Notes on Mathematical Methods in Physics

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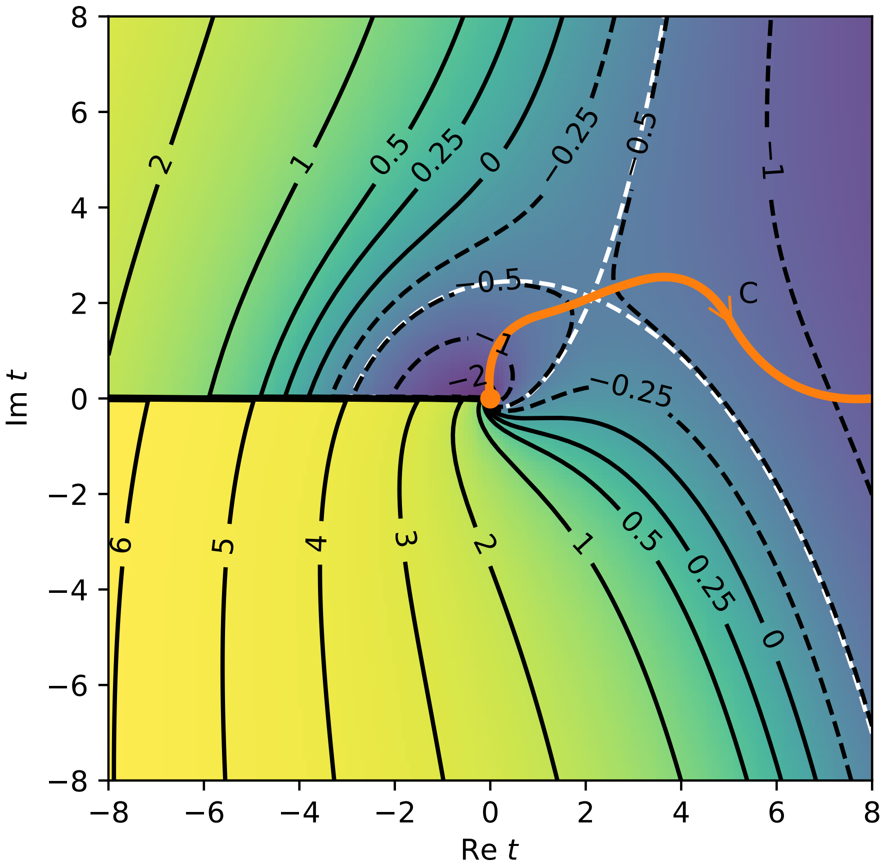

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Preface

These lecture notes are designed for a one-semester introductory graduate-level course in mathematical methods for Physics. The goal is to cover mathematical topics that will be needed in other core graduate-level Physics courses such as Classical Mechanics, Quantum Mechanics, and Electrodynamics. It is assumed that the student will have had undergraduate level courses in linear algebra, calculus, ordinary differential equations, partial differential equations, and complex analysis. However, each module in these notes begins at a point that is hopefully "too easy" — i.e., already covered in the undergraduate courses — and progresses to more advanced material.

These notes are based heavily on the book *Mathematical Methods of Physics* (2nd edition) by Jon Mathews and R. L. Walker (Addison-Wesley, 1970). Additional material was drawn from *Mathematical Methods for Physicists* (3rd edition) by George Arfken (Academic Press, 1985) and *Complex Variables and Applications* (5th edition) by Ruel V. Churchill and James Ward Brown.

Module I

Infinite Series

Motivation

In physics problems we often encounter infinite series. Sometimes we want to expand functions in power series, e.g., when we want to evaluate complex functions for small arguments. Sometimes we have solutions in the form of an infinite series and we want to sum the series.

This module reviews techniques for determining if a series will converge, for summing series, and recaps certain familiar series that are commonly encountered.

1 Geometric Series

The **geometric series** is

$$\boxed{\sum_{n=0}^{\infty} x^n = 1 + x + x^2 + x^3 + x^4 + \cdots.} \tag{1.1}$$

This series can be summed: consider

$$f(x) = 1 + x + x^2 + x^3 + x^4 + \cdots. \tag{1.2}$$

$$x\,f(x) = \quad x + x^2 + x^3 + x^4 + \cdots \tag{1.3}$$

and subtract the second equation from the first:

$$(1 - x)f(x) = 1. \tag{1.4}$$

If $x \neq 1$ then

$$f(x) = \frac{1}{1-x} \tag{1.5}$$

$$= 1 + x + x^2 + x^3 + x^4 + \cdots. \tag{1.6}$$

We'll see that the second equality holds only for $|x| < 1$.

We see geometric series in repeating fractions:

$$y = 0.345\,345\,345\cdots \tag{1.7a}$$

$$= 0.345 \cdot \left\{1 + \frac{1}{1000} + \frac{1}{(1000)^2} + \cdots\right\} \tag{1.7b}$$

$$= 0.345 \cdot \left(\frac{1}{1 - \frac{1}{1000}}\right) \tag{1.7c}$$

$$= 0.345 \cdot \frac{1000}{999} \tag{1.7d}$$

$$= \frac{345}{999}. \tag{1.7e}$$

The geometric series only **converges** for $|x| < 1$.
Consider, e.g., $x = 2$:

$$\frac{1}{1-2} = \underbrace{-1}_{\substack{\text{negative}\\ \text{number}}} \stackrel{?}{=} \underbrace{1+2+4+8+\cdots}_{\substack{\text{ever increasing}\\ \text{positive numbers}}} \tag{1.8}$$

therefore we see that

$$f(x) = 1 + x + x^2 + x^3 + x^4 + \cdots \tag{1.9}$$

is only valid for $|x| < 1$ (where it converges).
However, everywhere within this domain,

$$f(x) = \frac{1}{1-x}, \quad |x| < 1 \tag{1.10}$$

but the expression $(1-x)^{-1}$ is actually valid everywhere except $x = 1$.
Therefore we say that

$$g(x) = \frac{1}{1-x} \tag{1.11}$$

is the **analytic continuation** of the function

$$f(x) = \sum_{n=0}^{\infty} x^n, \quad |x| < 1. \tag{1.12}$$

We will talk more about analytic continuation in the section on complex analysis.

We can easily derive other infinte series from the geometric series:

- Let $x \to -x$:

$$\frac{1}{1+x} = 1 - x + x^2 - x^3 + \cdots \tag{1.13}$$

  which is an **alternating series**.

- Let $x \to x^2$:

$$\frac{1}{1-x^2} = 1 + x^2 + x^4 + x^6 + \cdots . \tag{1.14}$$

2 Convergence

An infinte series

$$\sum_{n=1}^{\infty} a_n = a_1 + a_2 + a_3 + \cdots \tag{2.1}$$

is said to **converge** to the sum S provided the sequence of partial sums has the limit S:

$$\lim_{N\to\infty} \sum_{n=1}^{N} a_n = S\,. \tag{2.2}$$

The series is said to **converge absolutely** if the related series

$$\sum_{n=1}^{\infty} |a_n| \tag{2.3}$$

converges.

Ex. 2.1. The geometric series has partial sums

$$S_N = \sum_{n=0}^{N} x^n = 1 + x + x^2 + \cdots + x^N \tag{2.4a}$$

$$x\,S_N = \qquad x + x^2 + \cdots + x^N + x^{N+1} \tag{2.4b}$$

subtract:

$$(1-x)S_N = \quad 1 - x^{N+1}\,. \tag{2.4c}$$

- If $x = 1$ then $S_N = N + 1$ which diverges in the limit $N \to \infty$.
- If $x \neq 1$ then

$$S_N = \frac{1 - x^{N+1}}{1 - x}\,. \tag{2.5}$$

Then, in the limit $N \to \infty$,

$$\lim_{N\to\infty} S_N = \frac{1}{1-x} - \frac{x}{1-x} \lim_{N\to\infty} x^N \tag{2.6}$$

note: $x^N \to 0$ as $N \to \infty$ for $-1 < x < 1$

$$\therefore \lim_{N\to\infty} S_N = \frac{1}{1-x} \quad \text{for } |x| < 1 \tag{2.7}$$

otherwise the series diverges.

