of } a \text{ and } b) \]

\[ F(a, c; z) = (1 - z)^{-a} \quad \text{(geometric series when } a = 1) \]

\[ (d/dz)F(a, b; c; z) = (ab/c)F(a + 1, b + 1; c + 1; z) \]

\[ F(a, b; c; 0) = 1 \]

\[ F(a, b; c; 1) = \frac{\Gamma(c)\Gamma(c - b - a)}{\Gamma(c - a)\Gamma(c - b)} \]

\[ \lim_{c \to -n} \frac{1}{\Gamma(c)} F(a, b; c; z) = \frac{(a)_{n+1}(b)_{n+1}}{(n + 1)!} \frac{z^{n+1}}{ \times F(a + n + 1, b + n + 1; n + 2; z)} \]

\[ F(-n, b; -n - l; z) = \sum_{k=0}^{n} \frac{n!}{(n - k)!} \frac{(n + l - k)!}{(n + l)!} \frac{b}_k \frac{z^k}{k!} \]

\[ (c - b - 1)F(a, b; c; z) + bF(a, b + 1; c; z) \]
\[ - (c - 1)F(a, b; c - 1; z) = 0 \]

\[ F(a, b; c; z) = (1 - z)^{-a}F \left( a, c - b; \frac{z}{z - 1} \right) \]

\[ = (1 - z)^{-b}F \left( c - a, b; \frac{z}{z - 1} \right) \]

\[ = (1 - z)^{a-b}F(c - a, c - b; c; z) \]

\[ = (-z)^{-a} \frac{\Gamma(c)\Gamma(b - a)}{\Gamma(b)\Gamma(c - a)} F(1 + a - c, a; 1 + a - b; 1/z) \]
\[ + \frac{\Gamma(c)\Gamma(a - b)}{\Gamma(a)\Gamma(c - b)} F(1 + b - c, b; 1 - a + b; 1/z), \]
\[ |\arg(-z)| < \pi \]

\[ \left\{ \frac{z(1 - z)}{dz^2} + [c - (a + b + 1)z] \frac{d}{dz} - ab \right\}F(a, b; c; z) = 0. \]
Gauss's hypergeometric series, Eqs. (8.45) and (8.46), results from the Taylor series for \((1 - xt)^{-a}\) [Eq. (8.40)] put into Eqs. (8.42)–(8.44), and then from Eqs. (8.18), (8.30), (8.19), and (8.6). The radius of convergence follows from \(\lim_{k \to \infty} \{(a)_k(b)_k/[(c)_k k!]\}^{1/k} = 1\).

Equations (8.48)–(8.50) follow easily from the series expansion. Note that the geometric series is a special case. The value at \(x = 1\) follows directly from the integral representation of \(B(b - a, c - b)\).

When \(c\) is a negative integer, \(F(a, b; c; z)\) is undefined, but the limit in Eq. (8.53) follows from, say, Eq. (8.43) and the observation

\[
\frac{\Gamma(-a + 1)(-z)^k}{\Gamma(-a + 1 - k) k!} B(b + k, -n - b) = \frac{(a)_k z^k}{k!} \frac{\Gamma(b + k) \Gamma(-n - b)}{\Gamma(-n + k)} = 0, \quad k \leq n \tag{8.61}
\]

\[
= \frac{(a)_k z^k}{k!} \frac{\Gamma(b + k) \Gamma(-n - b)}{(k - n - 1)!}, \quad k \geq n + 1. \tag{8.62}
\]

If, however, first \(a\) becomes a negative integer, \(-n\), so that \(F(-n, b; c; z)\) is a polynomial, and then \(c\) becomes an integer at least as negative as \(a\), then Eq. (8.54) results.

Note: \((-n)_k/(-n - l)_k = (n + 1 - k)_k/(n + l + 1 - k)_k\).

The six hypergeometric functions for which one of \(a, b,\) and \(c\) is increased or decreased by 1 are said to be contiguous to \(F(a, b; c; z)\). Any contiguous function can be expressed as a linear combination of \(F(a, b; c; z)\) and any other contiguous function, where the coefficients are rational functions in \(a, b, c, z\). Equation (8.55) is typical. It follows from

\[
t^{b-1}(1 - t)^{c-b-1}(1 - xt)^{-a} = t^{b-1}(1 - t)^{c-b-2}(1 - xt)^{-a} - t^{b}(1 - t)^{c-b-2}(1 - xt)^{-a}. \tag{8.63}
\]

Equations (8.56)–(8.59) are examples of linear transformation formulas. Equation (8.56) results from the substitution \(t \to 1 - t\). Equation (8.57) is (8.56) with \(a\) and \(b\) interchanged, while Eq. (8.58) is (8.56) applied to (8.57). Equation (8.59) is a little more subtle. Refer to Fig. 10, and note
that \( \int_0^1 dt = \int_0^{1/z} dt + \int_{1/z}^1 dt \). By straightforward changes of variable,

\[
\int_0^{1/z} t^{b-1}(1 - t)^{c-b-1}(1 - zt)^{-a} \, dt = \frac{\Gamma(b)\Gamma(1 - a)}{\Gamma(1 - a + b)} \, z^{-b} F(1 + b - c, b; 1 - a + b; 1/z) \tag{8.64}
\]

\[
\int_{1/z}^1 t^{b-1}(1 - t)^{c-b-1}(1 - zt)^{-a} \, dt = \frac{\Gamma(c - b)\Gamma(1 - a)}{\Gamma(1 - a - b + c)} \, (-1)^a z^{1-a-b}(1 - 1/z)^{c-a-b}
\times F(1 - a, 1 - b; 1 - a - b + c; 1 - z), \tag{8.65}
\]

so that

\[
F(a, b; c; z) = \frac{\Gamma(c)\Gamma(1 - a)}{\Gamma(c - b)\Gamma(1 - a + b)} \, z^{-b} F(1 + b - c, b; 1 - a + b, 1/z)
+ \frac{\Gamma(c)\Gamma(1 - a)}{\Gamma(b)\Gamma(1 - a - b + c)} \, (-1)^a z^{1-a-b}(1 - 1/z)^{c-a-b}
\times F(1 - a, 1 - b; 1 - a - b + c; 1 - z). \tag{8.66}
\]

Here, \((-1)^a = \exp(\pm \pi ia)\), where the sign is taken to be the same as for \(\arg z\). By switching \(a\) and \(b\), a similar equation results. Elimination of \(F(1 - a, 1 - b; 1 - a - b + c; 1 - z)\) from the two gives Eq. (8.59.)

The proof that \(F(a, b; c; z)\) is a solution of the hypergeometric differential equation (8.60) is typical for integral representations of solutions to linear differential equations.

The gist is that:

1. Eq. (8.60) is of the form

\[
\mathcal{L}_z \int_\gamma f(t, z) \, dt = 0, \tag{8.67}
\]

where \(\mathcal{L}_z\) is the differential operator in braces, and \(f(t, z)\) is \(t^{b-1}(1 - t)^{c-b-1} \times (1 - zt)^{-a}\);

2. \(\mathcal{L}_z f(t, z) = (\partial/\partial t) g(t, z)\), where \(g(t, z) = -at^b(1 - t)^{c-b}(1 - zt)^{-a-1}\); and

3. \(g(t, z)\) has the same value at both endpoints of \(\gamma\). Thus,

\[
\mathcal{L}_z \int_\gamma f(t, z) \, dt = g(t, z) \bigg|_{t_{\text{final}}}^{t_{\text{initial}}} = 0 \tag{8.68}
\]

and \(\int_\gamma f(t, z) \, dt\) is the desired solution.
D. Legendre Polynomials and Associated Legendre Functions as Examples of the Hypergeometric Function

Important and somewhat typical examples of the hypergeometric function are the Legendre polynomials and associated Legendre functions. We show how some of their properties are special cases of those of the hypergeometric function, and how other properties can be derived using complex variable theory. These functions are met again in Chapter 4, Section VII.

1. Legendre Polynomials

a. Definition

\[
P_n(x) = F(-n, n + 1; 1; (1 - x)/2).
\]

(8.69)

b. Important Formulas

\[
P_n(x) = (2^{n+1}n!)^{-1} \int_{(1 - 1 < 2)}^z (t - z)^{-n-1}(t^2 - 1)^n \, dt \quad \text{(Schläfli)}
\]

(8.70)

\[
= 2^n(n!)^{-1} \int_{(1 - 1 < 2)}^{(1 + 1)} (t - z)^n(t^2 - 1)^{-n-1} \, dt
\]

(8.71)

\[
= (2^n n!)^{-1}(d/dz)^n(z^2 - 1)^n \quad \text{(Rodrigues)}
\]

(8.72)

\[
= \pi^{-1} \int_0^\pi (x + (z^2 - 1)^{1/2} \cos \phi)^n \, d\phi \quad \text{(Laplace)}
\]

(8.73)

\[
= \pi^{-1} \int_0^\pi (x + (z^2 - 1)^{1/2} \cos \phi)^{-n-1} \, d\phi \quad \text{(Jacobi),} \quad |\arg z| < \pi/2,
\]

(8.74)

\[
\int_{-1}^1 P_n(x)P_m(x) \, dx = \delta_{nm}/(2n + 1) \quad \text{(orthogonality)}
\]

(8.75)

\[
(n + 1)P_{n+1}(x) - (2n + 1)xP_n(x) + nP_{n-1}(x) = 0 \quad \text{(recurrence)}
\]

(8.76)

\[
\{(1 - x^2)(d/dz)^2 - 2x(d/dz) + n(n + 1)\}P_n(x) = 0,
\]

(8.77)

\[
(1 + h^2 - 2hx)^{-1/2} = \sum_{k=0}^\infty h^k P_k(x), \quad |h|^2 + 2|hx| < 1 \quad \text{(generating function)}.
\]

(8.78)
representations corresponding to the contour of Fig. 9c [cf. Eq. (8.29)]:

\[
F(-n, n + 1; 1; \frac{1 - z}{2}) = \frac{1}{2\pi i} \oint_{|\tau| = \tau > 1} \tau^{n} (\tau - 1)^{-n-1} \left(1 - \frac{1 - z}{2} \tau\right)^{n} d\tau
\]  
(8.79)

\[
F(n + 1, -n; 1; \frac{1 - z}{2}) = \frac{1}{2\pi i} \oint_{(|\tau| < 2/(1 - z))} \tau^{-n-1} (\tau - 1)^{n} \left(1 - \frac{1 - z}{2} \tau\right)^{-n-1} d\tau.
\]  
(8.80)

[It is necessary to use \(\Gamma(-n) \sin \pi n = -\pi/\Gamma(n + 1)\).] The substitution \(\tau = (1 - t)/(1 - z)\) yields Eqs. (8.70) and (8.71). The residue theorem applied to Schl"{a}fli's formula yields Rodrigues's formula. The Laplace integrals (the one found by Jacobi is called Laplace's integral of the second kind) are Eqs. (8.70) and (8.71) with the substitution \(t = z + (z^2 - 1)^{1/2} e^{i\phi}\). The orthogonality is obtained by using Rodrigues's formula and integrating by parts. Note that \(\int_{-1}^{1} (1 - t^2)^n dt = 2^{2n+1} B(n + 1, n + 1)\). The recurrence formula (8.76) is related to Eq. (8.55); it is a special case of such a relation among \(F(a + 1, b - 1; c; z)\), \(F(a, b; c; z)\), and \(F(a - 1, b + 1; c; z)\). Equation (8.76) is also a reflection of the relation

\[
[(1 + h^2 - 2hz)(d/dh) + h - z](1 + h^2 - 2hz)^{-1/2} = 0.
\]  
(8.81)

The differential equation (8.77) is Eq. (8.60) with appropriate substitutions.

The generating function can be obtained by directly summing the right-hand side of Eq. (8.78) via Schl"{a}fli's integral:

\[
\sum_{k=0}^{\infty} h^k P_k(z) = \frac{1}{2\pi i} \sum_{k=0}^{\infty} \oint_{|t-z|=1} (t-z)^{-1} \left(\frac{h}{2} - \frac{t^2 - 1}{t - z}\right)^n dt
\]  
(8.82)

\[
= \frac{1}{2\pi i} \oint_{|t-z|=1} [t - z - \frac{1}{2}h(t^2 - 1)]^{-1} dt,
\]  
(8.83)

which converges for small enough \(h\); the circle \(|t - z| = 1\) is chosen for convenience. The quadratic is factorable:

\[
t - z - \frac{1}{2}h(t^2 - 1) = -\frac{1}{2}h \left(t - \frac{1 + (1 + h^2 - 2hz)^{1/2}}{h}\right) \times \left(t - \frac{1 - (1 + h^2 - 2hz)^{1/2}}{h}\right).
\]  
(8.84)

The root \((1 - (1 + h^2 - 2hz)^{1/2})/h \approx z\) lies inside the contour, while \((1 + (1 + h^2 - 2hz)^{1/2})/h \approx 2/h\) lies outside. The residue at \((1 - (1 + h^2 - 2hz)^{1/2})/h\) is \(1/(1 + h^2 - 2hz)^{1/2}\).
2. Associated Legendre Functions

a. Definition, Important Equations. The analogs of Eqs. (8.69)–(8.78) are similarly derived. In physical applications, \( z \) is usually real, and \( |z| \leq 1 \). Where \((1 - z^2)^{1/2}\) appears below, the principal branch and \(|z^2| \leq 1\) are assumed. The definition and consequences, stated without further comment, are

\[
P_n^m(z) = (1 - z^2)^{m/2} (d/dz)^m F(-n; n + 1; 1; (1 - z)/2) \quad (8.85a)
\]

\[
= (1 - z^2)^{m/2} 2^{-m} \frac{(n + m)!}{(n - m)!} \frac{1}{m!} \times F\left(-n + m, n + 1 + m; 1 + m; \frac{1 - z}{2}\right), \quad m = 0, 1, 2, \ldots, n \quad (8.85b)
\]

\[
= (1 - z^2)^{m/2} (1 + z)^{-m} \frac{(n + m)!}{(n - m)!} \frac{1}{m!} \times F\left(-n, n + 1; 1 + m; \frac{1 - z}{2}\right) \quad [\text{cf. Eq. (8.58)}] \quad (8.86)
\]

\[
= (1 - z^2)^{m/2} 2^{-n - 1} (\pi i)^{-1} (n + m)! (n!)^{-1} \times \oint_{[z=1]} (t - z)^{-n - m - 1} (t^2 - 1)^n \, dt \quad (8.87a)
\]

\[
= (1 - z^2)^{-m/2} (-1)^m 2^{-n - 1} (\pi i)^{-1} (n + m)! (n!)^{-1} \times \oint_{[z=1]} (t - z)^{-n + m - 1} (t^2 - 1)^n \, dt \quad (8.87b)
\]

\[
= (1 - z^2)^{-m/2} (-1)^m 2^n (\pi i)^{-1} (n - m)! (n!)^{-1} \times \oint_{[t=1]} (t - z)^{-n - m} (t^2 - 1)^{-n - 1} \, dt \quad (8.88)
\]

\[
= 2^{-n} (n!)^{-1} (1 - z^2)^{m/2} (d/dz)^{n + m} (z^2 - 1)^n \quad (8.89a)
\]

\[
= 2^{-n} (n!)^{-1} [(-1)^m (n + m)!/(n - m)!] (1 - z^2)^{-m/2} \times (d/dz)^{n - m} (z^2 - 1)^n \quad (8.89b)
\]

\[
= (1 - z^2)^{m/2} (d/dz)^m P_n(z) \quad (8.90)
\]

\[
= i^{-m} (n + m)! (2\pi n!)^{-1} \int_0^{2\pi} e^{im\phi} (z + i(1 - z^2)^{1/2} \cos \phi)^n \, d\phi \quad (8.91)
\]

\[
= i^{m n} [2\pi (n - m)!]^{-1} \int_0^{2\pi} e^{im\phi} (z + i(1 - z^2)^{1/2} \cos \phi)^{-n - 1} \, d\phi, \quad \text{Re} \ z > 0, \quad (8.92)
\]
\[ \int_{-1}^{1} P_{n'}^m(z) P_{n}^{-m}(z) \, dz = \delta_{nn'}(-1)^m 2/(2n + 1) \] \hspace{1cm} (8.93) \\
\[ \int_{-1}^{1} P_{n'}^m(z) P_{n}^m(z) \, dz = \delta_{nn'} \frac{(n + m)!}{(n - m)!} \frac{2}{2n + 1}, \] \hspace{1cm} (8.94) \\

\[(n + 1 - m)P_{n+1}^m(z) - (2n + 1)z P_n^m(z) + (n + m)P_{n-1}^m(z) = 0 \] \hspace{1cm} (8.95) \\
\[(1 - z)^{1/2}P_{n}^{m+1}(z) - 2mzP_{n}^m(z) + (n + m)(n - m + 1)(1 - z^2)^{1/2}P_{n}^{m-1}(z) = 0 \] \hspace{1cm} (8.96) \\
\[\{(1 - z^2)(d/dz)^2 - 2z(d/dz) + n(n + 1) - m^2/(1 - z^2)\} P_n^m(z) = 0, \] \hspace{1cm} (8.97) \\
\[1 + h^2 - 2hz)^{-m-1/2}h^m(1 - z^2)^{m/2}(2m - 1)!! = \sum_{k=0}^{\infty} h^{k+m} P_{k+m}^m(z), \] \hspace{1cm} (8.98)

where 
\[(2m - 1)!! = (2m)!/(2^m m!) = 1 \cdot 3 \cdot 5 \cdots (2m - 1). \] \hspace{1cm} (8.99)

b. Negative Order, \(P_n^{-m}(z)\). Equation (8.85b) defines \(P_n^m(z)\) when \(m\) is a negative integer, if Eq. (8.53) is appropriately invoked:

\[P_n^{-M}(z) \equiv \lim_{\epsilon \to 1-M} (1 - z^2)^{m/2} 2^{-m} \frac{(n + m)!}{(n - m)!} \frac{1}{\Gamma(c)} \times F\left(-n + m; n + 1 + m; c; \frac{1 - z}{2}\right), \]
\[M \geq 0, \quad m = -M \] \hspace{1cm} (8.100) \\
\[= (-1)^M (1 - z^2)^{-M/2} (1 - z)^M \frac{1}{M!} \times F\left(-n, n + 1; 1 + M; \frac{1 - z}{2}\right) \] \hspace{1cm} (8.101) \\
\[= (-1)^M \frac{(n - M)!}{(n + M)!} P_n^M(z) \] \hspace{1cm} (8.102) \\
\[P_n^{-m}(z) = (-1)^m \frac{(n + m)!}{(n - m)!} P_n^{-m}(z), \] \hspace{1cm} (8.103)

Thus \(P_n^{-m}\) is a multiple of \(P_n^m\), and vice versa. Equations (8.85b)–(8.89) and (8.91)–(8.97) are valid for positive and negative \(m\); Eqs. (8.90) and (8.98) are valid only for positive \(m\).
c. Addition Formula. An extremely useful equation in applications is the addition formula:

\[
P_n(\cos \theta) = \sum_{m=-n}^{n} (-1)^m P_n^m(\cos \theta_1)P_n^{-m}(\cos \theta_2) \exp[i m(\phi_1 - \phi_2)],
\]

(8.104)

\[
\cos \theta = \cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2).
\]

(8.105)

By the addition formula, a function of the relative angle between two vectors is reduced to products in which the angular coordinates of the two vectors appear in separate factors. A derivation follows:

\[
\sum_{m=-n}^{n} (-1)^m P_n^m(z_1)P_n^{-m}(z_2)e^{im\psi}
\]

\[
= \frac{e^{im\psi}}{\pi i} \left( \frac{1 - z_1^2}{1 - z_2^2} \right)^{n/2} \int_{|t_1-1|<2} (t_1^2 - 1)^{-n-1} dt_1
\]

\[
\times \left\{ \sum_{m=-n}^{n} \left[ (t_1 - z_1)e^{-i\psi} \left( \frac{1 - z_2^2}{1 - z_1^2} \right)^{1/2} \right]^{n-m} \right\}
\]

\[
\times \frac{1}{2\pi i} \int_{|t-1|<2} \left( t_2 - z_2 \right)^{-(n-m)-1}(t_2^2 - 1)^n dt_2
\]

(8.106)

\[
= \frac{e^{im\psi}}{\pi i} \left( \frac{1 - z_1^2}{1 - z_2^2} \right)^{n/2} \int_{|t-1|<2} (t^2 - 1)^{-n-1}
\]

\[
\times \left\{ \left[ z_2 + (t - z_1)e^{-i\psi} \left( \frac{1 - z_2^2}{1 - z_1^2} \right)^{1/2} \right]^2 - 1 \right\}^n dt,
\]

(8.107)

\[
\sum_{n=0}^{\infty} h^n \sum_{m=-n}^{n} (-1)^m P_n^m(z_1)P_n^{-m}(z_2)e^{im\psi}
\]

\[
= \frac{1}{\pi i} \int_{|t-1|<2} \left[ t^2 - 1 - he^{i\psi} \left( \frac{1 - z_1^2}{1 - z_2^2} \right)^{1/2} \right]
\]

\[
\times \left\{ \left[ z_2 + (t - z_1)e^{-i\psi} \left( \frac{1 - z_2^2}{1 - z_1^2} \right)^{1/2} \right]^2 - 1 \right\}^{-1} dt
\]

(8.108)

\[
= \frac{1}{\pi i} \int_{|t-1|<2} \left\{ t^2 \left[ 1 - he^{-i\psi} \left( \frac{1 - z_2^2}{1 - z_1^2} \right)^{1/2} \right]
\]

\[- 2ht \left[ z_2 - z_1 e^{-i\psi} \left( \frac{1 - z_2^2}{1 - z_1^2} \right)^{1/2} \right]
\]

\[- \left[ 1 - 2hz_1z_2 - he^{i\psi}(1 - z_1^2)^{1/2}(1 - z_2^2)^{1/2} \right.
\]

\[+ hz_1^2 e^{-i\psi} \left( \frac{1 - z_2^2}{1 - z_1^2} \right)^{1/2} \right] \right\}^{-1} dt
\]

(8.109)

\[
= \{1 + h^2 - 2h[z_1z_2 + (1 - z_1^2)^{1/2}(1 - z_2^2)^{1/2} \cos \psi] \}^{-1/2}.
\]

(8.110)
Equation (8.106) uses both representations (8.87) and (8.88). Equation (8.107) follows from Eqs. (4.77), (5.28), and the observation that the first \((2n + 1)\) terms of the Taylor series for a polynomial of degree \(2n\) are the Taylor series. The right-hand side of Eq. (8.108) is the sum of the geometric series, which converges for sufficiently small \(|h|\). The denominator of Eq. (8.109) is just a quadratic polynomial in \(t\). The two roots are at
\[
t = t_\pm = \left[ 1 - he^{-i\psi} \left( \frac{1 - z_2^2}{1 - z_1^2} \right)^{1/2} \right]^{-1} \left\{ \frac{z_2}{z_1} e^{-i\psi} \left( \frac{1 - z_2^2}{1 - z_1^2} \right)^{1/2} \right\} \pm \left[ 1 + h^2 - 2h(z_1 z_2 + (1 - z_1^2)^{1/2}(1 - z_2^2)^{1/2} \cos \psi) \right]^{1/2}\]
\approx \pm 1 + O(h). \quad (8.112)

The root \(t_+\) (near 1 for small \(h\)) lies inside the contour, the root \(t_-\) lies outside, and the result is \(2ni \times \text{residue at } t_+ [\text{Eq. (8.110)]}\). Finally, (8.110) is the generating function for the \(P_n(cos \Theta)\), by Eqs. (8.105) and (8.78).

An alternative derivation of the addition theorem is given by Henderson in Chapter 4.

E. THE CONFLUENT HYPERGEOMETRIC FUNCTIONS

1. Definition of \(M(a, b, z)\)

The confluent hypergeometric function of the first kind, Kummer's function, is defined by
\[
M(a, b, z) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b - a)} \int_0^1 t^{a-1}(1 - t)^{b-a-1} e^{zt} dt,
\]
\[\text{Re } b > \text{Re } a > 0. \quad (8.113)\]

It may be obtained as a limit of a hypergeometric function:
\[
\lim_{n \to \infty} F(-n, a; b; -z/n) = \lim_{n \to \infty} \frac{\Gamma(b)}{\Gamma(a)\Gamma(b - a)} \int_0^1 t^{a-1}(1 - t)^{b-a-1}(1 + zt/n)^n dt
\]
\[= \frac{\Gamma(b)}{\Gamma(a)\Gamma(b - a)} \int_0^1 t^{a-1}(1 - t)^{b-a-1} e^{zt} dt. \quad (8.114)\]

The nomenclature reflects the formation of an irregular singular point.
at \( \infty \) by the \textit{confluence} of two regular singular points \((1/z \text{ and } \infty)\) of the hypergeometric differential equation.

As with \( F(a, b; c; z) \), \( M(a, b, z) \) is an analytic function of the parameters \( a, b \), and the variable \( z \). Any of the contours of Fig. 9 introduced for \( B(a, b) \) can be used, when appropriate, for \( M(a, b, z) \). For example, the equation

\[
M(a, b, z) = -\frac{1}{2\pi i} e^{-\pi i b} \Gamma(b) \Gamma(1 - a) \Gamma(1 + a - b) \times \int_{t_0}^{(1+0+1,0-)} t^{a-1}(1 - t)^{b-a-1} e^{zt} \, dt \tag{8.116}
\]

is valid when neither \( b, 1-a \), nor \( 1+a-b \) is a negative integer. \( M(a, b, z) \) is an entire function of \( z \) [cf. Eq. (8.123)].

Comprehensive treatments of confluent hypergeometric functions include those by Slater (1960), Erdélyi (1953), and Whittaker and Watson (1927). Here we sketch how some of the important results follow from the integral representation.

\section*{2. Differential Equation}

\( M(a, b, z) \) satisfies Kummer's differential equation:

\[
\{z(d/dz)^2 + (b - z)(d/dz) - a\} M(a, b, z) = 0. \tag{8.117}
\]

In the notation of Section VIII.C.3, Eq. (8.67), take \( f(t, z) = t^{a-1} \times (1 - t)^{b-a-1} e^{zt} \) and \( g(t, z) = -t^a(1 - t)^{b-a} e^{zt} \).

\section*{3. Definition of \( U(a, b, z) \)}

The confluent hypergeometric function of the second kind, \( U(a, b, z) \), is also a solution of Kummer's equation:

\[
U(a, b, z) = [\Gamma(a)]^{-1} \int_0^\infty t^{a-1}(1 + t)^{b-a-1} e^{-zt} \, dt, \quad \text{Re } a > 0. \tag{8.118}
\]

[Take \( f(t, z) = t^{a-1}(1 + t)^{b-a-1} e^{-zt} \) and \( g(t, z) = -t^a(1 + t)^{b-a} e^{-zt} \).]