Ex. 2.2. The alternating series

$$1-\frac{1}{2}+\frac{1}{3}-\frac{1}{4}+\cdots \tag{2.8}$$

converges. To see this, note that

$$S_{2N}=\left(1-\frac{1}{2}\right)+\left(\frac{1}{3}-\frac{1}{4}\right)+\cdots+\left(\frac{1}{2N-1}-\frac{1}{2N}\right)>0 \tag{2.9}$$

since each term in parentheses is positive, but also

$$S_{2N}=1-\left(\frac{1}{2}-\frac{1}{3}\right)-\left(\frac{1}{4}-\frac{1}{5}\right)-\cdots-\left(\frac{1}{2N-2}-\frac{1}{2N-1}\right)-\frac{1}{2N}<1 \tag{2.10}$$

since each term in parentheses is positive. Therefore

$$0<\lim_{N\to\infty} S_{2N}<1. \tag{2.11}$$

Also

$$\lim_{N\to\infty} S_{2N+1}=\lim_{N\to\infty}\left(S_{2N}+\frac{1}{2N+1}\right)=\lim_{N\to\infty} S_{2N} \tag{2.12}$$

so the partial sums converge as $N\to\infty$.

However this alternating series does *not* converge absolutely because the series

$$1+\frac{1}{2}+\frac{1}{3}+\frac{1}{4}+\cdots \tag{2.13}$$

diverges:

$$S_N=\sum_{n=1}^{N}\frac{1}{n} \qquad \text{(harmonic series)} \tag{2.14a}$$

$$S_1=1 \tag{2.14b}$$

$$S_2=1+\frac{1}{2} \tag{2.14c}$$

$$S_4=1+\frac{1}{2}+\left(\frac{1}{3}+\frac{1}{4}\right) \tag{2.14d}$$

$$>1+\frac{1}{2}+\left(\frac{1}{4}+\frac{1}{4}\right) \tag{2.14e}$$

$$=1+\frac{2}{2} \tag{2.14f}$$

$$S_8=1+\frac{1}{2}+\left(\frac{1}{3}+\frac{1}{4}\right)+\left(\frac{1}{5}+\frac{1}{6}+\frac{1}{7}+\frac{1}{8}\right) \tag{2.14g}$$

$$>1+\frac{1}{2}+\left(\frac{1}{4}+\frac{1}{4}\right)+\left(\frac{1}{8}+\frac{1}{8}+\frac{1}{8}+\frac{1}{8}\right) \tag{2.14h}$$

$$=1+\frac{3}{2} \tag{2.14i}$$

$$\therefore S_{2^N}>1+\frac{N}{2} \quad \to\infty \text{ as } N\to\infty \tag{2.14j}$$

The simplest way to tell if a series converges or diverges is to compare it to a series that is known to converge and diverge.

For example, the geometric series converges for $|x| < 1$ and diverges for $|x| > 1$ so compare

$$\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n = 1 + x + x^2 + x^3 + \cdots \tag{2.15}$$

with the series of interest

$$\sum_{n=0}^{\infty} a_n = a_0 + a_1 + a_2 + a_3 + \cdots \tag{2.16}$$

and we see that if, as $n \to \infty$, $|a_{n+1}/a_n| < 1$ then our series converges just as the geometric series does. Thus we obtain the **ratio test**:

Ratio Test

- If $\lim_{n\to\infty} \left|\frac{a_{n+1}}{a_n}\right| < 1$ the series converges (absolutely).
- If $\lim_{n\to\infty} \left|\frac{a_{n+1}}{a_n}\right| > 1$ the series diverges.
- If $\lim_{n\to\infty} \left|\frac{a_{n+1}}{a_n}\right| = 1$ (or doesn't exist) we must investigate further.

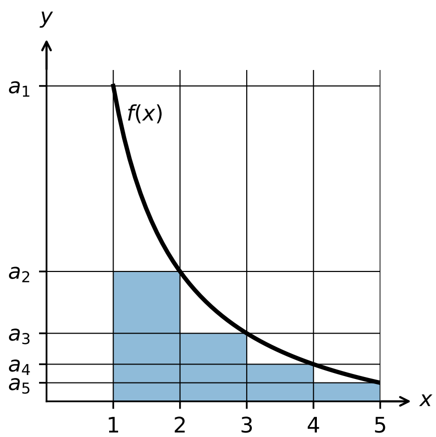


Figure 2.1: Riemann sums used in the integral test, where $f(x)$ is a monotonically-decreasing function. Left: $a_2+a_3+a_4+a_5 < \int_1^5 f(x)\,dx$. Right: $a_1+a_2+a_3+a_4 > \int_1^5 f(x)\,dx$.

Another method: compare with an infinite integral.

The series

$$f(1) + f(2) + f(3) + \cdots \tag{2.17}$$

will converge or diverge depending on whether the integral

$$\int^{\infty} f(x)\,dx \tag{2.18}$$

converges or diverges provided $f(x)$ is monotonically decreasing.

Let $a_n = f(n)$. Then, as shown in the left panel of Fig. 2.1,

$$\sum_{n=2}^{N} a_n = a_2 + a_3 + \cdots + a_N < \int_1^N f(x)\,dx \tag{2.19}$$

so if the integral converges as $N \to \infty$ then the series must converge.

Also, as shown in the right panel of Fig. 2.1,

$$\sum_{n=1}^{N-1} a_n = a_1 + a_2 + \cdots + a_{N-1} > \int_1^N f(x)\,dx \tag{2.20}$$

so if the integral diverges as $N \to \infty$ then the series must diverge.

Ex. 2.3. Consider the **Riemann zeta function**

$$\zeta(s) = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{4^s} + \cdots . \tag{2.21}$$

Try the ratio test:

$$\begin{aligned} \frac{a_{n+1}}{a_n} &= \left(\frac{n}{n+1}\right)^s = \left(1 + \frac{1}{n}\right)^{-s} \underset{n\to\infty}{\sim} 1 - \frac{s}{n} + \cdots \\ &\to 1 \text{ as } n \to \infty \end{aligned} \tag{2.22}$$

so the ratio test is inconclusive. But note:

$$\zeta(s) = f(1) + f(2) + f(3) + \cdots \quad \text{for} \quad f(x) = \frac{1}{x^s} \tag{2.23}$$

(a monotonically-decreasing function). Now,

$$\int f(x)\,dx = \int \frac{dx}{x^s} = -\frac{1}{s-1}\frac{1}{x^{s-1}} \quad (s \neq 1) \tag{2.24}$$

and this converges as $x \to \infty$ if $\mathrm{Re}(s) > 1$ so the Riemann zeta function converges for $\mathrm{Re}(s) > 1$.

This suggests that we can sharpen the ratio test by comparison to the Riemann zeta function:

> If $\left|\frac{a_{n+1}}{a_n}\right| \underset{n\to\infty}{\sim} 1 - \frac{s}{n}$ with $s > 1$ then the series converges absolutely.

In fact, consider the more slowly converging series:

$$\sum_{n=2}^{\infty} \frac{1}{n(\ln n)^s} = \frac{1}{2(\ln 2)^s} + \frac{1}{3(\ln 3)^s} + \cdots . \tag{2.25}$$

Note:

$$\int \frac{dx}{x(\ln x)^s} = -\frac{1}{s-1}\frac{1}{(\ln x)^{s-1}} \tag{2.26}$$

so the series converges provided $s > 1$.

Apply the ratio test:

$$\frac{a_{n+1}}{a_n} = \frac{n}{n+1}\left[\frac{\ln n}{\ln(n+1)}\right]^s \tag{2.27a}$$

$$= \left(1 - \frac{1}{n} + \cdots\right)\left[\frac{\ln n + \ln(1+1/n)}{\ln n}\right]^{-s} \tag{2.27b}$$

$$= \left(1 - \frac{1}{n} + \cdots\right)\left[\frac{\ln n + 1/n + \cdots}{\ln n}\right]^{-s} \tag{2.27c}$$

$$\sim 1 - \frac{1}{n} - \frac{s}{n \ln n} \quad \text{as } n \to \infty . \tag{2.27d}$$

A series converges absolutely if

$$\left|\frac{a_{n+1}}{a_n}\right| \underset{n\to\infty}{\sim} 1 - \frac{1}{n} - \frac{s}{n \ln n}, \quad s > 1$$

(and it diverges if $s < 1$).

Ex. 2.4. The **Legendre differential equation**

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0 \tag{2.28}$$

has a power series solution

$$y = 1 - n(n+1)\frac{x^2}{2!} + n(n+1)(n-2)(n+3)\frac{x^4}{4!} - \cdots \tag{2.29}$$

(see Ex. 19.2).