\( U(a, b, z) \) is multiple valued [cf. Eq. (8.125)], with branch point at \( z = 0 \).

A more general integral representation for \( U(a, b, z) \) [cf. Eq. (8.15)] is

\[
U(a, b, z) = (2\pi i)^{-1} e^{-\pi i a} \Gamma(1 - a) \int_{0+}^\infty t^{a-1}(1 + t)^{b-a-1} e^{-zt} \, dt. \tag{8.119}
\]
4. Recurrence Formulas

The identity \((1 \pm t)^{b-a-1} = (1 \pm t)^{b-a-2} \pm t(1 \pm t)^{b-a-2}\) yields

\[
(1 + a - b)M(a, b, z) - aM(a + 1, b, z) + (b - 1)M(a, b - 1, z) = 0
\]

(8.120)

\[
U(a, b, z) - aU(a + 1, b, z) - U(a, b - 1, z) = 0
\]

(8.121)

which are analogous to Eq. (8.55) and typical of a number of such equations in the references cited above.

5. Series Expansion

Expansion of \(e^z\) and term-by-term integration of Eq. (8.115) [cf. Eqs. (8.45) and (8.46)] give

\[
M(a, b, z) = 1 + \frac{a}{b} z + \frac{a(a + 1)}{b(b + 1)} \frac{z^2}{2!} + \cdots
\]

(8.122)

\[
= \sum_{k=0}^{\infty} \frac{(a)_k}{(b)_k} \frac{z^k}{k!},
\]

(8.123)

which clearly has an infinite radius of convergence. \(F(a, b; c; z)\) and \(M(a, b, z)\) are special cases, \(_2F_1(a, b; c; z)\) and \(_1F_1(a; b; z)\), respectively, of the generalized hypergeometric function

\[
_2F_1(a_1, a_2, \ldots, a_k; b_1, b_2, \ldots, b_l; z) = \sum_{n=0}^{\infty} \frac{(a_1)_n(a_2)_n \cdots (a_k)_n}{(b_1)_n(b_2)_n \cdots (b_l)_n} \frac{z^n}{n!}.
\]

(8.124)

A series for \(U(a, b, z)\) is implicit in the formula

\[
U(a, b, z) = \frac{\pi \alpha}{\sin \pi \beta} \left[ \frac{M(a, b, z)}{\Gamma(1 + a - b)\Gamma(b)} \right.
\]

\[
- \frac{z^{1-b}M(1 + a - b, 2 - b, z)}{\Gamma(1)\Gamma(2 - b)} \left. \right],
\]

(8.125)

which clearly displays the nature of the multiple valuedness of \(U(a, b, z)\). The derivation is quite instructive. The manipulation of the contour is essentially \(\int_0^\infty = \int_0^{-1} + \int_{-1}^\infty\), and involves drawing both branch cuts to \(+\infty\) along the real axis. We treat the case \(\text{Re} \ a > 0\) for simplicity.
Then

\[ U(a, b, z) = (e^{2\pi i b} - 1)^{-1} [\Gamma(a)]^{-1} \times \left\{ \int_{\infty}^{(1+)} - \int_{0}^{(1+)} \right\} t^{a-1}(1 + t)^{b-a-1}e^{-zt} \, dt. \]  

(8.126)

For the first integral, deform the contour so that \(|t| > 1\) always. Then

\[ (e^{2\pi i b} - 1)^{-1} [\Gamma(a)]^{-1} \int_{\infty}^{(1+)} t^{b-2}(1 + t^{-1})^{b-a-1}e^{-zt} \, dt \]

\[ = (e^{2\pi i b} - 1)^{-1} [\Gamma(a)]^{-1} \times \int_{\infty}^{(0+)} \sum_{k=0}^{\infty} \frac{\Gamma(1 + a - b + k)(-1)^k}{k!} t^{b-2-k}e^{-zt} \, dt \]  

(8.127)

\[ = \sum_{k=0}^{\infty} \frac{(1 + a - b)_k \Gamma(1 - k)(-1)^k}{k!} \pi \sin \pi(b - 1 - k) \Gamma(2 - b + k) \]

\[ \times z^{-b+k} \frac{M(1 + a - b, 2 - b, z)}{\Gamma(a) \Gamma(2 - b)}. \]  

(8.128)

The second term is amenable to the substitution \(\tau = -t\):

\[ -(e^{2\pi i b} - 1)^{-1} [\Gamma(a)]^{-1} e^{\pi i(a-1)} \int_{0}^{(1+)} (-t)^{a-1}(1 + t)^{b-a-1}e^{-zt} \, dt \]

\[ = -(e^{2\pi i b} - 1)^{-1} [\Gamma(a)]^{-1} e^{\pi i a} \int_{0}^{(1+)} \tau^{a-1}(1 - \tau)^{b-a-1}e^{-z\tau} \, d\tau \]  

(8.130)

\[ = -(e^{2\pi i b} - 1)^{-1} \frac{\Gamma(b - a)}{\Gamma(b)} e^{\pi i a}[1 - e^{2\pi i(b-a)}]M(a, b, z) \]

(8.131)

\[ = \frac{\pi}{\sin \pi b} \frac{M(a, b, z)}{\Gamma(b) \Gamma(1 + a - b)}. \]  

(8.132)

6. Kummer’s Transformations

These are the analogs of the linear transformation formulas (8.56)–(8.59). Set \(\tau = 1 - t\) in Eq. (8.113). Then

\[ M(a, b, z) = e^{z}M(b - a, b, -z). \]  

(8.133)

The second Kummer transformation is a direct consequence of Eq. (8.125):

\[ U(a, b, z) = z^{a-b}U(1 + a - b, 2 - b, z). \]  

(8.134)
3. Complex Variable Theory

F. Spherical Bessel Functions as Examples of Confluent Hypergeometric Functions

The confluent hypergeometric family includes the Bessel function family, the Airy function, the Hermite and Laguerre polynomials, and the exponential integral, to mention a few. The spherical Bessel function is important in many applications—scattering in quantum mechanics being a good example. We show how some of its properties are special cases of those of the confluent hypergeometric function, and how others can be derived by complex variable theory. Bessel functions are encountered again in Chapter 4, Section VI.

1. Definition of $j_n(z)$. The Double Factorial

\[
j_n(z) = [(3/2)_n]^{-1}(\frac{i}{2}z)^n e^{-i\pi/2} M(n + 1, 2n + 2, 2iz). \tag{8.135}\]
\[
= [(2n + 1)!]^{-1} z^n e^{-i\pi z} M(n + 1, 2n + 2, 2iz). \tag{8.136}\]

The spherical Bessel function is a special case of Bessel's function:

\[
j_n(z) = [\pi/(2z)]^{1/2} J_{n+1/2}(z). \tag{8.137}\]

The double factorial, defined in Eq. (8.99) for add integers, appears repeatedly in formulas related to $j_n(z)$. It is completely characterized by

\[
(2n)!! = 2^nn! = 2^n \Gamma(n + 1) = 2^n(1)_n, \quad n = 0, 1, 2, \ldots \tag{8.138}\]
\[
(2n - 1)!! = (2n)/(2n)!! = 2^n \Gamma(n + \frac{1}{2})/\Gamma(\frac{1}{2}) = 2^n(\frac{1}{2})_n, \quad n = 0, 1, 2, \ldots \tag{8.139}\]
\[
(-2n - 1)!! = 2^{-n} \Gamma(-n + \frac{1}{2})/\Gamma(\frac{1}{2}) = (-1)^n/(2n - 1)!!, \quad n = 0, \pm 1, \pm 2, \ldots \tag{8.140}\]

\[
1/(2n)!! = 0, \quad n = -1, -2, \ldots \tag{8.141}\]

2. Differential Equation and Integral Representation

Directly from Eqs. (8.136), (8.117), and (8.113), one has

\[
\{(d/dx)^2 + 2x^{-1}(d/dx) + 1 - n(n + 1)x^{-2}\} j_n(x) = 0, \tag{8.142}\]

\[
j_n(x) = x^n e^{-ix} 2^n (n!)^{-1} \int_0^1 t^n(1 - t)v^{i\pi s} dt \tag{8.143}\]

\[
= x^n (2n+1)!^{-1} \int_{-1}^1 (1 - s^2)^n e^{ist} ds, \quad t = (s + 1)/2. \tag{8.144}\]
3. Rayleigh's Formula, Power Series, Recurrence Formulas

Integration by parts of Eq. (8.144) and \(ise^{i\alpha s} = (d/d\alpha)x^{i\alpha s}\) gives

\[
j_n(\alpha) = (-\alpha)^{\alpha}(\alpha^{-1}d/d\alpha)^{\alpha-1}\sin \alpha \quad \text{(Rayleigh's formula).} \quad (8.145)
\]

In principle, a power series for \(j_n(\alpha)\) could be obtained from Eqs. (8.136), (8.123), and the power series for \(e^{-i\alpha}\). However, Rayleigh's formula and the power series for \(\sin \alpha\) give directly

\[
j_n(\alpha) = \sum_{k=0}^{\infty} (-1)^k \alpha^{n+2k}/[(2n + 2k + 1)!(2k)!]. \quad (8.146)
\]

Substitution in the appropriate recurrence formulas for \(M\) would yield recurrence formulas for \(j_n(\alpha)\). In this short exposition, an \textit{ad hoc} approach is more efficient. The result,

\[
(d/d\alpha)x^{-n}j_n(\alpha) = \alpha^{-n}[(d/d\alpha) - n/\alpha]j_n(\alpha) = -\alpha^{-n}j_{n+1}(\alpha), \quad (8.147)
\]

follows from Rayleigh's formula, while

\[
(d/d\alpha)x^{n+1}j_n(\alpha) = \alpha^{n+1}[(d/d\alpha) + (n + 1)/\alpha]j_n(\alpha) = \alpha^{n+1}j_{n-1}(\alpha) \quad (8.148)
\]

uses Rayleigh's formula and the identity

\[
(d/d\alpha)x^{2n+1}(\alpha^{-1}d/d\alpha)^{n-1} = \alpha^{2n}(\alpha^{-1}d/d\alpha)^{n-1}\alpha^{-1}(d/d\alpha)^{n}. \quad (8.149)
\]

Together, Eqs. (8.147) and (8.148) yield

\[
j_{n-1}(\alpha) - (n + 1)j_{n+1}(\alpha) = (2n + 1)(d/d\alpha)j_n(\alpha) \quad (8.150)
\]
\[
j_{n-1}(\alpha) + j_{n+1}(\alpha) = (2n + 1)\alpha^{-1}j_n(\alpha). \quad (8.151)
\]

4. Connection with Legendre Polynomials. Plane Wave Expansion

Equations (8.72) and (8.144) give immediately

\[
j_n(\alpha) = \frac{1}{2i^{n-1}} \int_{-1}^{1} P_n(s)e^{i\alpha s} \, ds. \quad (8.152)
\]

We derive additionally that

\[
e^{i\alpha s} = \sum_{n=0}^{\infty} (2n + 1)i^{n}j_n(\alpha)P_n(s). \quad (8.153)
\]
3. Complex Variable Theory

[Note that if we knew that the Legendre polynomials were complete, then Eq. (8.153) follows from Eq. (8.152) and the orthogonality of the Legendre polynomials, Eq. (8.75).] We substitute

\[ s^n/n! = \sum_{k=0}^{\infty} (2k + 1)P_k(s)/[(n + k + 1)!(n - k)!] \]  \hspace{1cm} (8.154)

[which is easily computed via Eqs. (8.152) and (8.75)] into the power series for \( e^{isz} \) and rearrange the terms. [The double series converges absolutely; an estimate of \(|P_n(s)|, |P_n(s)| \leq (|s| + |s^2 - 1|^{1/2})^n \) follows from Laplace's integral, Eq. (8.73).] The result is

\[ e^{isz} = \sum_{n=0}^{\infty} (iz)^n s^n/n! \]  \hspace{1cm} (8.155)

\[ = \sum_{n=0}^{\infty} \left[ \sum_{k=0}^{\infty} \frac{(iz)^n}{(n + k + 1)!(n - k)!} (2k + 1)P_k(s) \right] \]  \hspace{1cm} (8.156)

\[ = \sum_{k=0}^{\infty} \left( \sum_{m=0}^{\infty} \frac{(iz)^{k+2m}}{(2k + 2m + 1)!(2m)!} \right) (2k + 1)P_k(s) \]  \hspace{1cm} (8.157)

\[ = \sum_{k=0}^{\infty} (2k + 1)i^k j_k(s)P_k(s). \]  \hspace{1cm} (8.158)

Equation (8.158) often occurs combined with the addition formula (8.104), in a form called the "plane wave expansion":

\[ e^{ik \cdot r} = \sum_{l=0}^{\infty} (2l + 1)i^l j_l(kr)(-1)^m P_l^m(\cos \theta)P_l^{-m}(\cos \theta_k) \exp(\text{i}m(\phi - \phi_k)), \]  \hspace{1cm} (8.159)

where \((r, \theta, \phi)\) and \((k, \theta_k, \phi_k)\) are the spherical polar coordinates of \(r\) and \(k\).

G. SERIES FOR EXPONENTIAL-TYPE INTEGRAL

The exponential-type integral \(E_n(z)\) (Abramowitz and Stegun, 1964), which is defined by

\[ E_n(z) = \int_1^{\infty} t^{-n}e^{-zt} \, dt, \]  \hspace{1cm} (8.160)

is related to the confluent hypergeometric function \(U\) by

\[ E_n(z) = e^{-z}U(1, -n + 2, z). \]  \hspace{1cm} (8.161)
In Section X.E a series expansion is needed for $E_n(x)$, for $n$ a positive integer. The expansion is derived by first letting $n$ be nonintegral, by using Eqs. (8.125), (8.133), $[M(n, n, z) = e^z]$, and (8.123), then letting $n \to N = $ positive integer. With $\psi(n) = [(d/dn)\Gamma(n)]/\Gamma(n)$, one obtains

$$E_N(x) = \lim_{n \to N} e^{-x} \frac{\pi}{\sin \pi(2 - n)} \left[ \frac{M(1, 2 - n, z)}{\Gamma(n)\Gamma(2 - n)} - \frac{\pi^{n-1} M(n, n, z)}{\Gamma(1)\Gamma(n)} \right]$$

(8.162)

$$= \lim_{n \to N} \frac{\pi}{\sin \pi(2 - n)} \left[ \frac{M(1 - n, 2 - n, -z)}{\Gamma(n)\Gamma(2 - n)} - \frac{\pi^{n-1}}{\Gamma(n)} \right]$$

(8.163)

$$= \lim_{n \to N} \sum_{k=0}^{\infty} \frac{1}{(k - n + 1)k!} \left[ \frac{(-z)^k}{k!} \right] + \frac{\pi(-1)^{N-1}}{\sin \pi(N - n)} \frac{\pi^{n-1}}{\Gamma(n)}$$

(8.164)

$$= - \sum_{k=0}^{\infty} \frac{1}{(k - N + 1)(N-1)!} \frac{(-z)^k}{k!}$$

(8.165)

$$\frac{(N-1)!}{(N - 1)!} [\log x - \psi(N)]$$

---

**IX. On Fourier Transforms**

The Fourier transform of $f(x)$ is defined by

$$\text{FT}\{f(x)\} = \int_{-\infty}^{\infty} f(x)e^{ikx} \, dx.$$  

(9.1)

The central result, which is established below, is the *Fourier transform inversion formula*

$$(2\pi)^{-1} \int_{-\infty}^{\infty} e^{-ikx} \text{FT}\{f(x)\} \, dk = f(x);$$

(9.2)

that is,

$$(2\pi)^{-1} \int_{-\infty}^{\infty} e^{-ikx} \left( \int_{-\infty}^{\infty} e^{ikx'}f(x') \, dx' \right) \, dk = f(x).$$

(9.3)

Many computations are easier to carry out through the intermediacy of Fourier transforms.
In this section, the basic results on Fourier transforms are established for functions $f(x)$ that, together with their Fourier transforms, are analytic in a strip that includes the entire real axis, and that vanish strongly enough at $\infty$ both for the integrals below to exist, and for the integrated term in each integral by parts formula to vanish.

Given Eqs. (9.1)-(9.3), one may readily establish (interchange differentiation and integration)

$$\text{FT}\{(d/dx)^n f(x)\} = (-ik)^n \text{FT}\{f(x)\} \quad \text{(integrate by parts)} \quad (9.4)$$

$$\text{FT}\{x^nf(x)\} = (-id/dk)^n \text{FT}\{f(x)\} \quad (9.5)$$

$$\text{FT}\{f(x - x_0)\} = \exp(i k x_0) \text{FT}\{f(x)\} \quad (9.6)$$

$$\int_{-\infty}^{\infty} f_1(x)f_2(x) \, dx = (2\pi)^{-1} \int_{-\infty}^{\infty} \text{FT}\{f_1(x)\}_{(-k)} \text{FT}\{f_2(x)\} \, dk \quad (9.7)$$

$$\int_{-\infty}^{\infty} f_1^*(x)f_2(x) \, dx = (2\pi)^{-1} \int_{-\infty}^{\infty} \text{FT}^*\{f_1(x)\} \text{FT}\{f_2(x)\} \, dk. \quad (9.8)$$

Equations (9.7) and (9.8) are two versions of the Fourier transform convolution theorem. The asterisk (*) denotes complex conjugate, and $\text{FT}\{f_1(x)\}_{(-k)}$ denotes

$$\text{FT}\{f_1(x)\}_{(-k)} = \int_{-\infty}^{\infty} e^{-ikx} f_1(x) \, dx. \quad (9.9)$$

To derive the inversion formula under the assumptions given above, we use the extension of Cauchy’s theorem given in Section VII.B and the fact that the order of integration in a double integral can be interchanged when the integrand vanishes uniformly at $\infty$ in the two variables. Thus for real $x$,

$$(2\pi)^{-1} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx' \exp(ik(x' - x))f(x')$$

$$= \left( \int_{-\infty}^{0} dk \int_{-\infty}^{\infty} dx' \right. \left. + \int_{0}^{\infty} dk \int_{-\infty}^{\infty} dx' \right) \exp(ik(x' - x))f(x') \quad (9.10)$$

$$= \int_{-\infty}^{0} dk \int_{-\infty}^{\infty - ie} dx' \exp(ik(z' - x))f(z')$$

$$+ \int_{0}^{\infty} dk \int_{\infty + ie}^{\infty} dx' \exp(ik(z' - x))f(z'), \quad e > 0. \quad (9.11)$$
Since \( \text{Re}[ik(x' - x)] \) is less than 0 for both terms, the \( \int dk \) can be evaluated first. Then

\[
(2\pi)^{-1} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx' \exp[ik(x' - x)] f(x')
\]

\[
= (2\pi i)^{-1} \int_{-\infty-i\infty}^{\infty-i\infty} (x' - x)^{-1}f(x') \, dz'
\]

\[
- (2\pi i)^{-1} \int_{-\infty+i\infty}^{\infty+i\infty} (x' - x)^{-1}f(x') \, dz'
\]

\[
= (2\pi i)^{-1} \int_{(x^-)} (x' - x)^{-1}f(x') \, dz' = f(x). \quad (9.13)
\]

**Fourier Transforms in Three Dimensions** The three-dimensional Fourier transform of \( f(\mathbf{r}) \) \( [\mathbf{r} = (x, y, z)] \) is defined in the natural way by

\[
\text{FT}\{ f(\mathbf{r}) \} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \exp(i(k_x x + k_y y + k_z z)) f(\mathbf{r})
\]

\[
= \int e^{ik \cdot r} f(\mathbf{r}) \, dV, \quad dV = dx \, dy \, dz. \quad (9.15)
\]

An essential point is that if \( f(\mathbf{r}) \) vanishes rapidly and uniformly at \( \infty \), then the order of integration is immaterial. Indeed, in the next section we find it convenient to use spherical polar coordinates.

**A Special Form of the Convolution Theorem** A situation to which Eq. (9.8) is applicable, perhaps unexpectedly, is

\[
\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 f_1^*(x_1)f_{12}(x_1 - x_2)f_2(x_2)
\]

\[
= (2\pi)^{-1} \int_{-\infty}^{\infty} \text{FT}^*\{ f_1(x) \} \, \text{FT}\{ f_{12}(x) \} \, \text{FT}\{ f_2(x) \} \, dk, \quad (9.16)
\]

since

\[
\text{FT}\left\{ \int_{-\infty}^{\infty} dx_2 f_{12}(x - x_2)f_2(x_2) \right\} = \text{FT}\{ f_{12}(x) \} \, \text{FT}\{ f_2(x) \}. \quad (9.17)
\]
The three-dimensional version is

\[
\int dV_1 \int dV_2 f_1^\ast(r_1) f_{12}(r_1 - r_2) f_2(r_2) = (2\pi)^{-3} \int \text{FT}^\ast\{f_1(r)\} \text{FT}\{f_{12}(r)\} \text{FT}\{f_2(r)\} \, d^3k, \tag{9.18}
\]

where \(d^3k\) denotes \(dk_x \, dk_y \, dk_z\).

**X. Quantum Chemistry Integrals**

An important problem in quantum chemistry is the calculation of the energy levels of molecules. Frequently, it is necessary to evaluate integrals of the form

\[
I_{ab}(R) = \int \psi_a^\ast(r) A \psi_b(r - R) \, dV \tag{10.1}
\]

\[
I_{cd;ab}(\mathcal{R}_1, \mathcal{R}_2, R) = \int \int [\psi_a^\ast(r_2) \psi_b(r_2 - \mathcal{R}_2)]^* \times r_{12}^{-1} [\psi_c^\ast(r_1 - R) \psi_d(r_1 - R - \mathcal{R}_1)] \, dV_1 \, dV_2, \tag{10.2}
\]

where \(A\) denotes 1, \(-\frac{1}{2} V^2\), \(r^{-1}\), or \(|r - \mathcal{R}|^{-1}\), and the functions \(\psi(r)\) are so-called atomic orbitals.

Much has been written on the evaluation of these integrals using various approaches. The purpose here is to indicate how complex variable theory is applicable by working a few specific examples. The application is taken from Silverstone (1966, 1967, 1968a,b), Silverstone and Kay (1968), Silverstone and Todd (1971), Kay and Silverstone (1969a,b, 1970), Kay, Todd, and Silverstone (1969a,b), and Todd, Kay, and Silverstone (1970), to which the reader is referred for the general cases and more detailed discussions.

**A. Spherical Harmonics. Slater-Type Atomic Orbitals**

A commonly used atomic orbital is the so-called Slater-type atomic orbital:

\[
\psi(r) = \psi_{nlm}(r) = r^{n-\frac{1}{2}} e^{-\alpha r} Y_l^m(\theta, \phi) \tag{10.3}
\]
where \( \zeta \) is a constant, called the orbital exponent, and \( n, l, m \) are integers satisfying \( n - 1 \geq l \geq |m| \). The \( Y_l^m(\theta, \phi) \) are called spherical harmonics and are defined by

\[
Y_l^m(\theta, \phi) = (-1)^m \left[ \frac{2l + 1}{4\pi} \frac{(l - m)!}{(l + m)!} \right]^{1/2} P_l^m(\cos \theta) e^{im\phi} \tag{10.4}
\]

\[
= (-1)^m Y_{l-m}^m(\theta, \phi). \tag{10.5}
\]

By Eq. (8.94) and by \( \int_0^{2\pi} \exp(i(m' - m)\phi) \, d\phi = 2\pi \, \delta_{mm'} \), the \( Y_l^m \) are orthogonal and normalized to unity:

\[
\int_0^{2\pi} d\phi \int_0^{\pi} \sin \theta Y_{l-m}^m(\theta, \phi) Y_{l'}^{m'}(\theta, \phi) = \delta_{ll'} \, \delta_{mm'}. \tag{10.6}
\]

In the derivations below, we repeatedly use both the orthonormality of the \( Y_l^m \) [Eq. (10.6)], the relation between \( Y_{l-m}^m \) and \( Y_{l+m}^m \) [Eq. (10.5)], and the plane wave expansion [Eq. (8.159)] expressed in terms of the \( Y_l^m \),

\[
e^{ik \cdot r} = \sum_{l=0}^{\infty} 4\pi i l j_l(kr) \sum_{m=-l}^{l} (-1)^m Y_l^m(\theta, \phi) Y_{l-m}^m(\theta_k, \phi_k). \tag{10.7}
\]

Also, the spherical polar coordinates for the vectors \( \mathbf{r}, \mathbf{k}, \mathbf{R}, \mathbf{R}_1, \) and \( \mathbf{R}_2 \) are written \((r, \theta, \phi), (k, \theta_k, \phi_k), (R, \theta_R, \phi_R), (\mathbf{R}_1, \theta_{\mathbf{R}_1}, \phi_{\mathbf{R}_1}), \) and \((\mathbf{R}_2, \theta_{\mathbf{R}_2}, \phi_{\mathbf{R}_2})\).

**B. OUTLINE OF THE APPROACH**

The use of complex variable theory to evaluate integrals of the type \( I_{ab}(\mathbf{R}) \) and \( I_{cda}(\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}) \) is based on six equations: the Fourier transform inversion and convolution theorems, Eqs. (9.2) and (9.18); Eq. (9.6); the plane wave expansion, Eq. (10.7); the orthogonality of the \( Y_l^m \), Eq. (10.6); and the residue theorem, Eq. (7.1). In each case the fundamental steps are

1. transformation to Fourier transform variable via convolution theorem;
2. introduction of plane wave expansion to bring all angular dependence into spherical harmonics;
3. evaluation of angular integrations by orthogonality formula;
4. manipulation of final radial integration \( \int_0^{\infty} dk \) so as to be able to use the residue theorem.
C. Fourier Transform of a Slater-Type Atomic Orbital

Basic to this application is the FT\{ψ_{nlm}\}(r):

\[ \text{FT}\{ψ_{nlm}(r)\} = \int e^{ik \cdot r} ψ_{nlm}(r) \, dV \]

\[ = \int \sum_{\lambda, \mu} 4πi^2 j_\lambda(kr) Y_\lambda^\mu(\theta_k, \phi_k) Y_\mu^*(θ, φ) r^{n-1} e^{-itr} J_l^m(θ, φ) \, dV \]

\[ = f_{nlm}(k) Y_l^m(\theta_k, \phi_k), \]

\[ f_{nlm}(k) = 4πi^2 \int_0^∞ j_l(kr)r^{n-1}e^{-itr^2} dr \]

\[ = 4πi^2 \int_0^∞ (-k)(k^{-1} d/dk)k^{-1}r^{n-l} \sin kr e^{-itr} dr \]

\[ = 2πi^{l-1}(-k)(k^{-1} d/dk)k^{-1} \]

\[ \times \int_0^∞ r^{n-l}[\exp(-((ζ + ik)r) - \exp(-((ζ - ik)r)] dr \]

\[ = 2πi^{l-1}(n - l)(-k)(k^{-1} d/dk)k^{-1} \]

\[ \times [(ζ - ik)^{l-1-n} - (ζ + ik)^{l-1-n}]. \]

At this stage it is unnecessary to carry out the differentiations in Eq. (10.14). Rayleigh's formula for \( j_l(kr) \) and the definition of \( I(n - l + 1) \) were used in Eqs. (10.12) and (10.14). Note that the order of integration and differentiation was interchanged in Eqs. (10.12) and (10.13). Here and subsequently, we leave the justification to the reader.