Try the ratio test: if the series is $y = \sum_{m=1}^{\infty} a_m$ then

$$\frac{a_m}{a_{m-1}} = -\frac{(n-2m+4)(n+2m-3)}{(2m-3)(2m-2)}x^2 . \tag{2.30}$$

Check: take $a_1 = 1$ and then

$$\begin{aligned} a_2 &= -\frac{(n-4+4)(n+4-3)}{(4-3)(4-2)}x^2 a_1 \\ &= -\frac{1}{2}n(n+1)x^2 && \checkmark \\ a_3 &= -\frac{(n-6+4)(n+6-3)}{(6-3)(6-2)}x^2 a_2 \\ &= -\frac{1}{3\cdot 4}(n-2)(n+3)x^2 a_2 \\ &= \frac{1}{4!}n(n+1)(n-2)(n+3)x^4 . && \checkmark \end{aligned}$$

For large m,

$$\frac{a_m}{a_{m-1}} \underset{m\to\infty}{\sim} \left[1 - \frac{1}{m} + O\left(\frac{1}{m^2}\right)\right]x^2 . \tag{2.31}$$

Note that there is no $s/(m \ln m)$ term so $s = 0$. Therefore the series *diverges* if $x^2 = 1$ (unless $n - 2m + 4 = 0$ for some m, in which case this is actually a finite series).

3 Familiar Series

- **Binomial series**

$$\boxed{\begin{aligned}(1+x)^\alpha &= 1+\alpha x+\alpha(\alpha-1)\frac{x^2}{2!}+\alpha(\alpha-1)(\alpha-2)\frac{x^3}{3!}+\cdots\\ &= \sum_{n=0}^{\infty}\binom{\alpha}{n}x^n\end{aligned}} \tag{3.1}$$

where

$$\boxed{\binom{\alpha}{n}=\frac{\alpha(\alpha-1)(\alpha-2)\cdots(\alpha-n+1)}{n!}} \tag{3.2}$$

is the **binomial coefficient**.

If α is a non-negative integer then this is a *finite* series and so obviously converges for any finite x (except the case when $x=-1$ and $\alpha=0$, which is undefined).

The ratio test reveals that this series converges absolutely for $|x|<1$. In addition, it converges absolutely for $|x|=1$ and $\alpha>0$. It turns out that the series converges, but not absolutely, for $x=1$ and $-1<\alpha<0$.

- **Exponential series**

$$\boxed{\begin{aligned}e^x &= 1+x+\frac{x^2}{2!}+\frac{x^3}{3!}+\cdots\\ &= \sum_{n=0}^{\infty}\frac{x^n}{n!}\,.\end{aligned}} \tag{3.3}$$

The ratio test shows that this series always converges.

Generate new series:

- Use Euler's relation (see later) $e^{ix} = \cos x + i \sin x$ in the exponential series:

$$\cos x + i\sin x = e^{ix} = 1 + (ix) + \frac{(ix)^2}{2!} + \frac{(ix)^3}{3!} + \frac{(ix)^4}{4!} + \cdots \tag{3.4}$$

$$= 1 + ix - \frac{x^2}{2!} - i\frac{x^3}{3!} + \frac{x^4}{4!} + \cdots \tag{3.5}$$

$$= \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \cdots\right) + i\left(x - \frac{x^3}{3!} + \cdots\right) \tag{3.6}$$

  and identify the real and imaginary parts:

$$\boxed{\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \cdots} \tag{3.7}$$

$$\boxed{\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots .} \tag{3.8}$$

- Integrate the series for $(1+x)^{-1}$ term-by-term:

$$\underbrace{\int \frac{dx}{1+x}}_{\ln(1+x)} = \underbrace{\int \left\{1 - x + x^2 - x^3 + \cdots\right\} dx}_{x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \frac{1}{4}x^4 + \cdots} \tag{3.9}$$

  so

$$\boxed{\ln(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \frac{1}{4}x^4 + \cdots .} \tag{3.10}$$

  Take the average of $\ln(1+x)$ and $\ln(1-x)$:

$$\boxed{\frac{1}{2}\ln\left(\frac{1+x}{1-x}\right) = x + \frac{1}{3}x^3 + \frac{1}{5}x^5 + \frac{1}{7}x^7 \cdots .} \tag{3.11}$$

- Integrate the series for $(1+x^2)^{-1}$ term-by-term:

$$\underbrace{\int \frac{dx}{1+x^2}}_{\arctan x} = \underbrace{\int \left\{1 - x^2 + x^4 - x^6 + \cdots\right\} dx}_{x - \frac{1}{3}x^3 + \frac{1}{5}x^5 - \frac{1}{7}x^7 + \cdots} \tag{3.12}$$

  so

$$\boxed{\arctan x = x - \frac{1}{3}x^3 + \frac{1}{5}x^5 - \frac{1}{7}x^7 + \cdots .} \tag{3.13}$$

4 Transformation of Series

Series of constants can be summed by introducing a variable.

Ex. 4.1. Sum this series:

$$S = \frac{1}{2!} + \frac{2}{3!} + \frac{3}{4!} + \cdots . \tag{4.1}$$

Let

$$f(x) = \frac{x^2}{2!} + \frac{2x^3}{3!} + \frac{3x^4}{4!} + \cdots . \tag{4.2}$$

Note: $f(1) = S$ and $f(0) = 0$.
Now,

$$f'(x) = x + x^2 + \frac{x^3}{2!} + \frac{x^4}{3!} + \cdots \tag{4.3a}$$

$$= x\left\{1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots\right\} \tag{4.3b}$$

$$= x\,e^x . \tag{4.3c}$$

Therefore

$$f(x) = \int x\,e^x\,dx = x\,e^x - e^x + C . \tag{4.4}$$

The constant of integration is determined by

$$0 = f(0) = 0e^0 - e^0 + C = -1 + C \quad \Longrightarrow \quad C = 1 \tag{4.5}$$

so

$$f(x) = x\,e^x - e^x + 1 \tag{4.6}$$

and thus

$$S = f(1) = 1e^1 - e^1 + 1 = 1. \tag{4.7}$$

Ex. 4.2. Sum the alternating harmonic series:

$$S = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots \tag{4.8}$$

(recall this series converges, but not absolutely).
Let

$$f(x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \cdots . \tag{4.9}$$

Note: $S = f(1)$ and recall $f(x) = \ln(1+x)$ so

$$S = \ln 2 . \tag{4.10}$$

However, we can rearrange the series by putting two negative terms after each positive term:

$$\begin{aligned} S &= 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots && (4.11a) \\ &= 1 - \frac{1}{2} - \frac{1}{4} + \frac{1}{3} - \frac{1}{6} - \frac{1}{8} + \cdots && (4.11b) \\ &= \left(1 - \frac{1}{2}\right) - \frac{1}{4} + \left(\frac{1}{3} - \frac{1}{6}\right) - \frac{1}{8} + \cdots && (4.11c) \\ &= \frac{1}{2} - \frac{1}{4} + \frac{1}{6} - \frac{1}{8} + \cdots && (4.11d) \\ &= \frac{1}{2}\left(1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots\right) && (4.11e) \\ &= \frac{1}{2} \ln 2 . && (4.11f) \end{aligned}$$

Introduce the **Bernoulli numbers** by considering the series

$$\frac{x}{e^x - 1} = c_0 + c_1 x + c_2 x^2 + \cdots \qquad |x| < 2\pi \tag{4.12}$$

$$\implies x = \left(c_0 + c_1 x + c_2 x^2 + \cdots\right)\left(x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots\right). \tag{4.13}$$

Now divide both sides by x and define the Bernoulli numbers by $c_n = B_n/n!$:

$$1 = \left(B_0 + B_1 \frac{x}{1!} + B_2 \frac{x^2}{2!} + \cdots\right)\left(1 + \frac{x}{2!} + \frac{x^2}{3!} + \cdots\right). \tag{4.14}$$

Now equate powers in x:

$$1 = B_0 \tag{4.15a}$$

$$0 = \frac{B_0}{2!} + \frac{B_1}{1!} \qquad \implies \qquad B_1 = -\frac{1}{2} \tag{4.15b}$$

$$0 = \frac{B_0}{3!} + \frac{B_1}{1!2!} + \frac{B_2}{1!2!} \qquad \implies \qquad B_2 = \frac{1}{6} \tag{4.15c}$$

and so on. The first few Bernoulli numbers are

$$\begin{aligned} &B_0 = 1 \qquad B_2 = \frac{1}{6} \quad B_4 = -\frac{1}{30} \quad B_6 = \frac{1}{42} \quad \cdots \\ &B_1 = -\frac{1}{2} \quad B_3 = B_5 = B_7 = \cdots = 0\,. \end{aligned} \tag{4.16}$$

The Bernoulli numbers appear in series expansions of other common functions.

Ex. 4.3. Consider

$$\cot x = \frac{\cos x}{\sin x} = \frac{\frac{1}{2}(e^{ix} + e^{-ix})}{\frac{1}{2i}(e^{ix} - e^{-ix})} = i\,\frac{e^{ix} + e^{-ix}}{e^{ix} - e^{-ix}}\,. \tag{4.17}$$

Let $ix = y/2$:

$$\cot x = i\,\frac{e^{y/2} + e^{-y/2}}{e^{y/2} - e^{-y/2}} \tag{4.18a}$$

$$= i\,\frac{e^{y} + 1}{e^{y} - 1} \tag{4.18b}$$

$$= i\left(1 + \frac{2}{e^{y} - 1}\right) \tag{4.18c}$$

$$= \frac{2i}{y}\left(\frac{y}{2} + \frac{y}{e^{y} - 1}\right) \tag{4.18d}$$

$$= \frac{2i}{y}\left(-B_1 y + \sum_{n=0}^{\infty} B_n \frac{y^n}{n!}\right) \tag{4.18e}$$

note: $B_n = 0$ for n odd except B_1

$$= \sum_{n\ \text{even}} B_n \frac{y^n}{n!}\,. \tag{4.18f}$$

Now put back $y = 2ix$ and let $n = 2m$, $m = 0, 1, 2, \ldots$

$$\boxed{\begin{aligned} \cot x &= \frac{1}{x}\sum_{m=0}^{\infty}(-1)^m B_{2m}\frac{(2x)^{2m}}{(2m)!} \\ &= \frac{1}{x} - \frac{1}{3}x - \frac{1}{45}x^3 - \frac{2}{945}x^5 - \cdots \qquad 0 < |x| < \pi\,. \end{aligned}} \tag{4.19}$$

Deduce the series for $\tan x$ using $\tan x = \cot x - 2\cot 2x$:

$$\boxed{\begin{aligned} \tan x &= \frac{1}{x}\sum_{m=1}^{\infty}(-1)^{m-1}(2^{2n} - 1)B_{2m}\frac{(2x)^{2m}}{(2m)!} \\ &= x + \frac{1}{3}x^3 + \frac{2}{15}x^5 + \frac{17}{315}x^7 + \cdots \qquad |x| < \frac{\pi}{2}\,. \end{aligned}} \tag{4.20}$$

Ex. 4.4. And, just for fun, use Hardy's method to sum the series

$$S = \sum_{n=1}^{\infty} \frac{1}{n^2} = 1 + \frac{1}{4} + \frac{1}{9} + \frac{1}{16} + \cdots = \zeta(2)\,. \tag{4.21}$$

Consider the Fourier series (see Ex. 13.2 later):

$$\cos kx = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos nx + b_n \sin nx) \tag{4.22a}$$

$$= \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx \tag{4.22b}$$

where all the b_n coefficients are zero since $\cos kx$ is an even function, and where

$$a_n = \frac{2}{\pi} \int_0^{\pi} \cos nx \cos kx \, dx \tag{4.22c}$$

$$= (-1)^n \frac{2k \sin k\pi}{\pi(k^2 - n^2)} \tag{4.22d}$$

$$\therefore \quad \cos kx = \frac{2k \sin k\pi}{\pi} \left(\frac{1}{2k^2} - \frac{\cos x}{k^2 - 1} + \frac{\cos 2x}{k^2 - 4} - \frac{\cos 3x}{k^2 - 9} + \cdots \right). \tag{4.23}$$

Now set $x = \pi$:

$$\cos k\pi = \frac{2k \sin k\pi}{\pi} \left(\frac{1}{2k^2} + \frac{1}{k^2 - 1} + \frac{1}{k^2 - 4} + \frac{1}{k^2 - 9} + \cdots \right) \tag{4.24a}$$

and so

$$k\pi \cot k\pi = 2k^2 \left(\frac{1}{2k^2} + \frac{1}{k^2 - 1} + \frac{1}{k^2 - 4} + \frac{1}{k^2 - 9} + \cdots \right) \tag{4.24b}$$

$$= 1 + 2k^2 \left(-\frac{1}{1 - k^2} - \frac{1}{2^2} \frac{1}{1 - k^2/2^2} - \frac{1}{3^2} \frac{1}{1 - k^2/3^2} - \cdots \right) \tag{4.24c}$$

$$= 1 - 2k^2 \left[(1 + k^2 + k^4 + \cdots) + \frac{1}{2^2} \left(1 + \frac{k^2}{2^2} + \frac{k^4}{2^4} + \cdots \right) + \frac{1}{3^2} \left(1 + \frac{k^2}{3^2} + \frac{k^4}{3^4} + \cdots \right) + \cdots \right] \tag{4.24d}$$

$$= 1 - 2k^2 \left(1 + \frac{1}{2^2} + \frac{1}{3^2} + \cdots \right) - 2k^4 \left(1 + \frac{1}{2^4} + \frac{1}{3^4} + \cdots \right) + \cdots \tag{4.24e}$$

$$= 1 - 2 \sum_{n=1}^{\infty} \zeta(2n) k^{2n}\,. \tag{4.24f}$$

Now we have *two* series representations of cotangent: recall

$$\cot x = \frac{1}{x}\sum_{m=0}^{\infty}(-1)^m B_{2m}\frac{(2x)^{2m}}{(2m)!} \tag{4.25}$$

so

$$k\pi\cot k\pi = 1 + \sum_{m=1}^{\infty}(-1)^m\frac{B_{2m}(2\pi)^{2m}k^{2m}}{(2m)!} \tag{4.26}$$

and compare this to

$$k\pi\cot k\pi = 1 - 2\sum_{n=1}^{\infty}\zeta(2n)k^{2n}\,. \tag{4.27}$$

These are two equivalent power series so we must have

$$-2\zeta(2n) = (-1)^n\frac{B_{2n}(2\pi)^{2n}}{(2n)!} \tag{4.28}$$

or

$$\boxed{\zeta(2n) = (-1)^{n+1}\frac{B_{2n}(2\pi)^{2n}}{2(2n)!}\,.} \tag{4.29}$$

Hence:

$$1 + \frac{1}{4} + \frac{1}{9} + \cdots = \zeta(2) = \frac{B_2\,4\pi^2}{4} = \frac{\pi^2}{6} \tag{4.30}$$

$$1 + \frac{1}{16} + \frac{1}{81} + \cdots = \zeta(4) = -\frac{B_4\,16\pi^4}{48} = \frac{\pi^4}{90} \tag{4.31}$$

etc.

Problems

Problem 1.

a) For what values of x does the following series converge?

$$f(x) = 1 + \frac{4}{x^2} + \frac{16}{x^4} + \frac{64}{x^6} + \cdots$$

b) Does the following series converge or diverge?

$$\frac{(1\cdot 3)^2}{1\cdot 1\cdot (1)^2} + \frac{(1\cdot 3\cdot 5)^2}{4\cdot 2\cdot (1\cdot 2)^2} + \frac{(1\cdot 3\cdot 5\cdot 7)^2}{16\cdot 3\cdot (1\cdot 2\cdot 3)^2} + \frac{(1\cdot 3\cdot 5\cdot 7\cdot 9)^2}{64\cdot 4\cdot (1\cdot 2\cdot 3\cdot 4)^2} + \cdots$$

Problem 2.

a) Find the sum of the following series:

$$1 + \frac{1}{4} - \frac{1}{16} - \frac{1}{64} + \frac{1}{256} + \frac{1}{1024} - - + + \cdots$$

b) Find the sum of the following series:

$$\frac{1}{0!} + \frac{2}{1!} + \frac{3}{2!} + \cdots$$

Problem 3.

By repeatedly differentiating the geometric series

$$\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n$$

find a closed-form expression for the function

$$f(x) = \sum_{n=1}^{\infty} n^2 x^n.$$

For what values of x does the series converge?

Module II

Complex Analysis

Motivation

Complex numbers are encountered not only in quantum mechanics but are also a useful tool for many applications in physics. Complex analysis and contour integration give powerful mathematical techniques which we will encounter over and over in later modules.

5 Complex Variables

Basics

A **complex number** can be written as

$$z = x + iy \tag{5.1}$$

and where the **real part** and **imaginary part** are

$$\operatorname{Re} z = x \qquad \text{and} \qquad \operatorname{Im} z = y \tag{5.2}$$

respectively and where the **imaginary constant** i satisfies $i^2 = -1$.

The complex inverse, z^{-1}, which satisfies $z \cdot z^{-1} = 1$, is

$$z^{-1} = \frac{x - iy}{x^2 + y^2}\,. \tag{5.3}$$

A complex number can be represented as a point (x, y) on a two-dimensional plane known as the complex plane as shown in Fig. 5.1.