D. Two-Center Overlap-Type Integral

The integrals are named in part by the number of distinct atomic centers. The one-center integrals, characterized by \( R_1 = R_2 = R = 0 \), present no problem and are not discussed here. The simplest two-center integral is Eq. (10.1) with \( A = 1 \), and \( ψ_a \) and \( ψ_b \) both with \( n = 1 \), \( l = m = 0 \) [Eq. (10.3)]. We compute the "overlap integral"

\[ I_{ab} = \int ψ_{100l}^*(r) ψ_{100l}(r - R) \, dV. \]

In the course of computing \( I_{ab} \), we are led to consider four special functions of the confluent hypergeometric family.
Via the convolution theorem, Eq. (9.8), and Eqs. (9.6), (10.10), and (10.14), one obtains

\[
I_{ab} = (2\pi)^{-3} \int \mathcal{F}^{*}\{\psi_{100z_a}(r)\} \mathcal{F}\{\psi_{100z_b}(r - R)\} \, d^3k
\]  
(10.16)

\[
= (2\pi)^{-3} \int e^{ik \cdot R} \mathcal{F}^{*}\{\psi_{100z_a}(r)\} \mathcal{F}\{\psi_{100z_b}(r)\} \, d^3k
\]  
(10.17)

\[
= (2\pi)^{-3} \int e^{ik \cdot R} f_{10z_a}^*(k)f_{10z_b}(k)(Y_0^0)^2 \, d^3k.
\]  
(10.18)

We use the plane wave expansion, the orthonormality of the \(Y_{jm}\), and that \(Y_0^0 = (4\pi)^{-1/2}\), to obtain

\[
I_{ab} = (2\pi)^{-3} \int_0^\infty j_0(kR) 2\pi k^{-1}[\zeta_a - ik)^2 - (\zeta_a + ik)^2]^* \times [2\pi k^{-1}[\zeta_b - ik)^2 - (\zeta_b + ik)^2]k^2 \, dk
\]  
(10.19)

\[
= -2\pi k^{-1} \int_0^\infty \frac{\sin(kR)}{kR} \times [(\zeta_a - ik)^2 - (\zeta_a + ik)^2][2\pi k^{-1}[\zeta_b - ik)^2 - (\zeta_b + ik)^2] \, dk.
\]  
(10.20)

Since the integrand is an even function of \(k\), Eq. (10.20) can be written as a special case of Eq. (7.3) (note that the integrand is not singular at \(k = 0\)):

\[
I_{ab} = -\frac{1}{4\pi i} \int_{-\infty}^{\infty} e^{ikR(kR)^{-1}}[(\zeta_a - ik)^2 - (\zeta_a + ik)^2] \times [(\zeta_b - ik)^2 - (\zeta_b + ik)^2] \, dk
\]  
(10.21)

\[
= -\frac{1}{2} \sum \{\text{residues at } k = i\zeta_a, i\zeta_b\}
\]  
(10.22)

\[
= \frac{1}{2}(\partial/\partial \zeta_a) \exp(-\zeta_a R)(\zeta_a R)^{-1}[(\zeta_b + \zeta_a)^2 - (\zeta_b - \zeta_a)^2] + (\partial/\partial \zeta_b) \exp(-\zeta_b R)(\zeta_b R)^{-1}[(\zeta_a + \zeta_b)^2 - (\zeta_a - \zeta_b)^2],
\]  
(10.23)

\[
= -\frac{i}{2}(d/d\zeta_a)^8 \exp(-\zeta_a R)(\zeta_a R)^{-1} + (d/d\zeta_a) \exp(-\zeta_a R)(\zeta_a R)^{-1}(\zeta_a + \zeta_b)^2, \quad \zeta_a = \zeta_b.
\]  
(10.24)

The cases for more general values of the atomic orbital parameters work out similarly (Silverstone, 1966).

Despite the simplicity of the derivation of Eqs. (10.23) and (10.24), these equations do not exhibit clearly the behavior of \(I_{ab}(R)\) when either
3. Complex Variable Theory

$R \sim 0$ or $\zeta_a \sim \zeta_b$. An alternative approach, involving the exponential-type integral functions $\alpha_n$ and $\delta_n$, gives a more transparent formula (Todd, Kay, and Silverstone, 1970).

1. The Functions $\alpha_n(z)$ and $\delta_n(z)$

Define $\alpha_n(z)$ (Abramowitz and Stegun, 1964) and $\delta_n(z)$ (Silverstone, 1968a) by

$$\alpha_n(z) = \int_1^\infty t^n e^{-zt} \, dt = \sum_{k=0}^{n} \frac{n!}{(n-k)!} z^{-k-1} e^{-z}, \quad n = 0, 1, 2, \ldots \tag{10.25}$$

$$\delta_n(z) = -\int_0^1 t^n e^{-zt} \, dt = -\sum_{k=0}^{\infty} \frac{(-z)^k}{k!(n+k+1)}, \quad n = 0, 1, 2, \ldots \tag{10.26}$$

$$= \alpha_n(z) - n! / z^{n+1}. \tag{10.27}$$

$\delta_n(z)$ is an entire function of $z$ [Eq. (10.26)], while $\alpha_n(z)$ has a pole of order $n+1$ at the origin [Eq. (10.27)]. As $z \sim \infty$, $\alpha_n(z) \sim z^{-1} e^{-z}$ [Eq. (10.25)].

2. Alternative Formula

Returning to Eq. (10.20), we use the evenness of the integrand and Eq. (10.27) to write

$$I_{ab} = (2\pi)^{-1} \int_{-\infty}^{\infty} (kR)^{-1} \sin kR \left( (\zeta_a + ik)^{-2} - (\zeta_b - ik)^{-2} \right) \, dk$$

$$= (2\pi)^{-1} \int_{-\infty}^{\infty} k^{-1} R \sin kR \left\{ \alpha_1[(\zeta_a + ik)R] - \delta_1[(\zeta_a + ik)R] \right\}$$

$$\times \left[ (\zeta_b - ik)^{-2} - (\zeta_b + ik)^{-2} \right] \, dk \tag{10.28}$$

$$= (2\pi)^{-1} \int_{-\infty}^{\infty} k^{-1} R \sin kR \alpha_1[(\zeta_a + ik)R][(\zeta_b - ik)^{-2} - (\zeta_b + ik)^{-2}] \, dk$$

$$- (2\pi)^{-1} \int_{-\infty}^{\infty} k^{-1} R (-2i)^{-1} e^{-ikR} \delta_1[(\zeta_a + ik)R]$$

$$\times \left[ (\zeta_b - ik)^{-2} - (\zeta_b + ik)^{-2} \right] \, dk$$

$$- (2\pi)^{-1} \int_{-\infty}^{\infty} k^{-1} R (2i)^{-1} e^{ikR} \alpha_1[(\zeta_a + ik)R]$$

$$\times \left[ (\zeta_b - ik)^{-2} - (\zeta_b + ik)^{-2} \right] \, dk. \tag{10.29}$$

The integrands of the first two terms are bounded in the lower half-plane, and the third integrand is bounded in the upper half-plane. Closing the
contour at \( \infty \) in the appropriate half-plane, we evaluate each via the residue theorem. The poles inside the contour are either at \( k = i\zeta_b \) or \( k = -i\zeta_b \). The result is

\[
I_{ab} = \left( \frac{d}{d\zeta_b} \right) R \zeta_b^i \sin(i\zeta_b R) \alpha_1[(\zeta_a + \zeta_b)R] \\
- \frac{1}{2} \left( \frac{d}{d\zeta_b} \right) \zeta_b^{-1} \exp(-\zeta_b R) \hat{a}_1[(\zeta_a + \zeta_b)R] \\
+ \frac{1}{2} \left( \frac{d}{d\zeta_b} \right) \zeta_b^{-1} \exp(-\zeta_b R) \hat{a}_1[(\zeta_a - \zeta_b)R],
\]

(10.31)

\[
= -(d/d\zeta_b) R \zeta_b^{-1} \sinh(\zeta_b R) \alpha_1[(\zeta_a + \zeta_b)R] \\
-(d/d\zeta_b) R \zeta_b^{-1} \exp(-\zeta_b R) \hat{a}_1[(\zeta_a + \zeta_b)R] - \hat{a}_1[(\zeta_a - \zeta_b)R].
\]

(10.32)

Before taking the \((d/d\zeta_b)\) explicitly, we introduce two more functions.

3. Modified Spherical Bessel Functions

Still more concise formulas are obtained by introducing the modified spherical Bessel functions, \( \mathcal{K}_i \) and \( \mathcal{T}_i \):

\[
\mathcal{K}_i(z) = (-z)^i(z^{-1} d/dz)^i z^{-1} e^{-z}
\]

(10.33)

\[
= \sum_{m=0}^{l} ((l + m)!/(l - m)!(2m)!!) z^{-m-1} e^{-z}
\]

(10.34)

\[
\mathcal{T}_i(z) = z^i(z^{-1} d/dz)^i z^{-1} \sinh z = \sum_{m=0}^{\infty} \frac{z^{i+2m}}{(2l + 2m + 1)!!(2m)!!}
\]

(10.35)

\[
= i^{-l} j_i(i z)
\]

(10.36)

\[
= -\frac{1}{2} \left[ \mathcal{K}_i(-z) + (-1)^i \mathcal{K}_i(z) \right].
\]

(10.37)

With \( \mathcal{K}_i \) and \( \mathcal{T}_i \), \( I_{ab} \) becomes

\[
I_{ab} = -R^3 \left( \frac{d}{d\zeta_b} \right) (\mathcal{O}_0(\zeta_b R) \alpha_1[(\zeta_a + \zeta_b)R] \\
+ \mathcal{K}_0(\zeta_b R) \frac{1}{2} \{ \hat{a}_1[(\zeta_a + \zeta_b)R] - \hat{a}_1[(\zeta_a - \zeta_b)R] \})
\]

(10.38)

\[
= R^3 \mathcal{O}_0(\zeta_b R) \alpha_1[(\zeta_a + \zeta_b)R] - R^3 \mathcal{K}_1(\zeta_b R) \alpha_1[(\zeta_a + \zeta_b)R] \\
+ R^3 \mathcal{O}_0(\zeta_b R) \frac{1}{2} \{ \hat{a}_1[(\zeta_a + \zeta_b)R] + \hat{a}_1[(\zeta_a - \zeta_b)R] \} \\
+ R^3 \mathcal{K}_1(\zeta_b R) \frac{1}{2} \{ \hat{a}_1[(\zeta_a + \zeta_b)R] - \hat{a}_1[(\zeta_a - \zeta_b)R] \}.
\]

(10.39)

E. Fourier Transform of a Two-Center Product

The more complicated integrals represented by Eqs. (10.1) and (10.2) involve the Fourier transform

\[
G_{ab}(\mathcal{K}, \mathcal{R}) = \text{FT}\{\psi_a^*(\mathcal{R})\psi_b(\mathcal{R} - \mathcal{R})\}
\]

(10.40)

\[
= \int e^{i\mathcal{K} \cdot \mathcal{R}} \psi_a^*(\mathcal{R}) \psi_b(\mathcal{R} - \mathcal{R}) dV.
\]

(10.41)
We evaluate a simple case that illustrates the general considerations involved: We take $n_a = n_b = 1$, $l_a = m_a = l_b = m_b = 0$. Then

$$G_{ab}(k, R) = \int e^{ik \cdot r} \psi_{100}^* (r) \psi_{100} (r - R) \, dV$$

$$= (4\pi)^{-1} \int e^{ik \cdot r} \exp(-\zeta_a |r|) \exp(-\zeta_b |r - R|) \, dV.$$  

The functional dependence on $|r|$ and $|r - R|$ is somewhat inconvenient. A more convenient form is obtained at the cost of an infinite series. The $\exp(-\zeta_b |r - R|)$ is expanded in $Y_i^m(\theta, \phi)$ and functions of $r$:

$$\exp(-\zeta_b |r - R|) = \sum_{l=0}^{\infty} \nu_l (r, R) \sum_{m=-l}^{l} (-1)^m Y_l^{-m}(\theta, \phi) Y_l^m(\theta, \phi).$$

$$\nu_l (r, R) = 4\pi \left( -\frac{d}{d\zeta_b} \right) \zeta_b \mathcal{I}_l (\zeta_b r) \mathcal{H}_l (\zeta_b R), \quad r < R$$

$$= 4\pi \left( -\frac{d}{d\zeta_b} \right) \zeta_b \mathcal{I}_l (\zeta_b R) \mathcal{H}_l (\zeta_b r), \quad R < r.$$ 

A most straightforward way to derive this and similar expansions is via the inverse Fourier transform (Silverstone, 1967; Kay, Todd, and Silverstone, 1969a,b)

$$\exp(-\zeta_b |r - R|) = (2\pi)^{-3} \int \exp(-ik \cdot (r - R)) \text{FT}\{\exp(-\zeta_b r)\} \, dk$$

$$= (2\pi)^{-3} \int \{ \sum_{l_1, m_1} 4\pi i^{-l_1} j_{l_1} (kr) Y_{l_1}^{m_1} (\theta, \phi) Y_{l_1}^{-m_1} (\theta_k, \phi_k) \}