The **complex conjugate** $z^* = (x, -y)$
is the reflection of the point $z = (x, y)$ about the real axis.

In polar form, the point is (r, θ) where

$$r = |z| = \sqrt{x^2 + y^2} \tag{5.4}$$

is the **complex modulus** and

$$\theta = \arg z = \arctan(y/x) \tag{5.5}$$

is the **complex argument**. Then

$$z = r(\cos\theta + i\sin\theta). \tag{5.6}$$

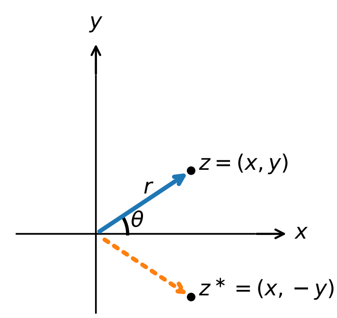


Figure 5.1: Representation of a complex number as a point on a two-dimensional plane.

Note: $\arg z$ is multiple valued.
Define the **principal value** $\operatorname{Arg} z$ such that

$$\arg z = \operatorname{Arg} z + 2n\pi, \quad n = 0, \pm1, \pm2, \ldots \tag{5.7}$$

where $-\pi < \operatorname{Arg} z \le \pi$.

Identities

$$|z|^2 = z \cdot z^* \qquad (z_1 + z_2)^* = z_1^* + z_2^* \qquad (z^*)^* = z$$
$$|z^*| = |z| \qquad (z_1 z_2)^* = z_1^* z_2^*$$
$$|z_1 z_2| = |z_1||z_2| \qquad \operatorname{Re} z = \frac{z + z^*}{2} \qquad \operatorname{Im} z = \frac{z - z^*}{2i} \tag{5.8}$$

Also,

$$\arg(z_1 z_2) = \arg z_1 + \arg z_2 \,. \tag{5.9}$$

Proof. Let $z_1 = r_1(\cos\theta_1 + i \sin\theta_1)$ and $z_2 = r_2(\cos\theta_2 + i \sin\theta_2)$; then

$$z_1 z_2 = r_1 r_2 [(\cos\theta_1 \cos\theta_2 - \sin\theta_1 \sin\theta_2) + i(\sin\theta_1 \cos\theta_2 + \cos\theta_1 \sin\theta_2)] \tag{5.10a}$$
$$= r_1 r_2 [\cos(\theta_1 + \theta_2) + i \sin(\theta_1 + \theta_2)] \,. \tag{5.10b}$$

This motivates the **exponential form**: define

$$e^{i\theta} = \cos\theta + i \sin\theta \tag{5.11}$$

which is **Euler's formula**; then

$$z = r(\cos\theta + i \sin\theta) = r e^{i\theta} \,. \tag{5.12}$$

We have:

$$e^{i\theta_1} e^{i\theta_2} = e^{i(\theta_1 + \theta_2)} \tag{5.13a}$$
$$\frac{1}{e^{i\theta}} = e^{-i\theta} \tag{5.13b}$$
$$e^{i\theta} = e^{i(\theta + 2n\pi)} \,, \quad n = 0, \pm 1, \pm 2, \ldots \,. \tag{5.13c}$$

Powers and Roots

Use induction to show:

$$z^{n+1} \equiv z \cdot z^n = r^{n+1} e^{i(n+1)\theta}, \qquad n = 1, 2, 3, \ldots \tag{5.14}$$

$$z^0 \equiv 1, \qquad z \neq 0 \tag{5.15}$$

$$z^n \equiv (z^{-1})^{(-n)}, \qquad n = -1, -2, -3, \ldots, \quad z \neq 0 \tag{5.16}$$

therefore

$$z^n = r^n e^{in\theta}, \quad n = 0, \pm 1, \pm 2, \ldots. \tag{5.17}$$

Use these to compute roots. E.g., the roots of unity are

$$z^n = 1 \implies r^n e^{in\theta} = 1 e^{i0} \tag{5.18a}$$

$$\implies r^n = 1 \quad \text{and} \quad n\theta = 0 + 2k\pi,\ k = 0, \pm 1, \pm 2, \ldots \tag{5.18b}$$

therefore

$$\boxed{z = e^{2\pi ik/n}, \qquad k = 0, \pm 1, \pm 2, \ldots.} \tag{5.19}$$

The distinct nth roots of unity are

$$1,\ \omega_n,\ \omega_n^2,\ \ldots,\ \omega_n^{n-1} \quad \text{where} \quad \omega_n = e^{2\pi i/n}. \tag{5.20}$$

Similarly, the roots of the equation $z^n = z_0$ are

$$c,\ c\omega_n,\ c\omega_n^2,\ \ldots,\ c\omega_n^{n-1} \quad \text{where} \quad c = \sqrt[n]{r_0}\, e^{i\theta_0/n}. \tag{5.21}$$

6 Complex Functions

Consider

$$w = f(z)\,. \tag{6.1}$$

Suppose $w = u + iv$ and $z = x + iy$; then

$$f(z) = u(x,y) + iv(x,y)\,. \tag{6.2}$$

E.g., if $f(z) = z^2$ then

$$f(x+iy) = \underbrace{x^2 - y^2}_{u(x,y)=x^2-y^2} + \underbrace{2ixy}_{v(x,y)=2xy}\,. \tag{6.3}$$

Think of this as a map from the x-y plane to the u-v plane as seen in Fig. 6.1.

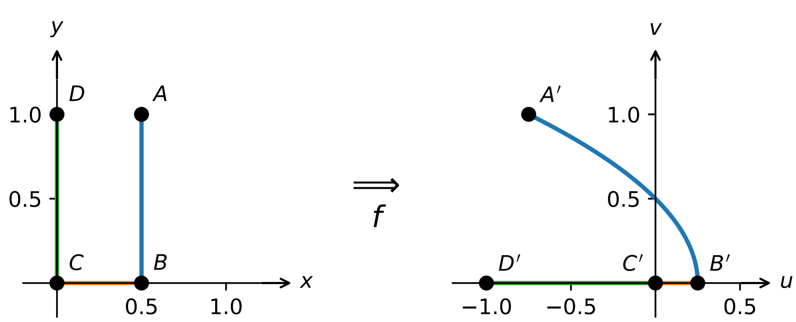


Figure 6.1: The complex map $w = z^2$.

Limits

If $f(z)$ is defined at all points z in some "deleted neighborhood" of z_0 (does not include z_0) then

$$\lim_{z\to z_0} f(z) = w_0 \tag{6.4a}$$

if and only if

$$\lim_{(x,y)\to(x_0,y_0)} u(x,y) = u_0 \qquad \text{and} \qquad \lim_{(x,y)\to(x_0,y_0)} v(x,y) = v_0 \tag{6.4b}$$

and $w_0 = u_0 + i v_0$.

Continuity

$f(z)$ is continuous at a point z_0 if

$$f(z_0)\text{ exists} \qquad \text{and} \qquad \lim_{z\to z_0} f(z) = f(z_0)\,. \tag{6.5}$$

Derivatives

$$\begin{aligned} f'(z_0) &= \lim_{z\to z_0} \frac{f(z)-f(z_0)}{z-z_0} \\ &= \lim_{\Delta z\to 0} \frac{f(z_0+\Delta z)-f(z_0)}{\Delta z}\,. \end{aligned} \tag{6.6}$$

The derivative only exists if it doesn't matter how $z \to z_0$ as illustrated in the following examples.

Ex. 6.1. The derivative of $f(z) = z^2$:

$$f'(z) = \lim_{\Delta z \to 0} \frac{(z + \Delta z)^2 - z^2}{\Delta z} \tag{6.7a}$$

$$= \lim_{\Delta z \to 0} (2z + \Delta z) \tag{6.7b}$$

$$= 2z\,. \tag{6.7c}$$

Ex. 6.2. The derivative of $f(z) = |z|^2 = z \cdot z^*$:

$$f'(z) = \lim_{\Delta z \to 0} \frac{(z + \Delta z)(z^* + (\Delta z)^*) - z \cdot z^*}{\Delta z} \tag{6.8a}$$

$$= \lim_{\Delta z \to 0} \left\{ z^* + (\Delta z)^* + z \frac{(\Delta z)^*}{\Delta z} \right\}. \tag{6.8b}$$

Here, $\Delta z = \Delta x + i\Delta y$. Consider two cases:

1. Approach the origin $\Delta z = 0$ along the real axis: $\Delta z = \Delta x$, $\Delta y = 0$:

$$f'(z) = \lim_{\Delta x \to 0} \{z^* + \Delta x + z\} = z^* + z\,. \tag{6.8c}$$

2. Approach the origin $\Delta z = 0$ along the imaginary axis: $\Delta z = i\Delta y$, $\Delta x = 0$:

$$f'(z) = \lim_{\Delta y \to 0} \{z^* - i\Delta y - z\} = z^* - z\,. \tag{6.8d}$$

These are different results if $z \neq 0$, therefore the only place the derivative exists is at $z = 0$.

Note: $f = |z|^2$ is continuous since

$$u(x, y) = x^2 + y^2 \qquad \text{and} \qquad v(x, y) = 0 \tag{6.9}$$

are both continuous.

Thus continuous $\not\Longrightarrow$ differentiable (though differentiable $\Longrightarrow$ continuous).

Cauchy-Riemann Equations

If $f(z) = u(x,y) + iv(x,y)$ then, if we approach z with y constant and $\Delta z = \Delta x$,

$$f'(z) = \frac{\partial u}{\partial x}(x,y) + i\frac{\partial v}{\partial x}(x,y) \tag{6.10a}$$

whereas if we approach z with x constant and $\Delta z = i\Delta y$,

$$f'(z) = \frac{\partial v}{\partial y}(x,y) - i\frac{\partial u}{\partial y}(x,y)\,. \tag{6.10b}$$

Therefore, a necessary condition for $f'(z)$ to exist is

$$\boxed{\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \qquad \text{and} \qquad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}\,.} \tag{6.11}$$

These are the **Cauchy-Riemann equations**.

The Cauchy-Riemann equations are also sufficient conditions for the existance of the derivative.

Analytic Functions

A function is said to be **analytic** at a point z_0 if its derivative exists in a neighborhood of z_0.

Ex. 6.3. $f(z) = 1/z$ is analytic everywhere except for $z = 0$. However, since $f(z)$ is analytic at some point in every neighborhood of $z = 0$, we call $z = 0$ a **singular point**.

Ex. 6.4. $f(z) = |z|^2$ is not analytic at any point.

A function is **entire** if it is analytic everywhere in the finite plane.
(Polynomials are entire.)

Harmonic Functions

A **harmonic function** $h(x,y)$ satisfies **Laplace's equation**

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = 0\,. \tag{6.12}$$

If $f(z) = u(x,y) + iv(x,y)$ is analyitic in some domain then u and v are harmonic functions in that domain and v is known as the **harmonic conjugate** of u.

Exponential Function

We seek something that behaves like e^x along the real axis, i.e.,

$$\frac{d}{dx}e^x = e^x \quad \forall x \text{ (real)}. \tag{6.13}$$

Define the **exponential function**, $\exp(z) = e^z$ by:

$$\boxed{e^z \text{ is entire} \qquad \text{and} \qquad \frac{d}{dz}e^z = e^z \quad \forall z\,.} \tag{6.14}$$

Consider the function

$$f(z) = e^x(\cos y + i \sin y) \tag{6.15}$$

so

$$u(x,y) = e^x \cos y \qquad \text{and} \qquad v(x,y) = e^x \sin y\,. \tag{6.16}$$

We see that

$$\frac{\partial u}{\partial x} = e^x \cos y \qquad \frac{\partial v}{\partial y} = e^x \cos y \qquad \Longrightarrow \qquad \frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \tag{6.17a}$$

$$\frac{\partial u}{\partial y} = -e^x \sin y \qquad \frac{\partial v}{\partial x} = e^x \sin y \qquad \Longrightarrow \qquad \frac{\partial u}{\partial x} = -\frac{\partial v}{\partial y} \tag{6.17b}$$

so the Cauchy-Riemann equations are satisfied everywhere. Furthermore,

$$\begin{aligned} f'(z) &= \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} = e^x(\cos y + i \sin y) \\ &= f(z) \end{aligned} \tag{6.18}$$

and therefore this is the exponential function:

$$\boxed{e^z = e^x(\cos y + i \sin y)\,.} \tag{6.19}$$

Note: this justifies our use of the symbol $e^{i\theta} = \cos\theta + i \sin\theta$ in the polar form of a complex number.

The exponential function has the familiar properties:

$$\begin{aligned} e^{z_1}e^{z_2} &= e^{z_1+z_2} & e^{z+2\pi i} &= e^z \\ |e^z| &= e^x & \arg e^z &= y + 2n\pi,\ n = 0, \pm 1, \pm 2, \dots \\ e^z &= \rho\, e^{i\phi} \quad \Longrightarrow & z &= \ln\rho + i(\phi + 2n\pi),\ n = 0, \pm 1, \pm 2, \dots\,. \end{aligned} \tag{6.20}$$

Therefore $w = e^z$ is a many-to-one mapping due to the periodicity of e^z.

Note: $e^z \neq 0$ so the range of $w = e^z$ is the entire w-plane except the origin $w = 0$.

Logarithm Function

The **logarithm function** is the inverse exponential function:

$$\boxed{\log z = \ln|z| + i\arg z, \quad z \neq 0\,.} \tag{6.21}$$

Since the complex argument is multi-valued, so is the logarithm function.
The logarithm function can be made single-valued by restricting it to a branch

$$|z| > 0,\ \alpha < \arg z < \alpha + 2\pi \tag{6.22}$$

where $|z| > 0$, $\arg z = \alpha$ is the **branch cut**.
The logarithm function is discontinuous across the branch cut.

The principal value of the logarithm is

$$\operatorname{Log} z = \ln|z| + i\operatorname{Arg} z, \quad z \neq 0\,. \tag{6.23}$$

Note: the logarithm function is analytic with

$$\frac{d}{dz}\log z = \frac{1}{z} \quad \text{for } z \neq 0\,. \tag{6.24}$$

The logarithm function has the following properties:

$$\exp(\log z) = z \tag{6.25a}$$

$$\log(\exp z) = z + 2\pi i n, \qquad n = 0, \pm1, \pm2, \ldots \tag{6.25b}$$

$$\operatorname{Log}(\exp z) = z \tag{6.25c}$$

$$\log(z_1 z_2) = \log z_1 + \log z_2 \qquad \text{(for some branch)} \tag{6.25d}$$

$$z^n = \exp(n \log z), \qquad n = 0, \pm1, \pm2, \ldots \tag{6.25e}$$

$$z^{1/n} = \exp\left(\frac{1}{n}\log z\right), \qquad z \neq 0,\ n = 0, \pm1, \pm2, \ldots \tag{6.25f}$$

(the last equation has n distinct values corresponding to the n roots.)

Use the logarithm function to define complex exponents:

$$z^c = \exp(c \log z)\,. \tag{6.26}$$

Find:

$$\frac{d}{dz} z^c = c z^{c-1}, \quad |z| > 0,\ \alpha < \arg z < \alpha + 2\pi\,. \tag{6.27}$$

The principal value of z^c is

$$z^c = \exp(c \operatorname{Log} z) \tag{6.28}$$

and the principal branch is $|z| > 0$, $-\pi < \operatorname{Arg} z < \pi$.

Trigonometric Functions

Define the **trigonometric functions** as

$$\boxed{\sin z = \frac{e^{iz} - e^{-iz}}{2i} \qquad \text{and} \qquad \cos z = \frac{e^{iz} + e^{-iz}}{2}\,.} \tag{6.29}$$

(Also define $\tan z = \sin z / \cos z$, etc.)

Hyperbolic Functions

Define the **hyperbolic functions** as

$$\boxed{\sinh z = \frac{e^{z} - e^{-z}}{2} \qquad \text{and} \qquad \cosh z = \frac{e^{z} + e^{-z}}{2}\,.} \tag{6.30}$$

Inverse Trigonometric Functions

Consider the arcsin function:

$$w = \arcsin z \qquad \text{when} \qquad z = \sin w\,. \tag{6.31}$$

Therefore, solve $z = \sin w$ for w:

$$z = \frac{e^{iw} - e^{-iw}}{2i} \tag{6.32a}$$

$$\implies (e^{iw})^2 - 2iz(e^{iw}) - 1 = 0 \tag{6.32b}$$

$$\implies e^{iw} = iz + (1 - z^2)^{1/2} \tag{6.32c}$$

$$\implies w = \arcsin z = -i \log[iz + (1 - z^2)^{1/2}]\,. \tag{6.32d}$$

Note: the square root is double-valued and the log is multiple-valued, so the arcsin function is multiple-valued.