\{ \sum_{l_2, m_2} 4\pi i^{l_2} j_{l_2} (kR) (-1)^{m_2} Y_{l_2}^{-m_2} (\theta, \phi) \}

\times Y_{l_2}^{m_2} (\theta_k, \phi_k) \, f_{100} (k) \, dk$$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (-1)^m Y_l^{-m}(\theta, \phi) Y_l^m(\theta, \phi) \nu_l (r, R)$$

$$\nu_l (r, R) = (2/\pi) \int_0^{\infty} j_l (kr) j_l (kR) 2\pi i^{-l} \, dk$$

$$\times [(\zeta_b - ik)^{-2} - (\zeta_b + ik)^{-2}] k^2 \, dk.$$
Equation (10.50) is of a type similar to Eq. (7.3). When $\mathcal{R} > r$, we write [via Eq. (8.145) and the evenness of the integrand of Eq. (10.50)]

$$
\psi_1(r, \mathcal{R}) = -2 \int_{-\infty}^{\infty} (-\mathcal{R}) (\mathcal{R}^{-1} d/d\mathcal{R}) \mathcal{R}^{-1} e^{ik\mathcal{R}} k^{-1} j_1(kr) \\
\times [(\zeta_b - ik)^{-2} - (\zeta_b + ik)^{-2}] dk.
$$

(10.51)

We close the contour at $\infty$ in the upper half-plane and take $2\pi i \times$ residue at $k = i\zeta_b$:

$$
\psi_1(r, \mathcal{R}) = -4\pi (-\mathcal{R}) (\mathcal{R}^{-1} d/d\mathcal{R}) \mathcal{R}^{-1} (d/d\zeta_b) \exp(-\zeta_b \mathcal{R})(i\zeta_b)^{-1} \\
\times j_1(i\zeta_b r) \\
= 4\pi (-d/d\zeta_b) \zeta_b \mathcal{K}_1(\zeta_b \mathcal{R}) \mathcal{I}_1(\zeta_b r), \quad \mathcal{R} > r.
$$

(10.52)

(10.53)

When $\mathcal{R} < r$, Eq. (10.46) results.

With the expansion (10.44), the Fourier transform of Eq. (10.43) reduces to a sum of one-dimensional integrals

$$
G_{ab}(k, \mathcal{R}) = (4\pi)^{-1} \int e^{ik \cdot r} \exp(-\zeta_a r) \sum_{l,m} \psi_1(r, \mathcal{R})(-1)^m \\
\times Y_l^m(\theta, \phi) Y_l^m(\theta, \phi) dV
$$

(10.54)

$$
= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (-1)^m Y_l^m(\theta, \phi) Y_l^m(\theta, \phi) G_1(k, \mathcal{R})
$$

(10.55)

$$
G_1(k, \mathcal{R}) = i^l \int_0^{\infty} j_1(kr) \psi_1(r, \mathcal{R}) \exp(-\zeta_a r) r^2 dr
$$

(10.56)

$$
= 4\pi i (-d/d\zeta_b) \zeta_b \mathcal{K}_1(\zeta_b \mathcal{R}) \int_0^\mathcal{R} j_1(kr) \mathcal{I}_1(\zeta_b r) \exp(-\zeta_a r) r^2 dr \\
+ 4\pi i (-d/d\zeta_b) \zeta_b \mathcal{K}_1(\zeta_b \mathcal{R}) \int_\mathcal{R}^{\infty} j_1(kr) \mathcal{I}_1(\zeta_b r) \\
\times \exp(-\zeta_a r) r^2 dr.
$$

(10.57)

The second integral is readily evaluated with the aid of Rayleigh's formula and the exponential integral (Section VIII.G):

$$
\int_\mathcal{R}^{\infty} j_1(kr) \mathcal{K}_1(\zeta_b r) \exp(-\zeta_a r) r^2 dr
$$

$$
= (-k)^l (k^{-1} d/dk) \mathcal{K}_1^{-1}(\zeta_b) \mathcal{I}_1^{-1}(\zeta_b r) \\
\times \int_\mathcal{R}^{\infty} r^{-2l} \exp(-(\zeta_a + \zeta_b) r) \sin kr dr
$$

(10.58)

$$
= (-k)^l (k^{-1} d/dk) \mathcal{K}_1^{-1}(\zeta_b) \mathcal{I}_1^{-1}(\zeta_b r) \mathcal{R}^{1-2l}(2i)^{-1} \\
\times \{E_{2l}[(\zeta_a + \zeta_b - ik) \mathcal{R}] - E_{2l}[(\zeta_a + \zeta_b + ik) \mathcal{R}]\}. \quad (10.59)
$$
The first integral, if we are careful about the lower limit, can be similarly treated:

\[
\int_0^\infty j_i(kr) J_1(\zeta_b r) \exp(-\zeta_a r) r^2 \, dr \\
= \lim_{\varepsilon \to 0} \int_\varepsilon^\infty j_i(kr) J_1(\zeta_b r) \exp(-\zeta_a r) r^2 \, dr \\
= \lim_{\varepsilon \to 0} (-k)^l (k^{-1} d/dk)^l k^{-1} \zeta_b^{-1} d/d\zeta_b) \zeta_b^{-1} (4i)^{-1} \\
\times r^{1-2l} [E_{2l}[(\zeta_a + \zeta_b - ik)r] - E_{2l}[(\zeta_a - \zeta_b - ik)r] \\
- E_{2l}[(\zeta_a + \zeta_b + ik)r] + E_{2l}[(\zeta_a - \zeta_b + ik)r]] \\
\bigg|_{\varepsilon}^\infty. 
\]

(10.60)

Before taking the limit, we define

\[
\tilde{E}_n(z) = E_n(z) + \frac{(-z)^{n-1}}{(n-1)!} [\log z - \psi(n)]. 
\]

(10.62)

By Eq. (8.165), $\tilde{E}_n(z)$ is an entire function of $z$. Moreover,

\[
r^{1-2l} E_{2l}[(\zeta_a + \zeta_b - ik)r] \\
= r^{1-2l} \tilde{E}_{2l}[(\zeta_a + \zeta_b + ik)r] \\
\bigg|_{\varepsilon}^\infty - \frac{[-(\zeta_a + \zeta_b - ik)]^{2l-1}}{(2l-1)!} \\
\times [\log \varepsilon - \log \varepsilon]; 
\]

(10.63)

that is, the terms in $\log(\zeta_a + \zeta_b - ik)$ cancel. Since

\[
\tilde{p}_{2l-1}(\zeta_b) = (\zeta_a + \zeta_b - ik)^{2l-1} - (\zeta_a - \zeta_b - ik)^{2l-1} \\
- (\zeta_a + \zeta_b + ik)^{2l-1} + (\zeta_a - \zeta_b + ik)^{2l-1} 
\]

(10.64)

is both a polynomial of degree $(2l - 1)$ in $\zeta_b$ and an odd function of $\zeta_b$, one finds that $(\zeta_b^{-1} d/d\zeta_b) \zeta_b^{-1} p_{2l-1}(\zeta_b) = 0$, and that the $E$'s in Eq. (10.61) can be replaced by $\tilde{E}$'s. Finally, since the first $2l$ terms in the series expansion of the four $\tilde{E}$'s vanish because of the $(\zeta_b d/d\zeta_b) \zeta_b^{-1}$, the limit $\varepsilon \to 0$ yields zero for the lower limit. The result for $G_l(h, \mathcal{R})$ is

\[
G_l(h, \mathcal{R}) = 4\pi h^{l-1} d/d\zeta_b) \zeta_b^{-1} d/d\zeta_b) \zeta_b^{-1} \\
\times (-h)^l (k^{-1} d/dk)^l k^{-1} \mathcal{R}^{2l-2l} \\
\times \frac{1}{2} \left( E_{2l}[(\zeta_a + \zeta_b - ik)\mathcal{R}] - E_{2l}[(\zeta_a + \zeta_b + ik)\mathcal{R}] \right) \\
+ 4\pi h^{l-1} \left( d/d\zeta_b) \zeta_b^{-1} d/d\zeta_b) \zeta_b^{-1} \\
\times (-h)^l (k^{-1} d/dk)^l k^{-1} \mathcal{R}^{2l-2l} \\
\times \frac{1}{2} \left( \tilde{E}_{2l}[(\zeta_a + \zeta_b - ik)\mathcal{R}] - \tilde{E}_{2l}[(\zeta_a - \zeta_b - ik)\mathcal{R}] ight) \\
- \tilde{E}_{2l}[(\zeta_a + \zeta_b + ik)\mathcal{R}] + \tilde{E}_{2l}[(\zeta_a - \zeta_b + ik)\mathcal{R}]. 
\]

(10.65)
A convenient shorthand notation is
\[
g^{(2)}(x \pm y) = g(x + y) - g(x - y) \tag{10.66}
g^{(3)}(x \pm y \pm z) = g(x + y + z) - g(x - y + z) - g(x + y - z) + g(x - y - z), \tag{10.67}
\]
\[
[\ldots \mathcal{I}(\xi_b R) \ldots] = (-d/d\xi_b)\xi_b \mathcal{I}(\xi_b R)\xi_b^{-1} d/d\xi_b \xi_b^{-1} R^{1-2i} \tag{10.68}
\]
\[
[\ldots \mathcal{K}(\xi_b R) \ldots] = (-d/d\xi_b)\xi_b \mathcal{K}(\xi_b R)\xi_b^{-1} d/d\xi_b \xi_b^{-1} R^{1-2i}. \tag{10.69}
\]
Then
\[
G_1(k, R) = 4\pi i^{l-1}[\ldots \mathcal{I}(\xi_b R) \ldots] \\
\times k^l(k^{-1} d/dk) k^{-1} E_2^{(i)}[(\xi_a \pm \xi_b \pm ik) R] \\
+ 4\pi i^{l-1}(-1)^l[\ldots \mathcal{K}(\xi_b R) \ldots] \\
\times k^l(k^{-1} d/dk) k^{-1} E_2^{(i)}[(\xi_a \pm \xi_b \pm ik) R]. \tag{10.70}
\]

**F. Evaluation of a (1-2)-Type Three-Center Integral**

The final integral we evaluate in this section is typical of the three- and four-center integrals. Its evaluation involves more details than in the preceding examples, but the basic manipulations are essentially similar. Consider
\[
I_{c,ab}(R, R) = \int \psi_{100c}^+(r_1) r_1^{-1} \psi_{100c}^+(r_2 - R) \psi_{100c}^-(r_2 - R - R) dV_1 dV_2 \tag{10.71}
\]
By Eqs. (9.18) and (9.6),
\[
I_{c,ab}(R, R) = (2\pi)^{-3} \int \text{FT} \{\psi_{100c}^+(r)\} \text{FT} \{r^{-1}\} \\
\times e^{ik \cdot R} \text{FT} \{\psi_{100c}^+(r) \psi_{100c}^-(r - R)\} d^{3k}. \tag{10.72}
\]
Two of the three FTs are given by Eqs. (10.10), (10.14), (10.55), and (10.70); the FT \{r^{-1}\} requires additional comment.
Fourier Transform of $1/r$. \( \text{Straightforwardly one calculates} \)
\[
\text{FT}\{r^{-1}\} = \int e^{ik \cdot r^{-1}} \, dV = 4\pi \int_0^\infty j_0(kr) \, r \, dr \tag{10.73}
\]
\[
= 4\pi k^{-1} \int_0^\infty \sin kr \, dr. \tag{10.74}
\]
Clearly, the usual definition of \(\text{FT}\{f(r)\}\) fails. On the other hand, from Eq. (10.14),
\[
\lim_{\zeta \to 0} \text{FT}\{r^{-1}e^{-\zeta r}\} = \lim_{\zeta \to 0} 2\pi i^{-1}k^{-1}[(\zeta - ik)^{-1} - (\zeta + ik)^{-1}] \tag{10.75}
\]
\[
= 4\pi k^{-2}. \tag{10.76}
\]
Thus we define \(\text{FT}\{r^{-1}\}\) to be
\[
\text{FT}\{r^{-1}\} = \lim_{\zeta \to 0} \text{FT}\{r^{-1}e^{-\zeta r}\} = 4\pi k^{-2}. \tag{10.77}
\]
Note that the inverse Fourier transform of $4\pi k^{-2}$ is $r^{-1}$. A more rigorous justification of Eq. (10.77) can be given in the theory of generalized functions [Chapter 2 of this volume; Lighthill (1958)].