Similarly can compute the other **inverse trigonometric functions**:

$$\boxed{\begin{aligned} \arcsin z &= -i \log[iz + (1 - z^2)^{1/2}] \\ \arccos z &= -i \log[z + i(1 - z^2)^{1/2}] \\ \arctan z &= \frac{i}{2} \log \frac{i + z}{i - z}\,. \end{aligned}} \tag{6.33}$$

We can now compute the derivatives of these functions.

We can similarly find the **inverse hyperbolic functions**.

7 Complex Integrals

A **contour** C is a set of points

$$C = \{(x(t), y(t)) : a \le t \le b\} \tag{7.1}$$

(see Fig. 7.1). The length of C is

$$L = \int_a^b |z'(t)|\, dt \tag{7.2}$$

where $z'(t) = x'(t) + i y'(t)$.

A **simple contour** does not self-intersect.

A **simple closed contour** does not self-intersect except at the end points, which are the same.

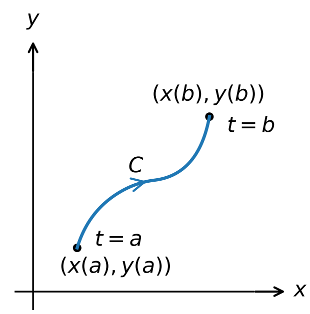


Figure 7.1: Contour.

Contour Integral

A **contour integral** is

$$\int_C f(z)\, dz = \int_a^b f[z(t)]\, z'(t)\, dt\,. \tag{7.3}$$

This integral is invariant under re-parameterization of the contour.

Properties of contour integrals:

- $$\int_{-C} f(z)\, dz = -\int_C f(z)\, dz \tag{7.4a}$$
- $$\int_{C=C_1+C_2} f(z)\, dz = \int_{C_1} f(z)\, dz + \int_{C_2} f(z)\, dz \tag{7.4b}$$
- $$\left|\int_C f(z)\, dz\right| \le \int_a^b |f[z(t)]\, z'(t)|\, dt \tag{7.4c}$$
- If M is a non-negative constant such that $|f(z)| \le M$ on C then

$$\left|\int_C f(z)\, dz\right| \le M \int_a^b |z'(t)|\, dt = ML\,. \tag{7.4d}$$

Ex. 7.1. Let C be the path (see Fig. 7.2)

$$z = 3e^{i\theta}, \quad 0 \le \theta \le \pi \,. \tag{7.5}$$

Let

$$f(z) = z^{1/2} = \sqrt{r}e^{i\theta/2}, \quad r > 0,\, 0 < \theta < 2\pi \,. \tag{7.6}$$

Note: this branch of the square root is not defined at the initial point, but we can still integrate $f(z)$ because it only needs to be piecewise continuous.

Therefore

$$f[z(\theta)] = \sqrt{3}e^{i\theta/2} = \sqrt{3}\cos\frac{\theta}{2} + i\sqrt{3}\sin\frac{\theta}{2}, \quad 0 < \theta \le \pi \,. \tag{7.7}$$

As $\theta \to 0$, $f[z(\theta)] \to \sqrt{3}$ so just define this to be its value at $\theta = 0$. Then

$$I = \int_C f(z)\,dz = \int_C z^{1/2}\,dz = \int_0^{\pi} \sqrt{3}e^{i\theta/2}(3ie^{i\theta})\,d\theta \tag{7.8a}$$

$$= 3\sqrt{3}i\int_0^{\pi} e^{i3\theta/2}\,d\theta = 3\sqrt{3}\left[\frac{2}{3i}e^{i3\theta/2}\right]_0^{\pi} = 3\sqrt{3}\left[-\frac{2}{3i}(1+i)\right] \tag{7.8b}$$

$$= -2\sqrt{3}(1+i)\,. \tag{7.8c}$$

If we had just wanted to bound the integral, we note that $|z^{1/2}| = \sqrt{3}$ and $L = 3\pi$, therefore

$$|I| \le 3\sqrt{3}\pi \,. \tag{7.9}$$

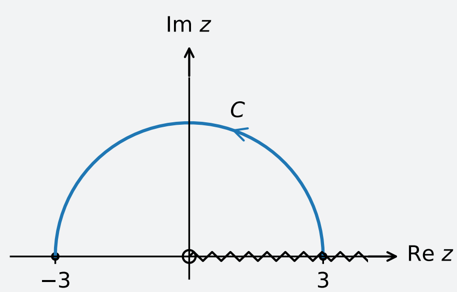


Figure 7.2: Contour for Ex. 7.1

Cauchy-Goursat Theorem

Theorem 1 (Cauchy-Goursat)**.** If a function f is analytic at all points interior to and on a simple closed curve C then

$$\oint_C f(z)\,dz = 0\,. \tag{7.10}$$

Sketch of proof.

$$\oint_C f(z)\,dz = \int_a^b f[z(t)]\,z'(t)\,dt \tag{7.11a}$$

let $f(z) = u(x,y) + i\,v(x,y)$ and $z(t) = x(t) + i\,y(t)$

$$= \int_a^b [(ux' - vy') + i(vx' + uy')]\,dt \tag{7.11b}$$

$$= \oint_C (u\,dx - v\,dy) + i\oint_C (v\,dx + u\,dy) \tag{7.11c}$$

by Green's theorem where C is the boundary of region R

$$= \iint_R \left(-\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) dx\,dy + i\iint_R \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) dx\,dy \tag{7.11d}$$

by the Cauchy-Riemann equations

$$= 0\,. \tag{7.11e}$$

□

Cauchy Integral Formula

If f is analytic everywhere within and on a simple closed contour C, take in a positive (counterclockwise) sense, and if z_0 is any point interior to C, then

$$\boxed{f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0}\, dz\,.} \tag{7.12}$$

This is the **Cauchy integral formula.**

Proof. Consider C_ϵ wich is a circle of radius ϵ about z_0: $z(\theta) = z_0 + \epsilon e^{i\theta}$, $z'(\theta) = \epsilon i e^{i\theta}$:

$$\oint_{C_\epsilon} \frac{f(z)}{z - z_0}\, dz \approx f(z_0) \oint_{C_\epsilon} \frac{dz}{z - z_0} = f(z_0) \int_0^{2\pi} \frac{\epsilon i e^{i\theta}}{\epsilon e^{i\theta}}\, d\theta \tag{7.13a}$$

$$= 2\pi i f(z_0). \tag{7.13b}$$

Now divide C into the modified contour $C + L - C_\epsilon - L$ as shown in Fig. 7.3. The integrand is analytic everywhere inside this contour so, by the Cauchy-Goursat theroem,

$$0 = \oint_C \frac{f(z)}{z - z_0}\, dz + \cancel{\int_L \frac{f(z)}{z - z_0}\, dz} - \oint_{C_\epsilon} \frac{f(z)}{z - z_0}\, dz - \cancel{\int_L \frac{f(z)}{z - z_0}\, dz} \tag{7.14}$$

$$\implies \oint_C \frac{f(z)}{z - z_0}\, dz = \oint_{C_\epsilon} \frac{f(z)}{z - z_0}\, dz = 2\pi i f(z_0) \tag{7.15}$$

□

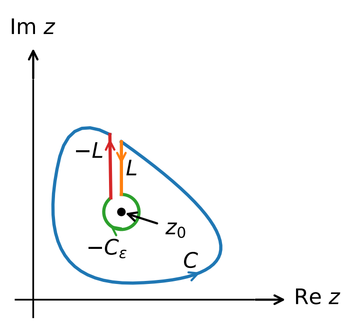


Figure 7.3: Contour for Cauchy integral formula

Derivatives of Analytic Functions

Assume f is analytic on and within a positively-oriented closed contour C about z. Then:

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(s)}{s-z}\, ds\,. \tag{7.16}$$

Now,

$$f'(z) = \frac{1}{2\pi i} \oint_C \frac{f(s)}{(s-z)^2}\, ds \tag{7.17a}$$

$$f''(z) = \frac{1}{\pi i} \oint_C \frac{f(s)}{(s-z)^3}\, ds \tag{7.17b}$$

etc.

This establishes the existance of all derivatives of f at z and shows that all derivatives are also analytic at z:

$$\boxed{f^{(n)}(z) = \frac{n!}{2\pi i} \oint_C \frac{f(s)}{(s-z)^{n+1}}\, ds\,.} \tag{7.18}$$

Ex. 7.2. Take $f(z) = 1$:

$$\oint_C \frac{dz}{(z-z_0)^{n+1}} = \begin{cases} 2\pi i, & n = 0 \\ 0, & n = 1, 2, 3 \ldots\,. \end{cases} \tag{7.19}$$

Maximum Moduli of Functions

Suppose $|f(z)| \le |f(z_0)|$ everywhere in the disk $|z - z_0| < \epsilon$ and suppose $f(z)$ is analytic in this neighborhood.