Reduction to a Radial Integration \(\text{Equation (10.72) becomes} \)
\[
I_{e,ab}(\mathcal{R}, \mathcal{P}) = (2\pi)^{-3} \int \{f_{10c}(k)(4\pi)^{-1/2}\} \{4\pi k^{-2}\}
\times \left\{ \sum_{l_1,m_1} 4\pi i^{l_1} j_{l_1}(kR) Y_{l_1}^{m_1}(\theta_R, \phi_R) Y_{l_1}^{m_1*}(\theta_k, \phi_k) \right\}
\times \left\{ \sum_{l_2,m_2} (-1)^{m_2} Y_{-m_2}(\theta_{\mathcal{P}}, \phi_{\mathcal{P}}) Y_{l_2}^{m_2}(\theta_k, \phi_k) G_l(k, \mathcal{P}) \right\} \, d^3k
\tag{10.78}
\]
\[
= \sum_{l=0}^{\infty} \frac{i}{l} \pi^{3/2} (-1)^{m} Y_{l}^{m}(\theta_R, \phi_R) Y_{-l}^{m}(\theta_{\mathcal{P}}, \phi_{\mathcal{P}}) I_{e,ab}^l
\tag{10.79}
\]
\[
I_{e,ab}^l = \pi^{-3/2} \int_0^\infty f_{10c}(k) j_l(kR) G_l(k, \mathcal{P}) \, dk
\]
\[
= \frac{1}{2\pi} \pi^{-3/2} \int_{-\infty}^{\infty} f_{10c}(k) j_l(kR) G_l(k, \mathcal{P}) \, dk. \tag{10.80}
\]
This last integral is like Eq. (7.3), but more complicated. It can readily be evaluated by the residue theorem after closing the contour appropriately at \(\infty\). Note that the various terms in the integrand behave at \(\infty\) like
\[
\{k^{-3}\} \{e^{\pm ikRk^{-1}}\} \{e^{\pm ik\mathcal{P}k^{-1}}\} \tag{10.81}
\]
and

\[
\{k^{-3}\}\left\{e^{i\times k^{-1}}\right\}\{(\zeta_c^{-1}d/d\zeta_c)\zeta_c^{-1}k(-1)^{\zeta_c^{-1}}d/dk)k^{-1}(\zeta_c \pm \zeta_b + ik)^{R-1}
\times \log[\{\zeta_c \pm \zeta_b + ik\}]\}
\]

so that the appropriate half-plane will depend on whether \( R > R \) or \( R < R \). The only singularities of the integrand are second-order poles at \( k = \pm i\zeta_c \), logarithmic branch points at \( k = \pm i(\zeta_a + \zeta_b) \), and a nascent simple pole at the origin. Avoiding the logarithmic branch cuts requires some dexterity.

Via Eqs. (10.14) and (10.70), we put Eq. (10.80) in the form

\[
I_{c,ab} = I_{c,1} + I_{c,2}
\]

\[
I_{c,1} = (-1)^{i+1}4\pi^{-1}\int_{-\infty}^{\infty} k^{-1}[(\zeta_c - ik)^{-2} - (\zeta_c + ik)^{-2}]j_i(kR)
\]
\[
\times \left\{\cdots \mathcal{I}_{i}(\zeta_c R) \cdots \right\}k(-1)^{\zeta_c^{-1}}d/dk)k^{-1}\frac{1}{4}\tilde{E}_2(\zeta_a \pm \zeta_b + ik\zeta_c)\}
\]

\[
I_{c,2} = -4\pi^{-1}\int_{-\infty}^{\infty} k^{-1}[(\zeta_c - ik)^{-2} - (\zeta_c + ik)^{-2}]j_i(kR)
\]
\[
+ \left\{\cdots \mathcal{I}_{i}(\zeta_c R) \cdots \right\}k(-1)^{\zeta_c^{-1}}d/dk)k^{-1}\frac{1}{4}\tilde{E}_2(\zeta_a \pm \zeta_b + ik\zeta_c)\}
\]

\[
(10.84)
\]

**Evaluation of \( I_{c,1} \)** The integrand of \( I_{c,1} \) is an even function of \( k \), so that

\[
I_{c,1} = (-1)^{i+1}4\pi^{-1}\mathcal{P}\int_{-\infty}^{\infty} k^{-1}[(\zeta_c - ik)^{-2} - (\zeta_c + ik)^{-2}]j_i(kR)
\]
\[
\times \left\{\cdots \mathcal{I}_{i}(\zeta_c R) \cdots \right\}k(-1)^{\zeta_c^{-1}}d/dk)k^{-1}\tilde{E}_2(\zeta_a \pm \zeta_b - ik\zeta_c)\}
\]

\[
(10.86)
\]

The \( \mathcal{P} \) arises as in Eqs. (7.55) and (7.56). The integrand of Eq. (10.86) has a simple pole at \( k = 0 \). When \( R > R \), \( \tilde{E}_2[(\zeta_a + \zeta_b - ik\zeta_c)\zeta_c^{-1}+1] \) dominates the behavior at \( \infty \), the contour can be closed at \( \infty \) in the upper half-plane, and the residue theorem gives

\[
I_{c,1} = 2\pi i \times \{(\text{residue at } k = i\zeta_c) + \frac{1}{2} (\text{residue at } k = 0)\}
\]

\[
= \left\{\cdots \mathcal{I}_{i}(\zeta_c R) \cdots \right\}(8(-1)^i(d/d\zeta_c)\mathcal{I}_{i}(\zeta_c R)\zeta_c^{-1+i}
\times \left\{\zeta_c^{-1}d/d\zeta_c)^{\zeta_c^{-1}}E_2[(\zeta_a + \zeta_b + \zeta_c)\zeta_c^{-1}+1}
\times \left\{16\zeta_c^{-3}R^{1}(2l + 1)E_2[(\zeta_a + \zeta_b)\zeta_c^{-1}+1], \quad R > R.
\]

\[
(10.88)
\]
For $I^{1,1}$ when $R > \mathcal{R}$, first add and subtract a term and manipulate as follows:

$$I^{1,1} = (-1)^{i+1}4\pi^{-1} \int_{-\infty}^{\infty} k^{-1}[(\zeta_e - ik)^{-2} - (\zeta_e + ik)^{-2}] j_i(kR)$$

$$\times \left[ \cdots \mathcal{I}_i(\zeta_b \mathcal{R}) \cdots \right] k^{i(k-1)} \frac{d}{dk} k^{-1} [(\zeta_a + \zeta_b = \pm ik) \mathcal{R}]$$

$$- (\mathcal{R}/R)^{2l_1} E_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})]$$

$$+ (\mathcal{R}/R)^{2l_1} E_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] \right] \frac{d}{dk} \right] dk$$

$$= i^{4\pi^{-1}} \mathcal{P} \int_{-\infty}^{\infty} k^{-1}[(\zeta_e - ik)^{-2} - (\zeta_e + ik)^{-2}] \mathcal{I}_i(-ikR)$$

$$\times \left[ \cdots \mathcal{I}_i(\zeta_b \mathcal{R}) \cdots \right] k^{i(k-1)} \frac{d}{dk} k^{-1} [(\zeta_a + \zeta_b = \pm ik) \mathcal{R}]$$

$$- (\mathcal{R}/R)^{2l_1} E_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] + (-1)^{i+1} 4\pi^{-1}$$

$$\times \mathcal{P} \int_{-\infty}^{\infty} k^{-1}[(\zeta_e - ik)^{-2} - (\zeta_e + ik)^{-2}] j_i(kR) \left[ \cdots \mathcal{I}_i(\zeta_b \mathcal{R}) \cdots \right]$$

$$\times k^{i(k-1)} \frac{d}{dk} k^{-1} (\mathcal{R}/R)^{2l_1} E_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] \right]$$

$$= i^{4\pi^{-1}} \mathcal{P} \int_{-\infty}^{\infty} k^{-1} [(\zeta_a + \zeta_b = \pm ik) \mathcal{R}] - (\mathcal{R}/R)^{2l_1} E_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})]$$

$$= (k^{-1} \frac{d}{dk}) k^{-1} \left[ \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] - (\mathcal{R}/R)^{2l_1} \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] \right]$$

$$= (k^{-1} \frac{d}{dk}) k^{-1} \left[ \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] - (\mathcal{R}/R)^{2l_1} \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] \right]$$

$$= (k^{-1} \frac{d}{dk}) k^{-1} \left[ \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] - (\mathcal{R}/R)^{2l_1} \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] \right]$$

The behavior at $\infty$ is dominated by $e^{\pm ikR}$. The first integral of Eq. (10.90) can be closed at $\infty$ in the upper half-plane. The subtracted term has been chosen to cancel out the logarithmic branch point at $k = i(\zeta_a + \zeta_b)$, and the residue theorem applies. Indeed, from Eq. (8.165) [cf. Eqs. (10.61)–(10.65)],

$$(k^{-1} \frac{d}{dk}) k^{-1} \left[ \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] - (\mathcal{R}/R)^{2l_1} \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] \right]$$

$$= (k^{-1} \frac{d}{dk}) k^{-1} \left[ \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] - (\mathcal{R}/R)^{2l_1} \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm ik) \mathcal{R})] \right]$$

The second integral vanishes uniformly at $\infty$ and can be treated like $I^{1,1}$ in the $\mathcal{R} > R$ case. The result is

$$I^{1,1} = \left[ \cdots \mathcal{I}_i(\zeta_b \mathcal{R}) \cdots \right] \left[ -8(d/d\zeta_e) \mathcal{I}_i(\zeta_e R) \zeta_e^{-1} \right.$$

$$\times (\zeta_e^{-1} d/d\zeta_e) \zeta_e^{-1} \left[ \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm \zeta_e) \mathcal{R})] - (\mathcal{R}/R)^{2l_1} \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b = \pm \zeta_e) \mathcal{R})] \right.$$

$$+ 8(-1)^{i(l\zeta_e)} \mathcal{I}_i(\zeta_e R) \zeta_e^{-1} (d/d\zeta_e) \zeta_e^{-1} (\mathcal{R}/R)^{2l_1}$$

$$\times \mathcal{E}_{2l_1}[((\zeta_a + \zeta_b + \zeta_e) \mathcal{R})]$$

$$+ 16(2l + 1)^{-1} R^{1-l-1} \mathcal{R}^{2l+1} \mathcal{E}_{2l+1}[((\zeta_a + \zeta_b) \mathcal{R})]$$

$$- \mathcal{R}^{2l+1} \mathcal{E}_{2l+1}[((\zeta_a + \zeta_b) \mathcal{R})]$$

$$+ 16(2l + 1)^{-1} R^{1-l-1} \mathcal{R}^{2l+1} \mathcal{E}_{2l+1}[((\zeta_a + \zeta_b) \mathcal{R})], \quad R > \mathcal{R}.$$
We have used the fact [cf. Eqs. (10.62), (8.160), and (10.25)–(10.27)]

\[-d/dz^{a+m}\hat{E}_n(z) = \hat{\alpha}_m(z).\]  

(10.93)

**Evaluation of \(I^{1,2}\)** When \(R > \mathbb{R}\), the \(e^{\pm ikR}\) dominates the integrand of \(I^{1,2}\), Eq. (10.85). The sequence of steps to evaluate \(I^{1,2}\) is \(j_i(kR) \rightarrow -\mathbb{P}_{-1}^l K_i(-ikR) \rightarrow 2\pi i \times \{\text{residue at } k = i\xi_o + \frac{1}{2} \text{(residue at } k = 0)\}\). The result is

\[
I^{1,2} = \cdots K_i(\xi_b \mathbb{R}) \cdots \{-8(-1)^l i/(d/d\xi_o)K_i(\xi_o R)\xi_o^{-1+1} \\
\times (\xi_o^{-1} d/d\xi_o)\xi_o^{-1+1/2}E_{2l}^{(q)}[(\xi_a \pm \xi_b \pm \xi_o) \mathbb{R}] \\
+ 16(-1)^l i^{-3}(2l + 1)^{-1}R^{-l+1/2}E_{2l+1}^{(q)}[(\xi_a \pm \xi_b \pm \xi_o) \mathbb{R}].\}
\]

(10.94)

When \(\mathbb{R} > R\), \(I^{1,2}\) is analogous to \(I^{1,1}\) with \(R > \mathbb{R}\). The "E part" of the \(\hat{E}\) factors in Eq. (10.85) dominates the \(j_i(kR)\) at \(\infty\), but the "log part" is dominated by the \(j_i(kR)\). We add and subtract a term with \(E_{2l}^{(q)}[(\xi_a \pm \xi_b \mp ik) \mathbb{R}]\) replaced by \((\mathbb{R}/R)^{2l-1}E_{2l}^{(q)}[(\xi_a \pm \xi_b \mp ik)R]\), and note that

\[
(k^{-1} d/dk)^l k^{-1}[E_{2l}^{(q)}[(\xi_a \pm \xi_b \mp ik) \mathbb{R}] - (\mathbb{R}/R)^{2l-1} \\
\times E_{2l}^{(q)}[(\xi_a \pm \xi_b \mp ik)R]] \\
= (k^{-1} d/dk)^l k^{-1}[E_{2l}^{(q)}[(\xi_a \pm \xi_b \mp ik) \mathbb{R}] - (\mathbb{R}/R)^{2l-1} \\
\times E_{2l}^{(q)}[(\xi_a \pm \xi_b \mp ik)R]].
\]

(10.95)

For the moment, we assume that \(\xi_a > \xi_b\), so that the logarithmic branch cuts from \(\pm i(\xi_a - \xi_b)\) to \(\pm i\infty\) do not cross the real axis (the integration path). Then \(I^{1,2}\) becomes

\[
I^{1,2} = 4\pi^{-1} i^{-l} \mathbb{P} \int_{-\infty}^{\infty} k^{-1}[(\xi_o - ik)^{-2} - (\xi_o + ik)^{-2}]K_i(-ikR) \\
\times [\cdots K_l(\xi_b \mathbb{R}) \cdots]k^{l-1} d/dk)k^{-1}(\mathbb{R}/R)^{2l-1} \\
\times \frac{1}{2}E_{2l}^{(q)}[(\xi_a \pm \xi_b \mp ik)R] \, dk \\
- 4\pi^{-1} \mathbb{P} \int_{-\infty}^{\infty} k^{-1}[(\xi_o - ik)^{-2} - (\xi_o + ik)^{-2}]j_i(kR) \\
\times [\cdots K_l(\xi_b \mathbb{R}) \cdots]k^{l-1} d/dk)k^{-1}\frac{1}{2}E_{2l}^{(q)}[(\xi_a \pm \xi_b - ik) \mathbb{R}] \\
- (\mathbb{R}/R)^{2l-1}E_{2l}^{(q)}[(\xi_a \pm \xi_b - ik)R] \, dk.
\]

(10.96)

Both contours can be closed at \(\infty\) in the upper half-plane, and the result
is \(2\pi i \times \{(\text{residue at } k = i\zeta_o) + \frac{1}{2}(\text{residue at } k = 0)\}:

\[ I_{12} = [\cdots \mathcal{H}_i(\zeta_b R) \cdots ](-8(-1)^{l}(d/d\zeta_o)\mathcal{H}_i(\zeta_o R)\zeta_o^{-1+l} \]

\[ \times (\zeta_o^{-1} d/d\zeta_o)\zeta_o^{-1-\frac{1}{2}}(\mathcal{R}/R)^{2l-1}\mathcal{E}_{21}^{(q)}[(\zeta_a \pm \zeta_b \pm \zeta_o)R] \]

\[ + 8(d/d\zeta_o)\mathcal{Y}_i(\zeta_o R)\zeta_o^{1+l}(\zeta_o^{-1} d/d\zeta_o)\zeta_o^{-1-\frac{1}{2}} \]

\[ \times \{\mathcal{E}_{21}^{(p)}[(\zeta_a \pm \zeta_b + \zeta_o)R] - (\mathcal{R}/R)^{2l-1}\mathcal{E}_{21}^{(q)}[(\zeta_a \pm \zeta_b + \zeta_o)R]\} \]

\[ + 16(-1)^{l}\zeta_o^{-3}(2l + 1)^{-1}R^{-l+1}\mathcal{R}^{2l-1}d^i_1[(\zeta_a \pm \zeta_b)R] \]

\[ + 16(-1)^{l}\zeta_o^{-3}(2l + 1)^{-1}R^{-l+1}\frac{1}{2}\mathcal{E}_{21}^{(p)}[(\zeta_a \pm \zeta_b)R] - (\mathcal{R}/R)^{2l-1} \]

\[ \times \mathcal{E}_{21}^{(q)}[(\zeta_a \pm \zeta_b)R]\}, \quad \mathcal{R} > R, \quad (10.97) \]

where

\[ (\zeta_b^{-1} d/d\zeta_b)^{l}\zeta_b^{-1} \]

\[ \times \{\mathcal{E}_{21}^{(p)}[(\zeta_a \pm \zeta_b + \zeta_o)R] - (\mathcal{R}/R)^{2l-1}\mathcal{E}_{21}^{(q)}[(\zeta_a \pm \zeta_b + \zeta_o)R]\} \]

\[ = (\zeta_b^{-1} d/d\zeta_b)^{l}\zeta_b^{-1} \]

\[ \times \{\mathcal{E}_{21}^{(p)}[(\zeta_a \pm \zeta_b + \zeta_o)R] - (\mathcal{R}/R)^{2l-1}\mathcal{E}_{21}^{(q)}[(\zeta_a \pm \zeta_b + \zeta_o)R]\}, \]

\[ \quad (10.98) \]

and similar equations have been used to replace the \(E^{(q)}\)'s by corresponding \(E^{(p)}\)'s in Eq. (10.97). Note that the right side of Eq. (10.97) is analytic at \((\zeta_a - \zeta_b) = 0\). One may infer that the restriction \((\zeta_a > \zeta_b)\) can be removed.

This completes the evaluation of \(I_{c;ab}\), Eq. (10.71).

G. ARBITRARY MULTICENTER INTEGRALS

The specific examples worked above illustrate how complex variable theory can be used in general to evaluate multizcenter integrals in quantum chemistry. The results given contain derivatives that must be dealt with systematically, but this belongs to the realm of ordinary differential calculus, not to complex analysis. The evaluation of the more general cases have been discussed in the references cited at the beginning of this section. The details are indeed more intricate, but the basic principles of the method are the same.
XI. A Formula of Lagrange
and Nondegenerate Perturbation Theory

In a mémoire read in 1770, Lagrange discussed finding roots of equations, and functions of these roots. The solution he gave is easily derived by complex variable theory. The formula itself gives a quick formal solution of Rayleigh-Schrödinger perturbation theory in quantum mechanics, an application discovered by Sack (1969) and by Silverstone and Holloway (1970).

A. Lagrange’s Formula

Let \( C \) be a simple closed curve, and let \( f(z) \) and \( \phi(z) \) both be analytic on and within \( C \). Let \( a \) be inside \( C \), and let \( \zeta = \zeta(t) \) be the only root inside \( C \) of the equation

\[
\zeta = a + t\phi(\zeta), \quad 0 \leq |t| < R. \tag{11.1}
\]

Lagrange’s formula is the expansion

\[
f(\zeta) = f(a) + \sum_{n=1}^{\infty} t^n (n!)^{-1} (d/d\alpha)^{n-1} \{ f'(a) [\phi(a)]^n \}. \tag{11.2}
\]

Derivation By assumption \( z - a - t\phi(z) \) has a simple zero at \( z = \zeta \), so that \( (1 - t\phi'(z))/(z - a - t\phi(z)) \) has a simple pole at \( z = \zeta \) (cf. Section VI.A). The Laurent series about \( z = \zeta \) is

\[
\frac{1 - t\phi'(z)}{z - a - t\phi(z)} = \frac{1}{z - \zeta} + \left[ -\frac{1}{2} \frac{t\phi''(\zeta)}{1 - t\phi'('\zeta)} \right] + \ldots. \tag{11.3}
\]

[\( 1 - t\phi'(\zeta) \neq 0 \), since \( \zeta \) is a simple zero.] By Cauchy’s theorem, the residue theorem, and integration by parts,

\[
f(\zeta) - f(a) = (2\pi i)^{-1} \int_{C} f(z) \left[ \frac{1 - t\phi'(z)}{z - a - t\phi(z)} - \frac{1}{z - a} \right] dz \tag{11.4}
\]

\[
= -(2\pi i)^{-1} \int_{C} f'(z) \log \left[ 1 - t \frac{\phi(z)}{z - a} \right] dz. \tag{11.5}
\]

For small enough \( t \),

\[
f(\zeta) - f(a) = (2\pi i)^{-1} \int_{C} \sum_{n=1}^{\infty} (1/n)t^n [\phi(z)/(z - a)]^n f'(z) dz \tag{11.6}
\]
and
\[ f(\zeta) = f(a) + \sum_{n=1}^{\infty} t^n (n!)^{-1} (d/d\zeta)^{n-1} \left\{ f'(a) [\phi(a)]^n \right\}, \] (11.7)

by the theorem of Section V.C on the integration of uniformly convergent series and by the residue theorem.

B. NONDEGENERATE PERTURBATION THEORY

This final section is intended only for the reader familiar with the formalism of quantum mechanics.

A standard quantum mechanical problem is to solve the eigenvalue equation
\[ H | \psi \rangle = E | \psi \rangle, \] (11.8)

where \( H \) is a Hermitian operator, \( E \) an eigenvalue, and \( | \psi \rangle \) the corresponding eigenvector. Perturbation theory refers to methods treating \( H \) as a perturbation of a Hermitian operator whose eigenvalue and eigenvector are known:
\[ H = H^{(0)} + \lambda V \] (11.9)
\[ (H^{(0)} - E^{(0)}) | \psi^{(0)} \rangle = 0 \] (11.10)
\[ \lim_{\lambda \to 0} | \psi \rangle = | \psi^{(0)} \rangle. \] (11.11)

We denote by \( Q \) the projection operator
\[ Q = 1 - | \psi^{(0)} \rangle \langle \psi^{(0)} |. \] (11.12)

We further assume that \( E^{(0)} \) is a nondegenerate eigenvalue of \( H^{(0)} \), and that \( E \) is a nondegenerate eigenvalue of \( H \). In particular, the operator \( Q/(E^{(0)} - H^{(0)}) \),
\[ Q \] (11.13)

exists. In the equations that follow, all quantities are assumed to exist, and all series to converge.

The Brillouin–Wigner series for \( E \) and \( \psi \) are
\[ E = E^{(0)} + \sum_{\ell=0}^{\infty} \langle \psi^{(0)} | \lambda V \left[ \frac{Q}{E - H^{(0)}} \lambda V \right]^k | \psi^{(0)} \rangle \] (11.14)
\[ \psi = \sum_{\ell=0}^{\infty} \left[ \frac{Q}{E - H^{(0)}} \lambda V \right]^k | \psi^{(0)} \rangle \] (11.15)
where Eq. (11.14) must first be solved for \( E \), then its solution used in Eq. (11.15). Note that Eq. (11.14) has the same form as Eq. (11.1) with \( z = E, \ a = E^{(0)} \), and

\[
\phi(z) = \sum_{k=0}^{\infty} \langle \psi^{(0)} \big| \lambda V \left[ \frac{O}{E - H^{(0)}} \right]^k \big| \psi^{(0)} \rangle.
\]

The Rayleigh–Schrödinger series for \( E \) and \( \psi \) are the power series expansions in \( \lambda \):

\[
E = \sum_{n=0}^{\infty} \lambda^n E^{(n)}
\]

\[
|\psi\rangle = \sum_{n=0}^{\infty} \lambda^n |\psi^{(n)}\rangle.
\]

The explicit form of the \( E^{(n)} \) and \( |\psi^{(n)}\rangle \) can be obtained from the Brillouin–Wigner series by first applying Lagrange’s formula

\[
E = E^{(0)} + \sum_{n=1}^{\infty} (n!)^{-1} \left( \frac{d}{dE^{(0)}} \right)^{n-1} \times \left\{ \sum_{k=0}^{\infty} \langle \psi^{(0)} \big| \lambda V \left[ \frac{O}{E^{(0)} - H^{(0)}} \right]^k \big| \psi^{(0)} \rangle \right\}^n
\]

\[
|\psi\rangle = \sum_{k=0}^{\infty} \left[ \frac{O}{E^{(0)} - H^{(0)}} \lambda V \right]^k |\psi^{(0)}\rangle
\]

\[
+ \sum_{n=1}^{\infty} (n!)^{-1} \left( \frac{d}{dE^{(0)}} \right)^{n-1} \left\{ \left[ \frac{d}{dE^{(0)}} \right] \sum_{k=0}^{\infty} \left[ \frac{O}{E^{(0)} - H^{(0)}} \lambda V \right]^k |\psi^{(0)}\rangle \right\} \times \left\{ \sum_{k=0}^{\infty} \langle \psi^{(0)} \big| \lambda V \left[ \frac{O}{E^{(0)} - H^{(0)}} \right]^k \big| \psi^{(0)} \rangle \right\}^n.
\]

Then use the multinomial expansion

\[
(x_1 + x_2 + \cdots)^n = \sum_{\sigma_1 + \sigma_2 + \cdots = n} \frac{n!}{\sigma_1! \sigma_2! \cdots} x_{1}^{\sigma_1} x_{2}^{\sigma_2} \cdots,
\]

and collect terms having the same power of \( \lambda \). We use the abbreviations

\[
R^{-1} = \frac{O}{E^{(0)} - H^{(0)}}
\]

\[
\langle V \rangle = \langle \psi^{(0)} \big| V \big| \psi^{(0)} \rangle
\]

\[
\langle \cdots \rangle = \langle \psi^{(0)} \big| \cdots \big| \psi^{(0)} \rangle.
\]
Note that
\[
\left( -\frac{d}{dE^{(0)}} \right)^n R^{-1} = n! \frac{Q}{(E^{(0)} - H^{(0)})^{n+1}} = n! R^{-n-1}.
\] (11.24)

The rearranged series are then
\[
E = E^{(0)} + \sum_{N=1}^{\infty} \lambda^N \sum_{\sigma_1+2\sigma_2+3\sigma_3+\cdots=N} \frac{(d/dE^{(0)})^{-1+\sigma_1+\sigma_2+\sigma_3+\cdots}}{\sigma_1!\sigma_2!\sigma_3! \cdots} \\
\times \langle V \rangle^{\sigma_1} \langle VR^{-1}V \rangle^{\sigma_2} \langle VR^{-1}VR^{-1}V \rangle^{\sigma_3} \cdots
\] (11.25)
\[
= E^{(0)} + \lambda \langle V \rangle + \lambda^2 \langle VR^{-2}V \rangle \\
+ \lambda^3 (\langle VR^{-1}VR^{-1}V \rangle - \langle V \rangle \langle VR^{-2}V \rangle) + \cdots
\] (11.26)

\[ |\psi\rangle = |\psi^{(0)}\rangle + \sum_{N=1}^{\infty} \lambda^N \{ (R^{-1}V)^N \langle V | \psi^{(0)} \rangle \\
+ \sum_{j=1}^{N-1} \sum_{\sigma_1+2\sigma_2+3\sigma_3+\cdots=N-j} \frac{(d/dE^{(0)})^{-1+\sigma_1+\sigma_2+\sigma_3+\cdots}}{\sigma_1!\sigma_2!\sigma_3! \cdots} \\
\times [ \langle V \rangle^{\sigma_1} \langle VR^{-1}V \rangle^{\sigma_2} \langle VR^{-1}VR^{-1}V \rangle^{\sigma_3} \cdots \\
\times (d/dE^{(0)})(R^{-1}V)^j \langle V | \psi^{(0)} \rangle ] \}
\] (11.27)
\[
= |\psi^{(0)}\rangle + \lambda R^{-1}V |\psi^{(0)}\rangle \\
+ \lambda^2 [R^{-1}VR^{-1}V |\psi^{(0)}\rangle - \langle V \rangle R^{-2}V |\psi^{(0)}\rangle ] + \cdots
\] (11.28)

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**Special References**