Let C_ρ be the oriented circle $|z - z_0| = \rho$ with $0 < \rho < \epsilon$ so $C_\rho = \{z_0 + \rho e^{i\theta} : 0 \le \theta \le 2\pi\}$. Then

$$f(z_0) = \frac{1}{2\pi i} \oint_{C_\rho} \frac{f(z)}{z - z_0}\, dz = \frac{1}{2\pi} \int_0^{2\pi} f(z_0 + \rho e^{i\theta})\, d\theta\,. \tag{7.20}$$

(This is **Gauss's mean value theorem**.)

We have:

$$|f(z_0)| \le \frac{1}{2\pi} \int_0^{2\pi} |f(z_0 + \rho e^{i\theta})|\, d\theta\,. \tag{7.21a}$$

Also, by assumption, $|f(z_0)| \ge |f(z_0 + \rho e^{i\theta})|$ so

$$\frac{1}{2\pi} \int_0^{2\pi} |f(z_0 + \rho e^{i\theta})|\, d\theta \le \frac{1}{2\pi} \int_0^{2\pi} |f(z_0)|\, d\theta = |f(z_0)|\,. \tag{7.21b}$$

By Eq. (7.21a) and Eq. (7.21b) we see that

$$|f(z_0)| = |f(z_0 + \rho e^{i\theta})|\,. \tag{7.21c}$$

It turns out that when the modulus of a function is constant in a domain, the function itself must be constant there.

Therefore we have the **maximum modulus principle**:

If a function f is analytic and not constant in a given domain then $|f(z)|$ has no maximum value in the domain.

Corollary. Suppose a function f is continuous in a closed bounded region R and that it is analytic and not constant in the interior of R. Then the maximum value of $|f(z)|$, which is always reached, occurs somewhere on the boundary of R and never in the interior.

Taylor's Theorem

Theorem 2 (Taylor's Theorem)**.** If f is analytic throughout an open disk $|z-z_0|<R_0$ centered at z_0 with radius R_0 then at each point in the disk

$$\boxed{f(z)=\sum_{n=0}^{\infty} a_n(z-z_0)^n \qquad \text{with} \qquad a_n=\frac{1}{n!}f^{(n)}(z_0)} \tag{7.22}$$

(the infinite series converges).

Proof. We prove it for the **Maclaurin series** where $z_0=0$.

Let C_0 be a positively-oreinted circle $|s|=r_0$ where $r<r_0<R_0$ with $|z|=r$ as shown in Fig. 7.4.

$$f(z)=\frac{1}{2\pi i}\oint_{C_0}\frac{f(s)}{s-z}\,ds=\frac{1}{2\pi i}\oint_{C_0}\frac{1}{s}\frac{1}{1-z/s}f(s)\,ds \tag{7.23a}$$

$$=\frac{1}{2\pi i}\oint_{C_0}\frac{1}{s}\left\{1+\frac{z}{s}+\left(\frac{z}{s}\right)^2+\cdots+\left(\frac{z}{s}\right)^{N-1}+\frac{(z/s)^N}{1-z/s}\right\}f(s)\,ds \tag{7.23b}$$

$$=f(0)+f'(0)z+\frac{1}{2!}f''(0)z^2+\cdots+\frac{1}{(N-1)!}f^{(N-1)}(0)z^{N-1}+\mathcal{R}_N(z) \tag{7.23c}$$

where the remainder term is

$$\mathcal{R}_N(z)=\frac{z^N}{2\pi i}\oint_{C_0}\frac{f(s)}{(s-z)s^N}\,ds\,. \tag{7.23d}$$

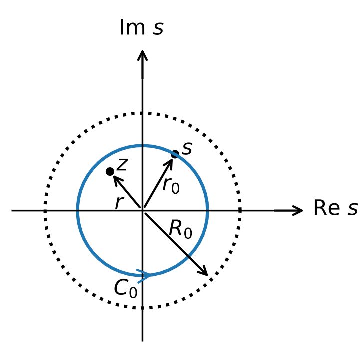


Figure 7.4: Contour for Taylor's theorem

Now $|s-z| \geq ||s|-|z|| = r_0 - r$ since $r_0 > r$ and let M be the maximum value of $|f(s)|$ on C_0. Then

$$|\mathcal{R}_N(z)| \leq \left|\frac{z^N}{2\pi i}\right| \frac{M}{(r_0-r)r_0^N} 2\pi r_0 = \frac{M r_0}{r_0 - r}\left(\frac{r}{r_0}\right)^N \tag{7.24}$$

$$\rightarrow 0 \text{ as } N \rightarrow \infty \text{ since } r_0 > r\,. \tag{7.25}$$

Therefore the Maclaurin series

$$f(z) = f(0) + f'(0)z + \frac{1}{2!}f''(0)z^2 + \cdots + \frac{1}{n!}f^{(n)}(0)z^n + \cdots \tag{7.26}$$

converges in the open disk $|z| < R_0$ provided that $f(z)$ is analytic in this disk.

(It is straightforward to shift the origin to obtain Taylor's theorem.)

□

Ex. 7.3. For the exponential function,

$$f(z) = e^z\,, \quad f'(z) = e^z\,, \quad \ldots\,, \quad f^{(n)}(z) = e^z \tag{7.27}$$

so

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!}\,. \tag{7.28}$$

Note: since e^z is entire, this series converges for all z.

Laurent's Theorem

If f is not analytic at a point z_0, we cannot apply Taylor's theorem there. However, we can use **Laurent's theorem**:

Theorem 3 (Laurent)**.** Suppose a function f is analytic throughout an annular domain $R_1 < |z - z_0| < R_2$ and let C donate any positively-oriented closed contour around z_0 and lying in that domain. Then, at each point z in the domain,

$$\boxed{f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n + \sum_{n=1}^{\infty} \frac{b_n}{(z - z_0)^n}, \qquad R_1 < |z - z_0| < R_2} \tag{7.29}$$

where

$$\boxed{\begin{aligned} a_n &= \frac{1}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}}\, dz, \qquad n = 0, 1, 2, \dots \\ b_n &= \frac{1}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{-n+1}}\, dz, \qquad n = 1, 2, \dots \end{aligned}} \tag{7.30}$$

or, more concisely,

$$\boxed{f(z) = \sum_{n=-\infty}^{\infty} c_n (z - z_0)^n, \qquad R_1 < |z - z_0| < R_2} \tag{7.31}$$

where

$$\boxed{c_n = \frac{1}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}}, \qquad n = 0, \pm 1, \pm 2, \dots .} \tag{7.32}$$

Sketch of proof. Take z_0 as before for simplicity. Refer to Fig. 7.5 for contours C, C_1, C_2, and Γ. First note:

$$\oint_{C_2} \frac{f(s)}{s - z}\, ds - \oint_{C_1} \frac{f(s)}{s - z}\, ds - \underbrace{\oint_{\Gamma} \frac{f(s)}{s - z}\, ds}_{-2\pi i f(z)} = 0 \tag{7.33}$$

$$\implies f(z) = \frac{1}{2\pi i} \oint_{C_2} \frac{f(s)}{s - z}\, ds - \frac{1}{2\pi i} \oint_{C_1} \frac{f(s)}{s - z}\, ds. \tag{7.34}$$

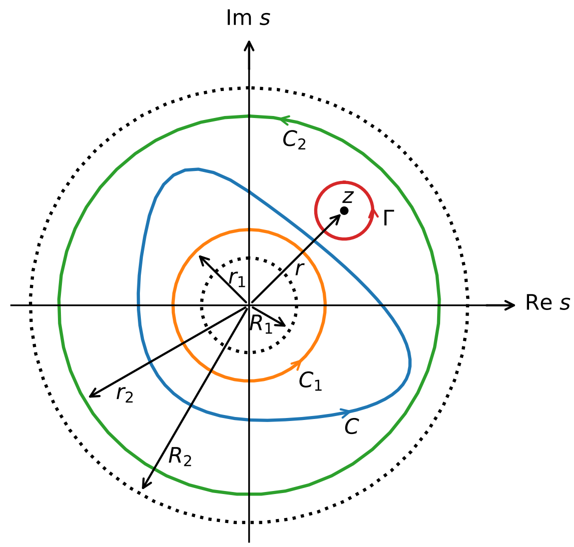


Figure 7.5: Contours for Laurent's theorem.

In the integrand of the first integral where $|s| > |z|$ expand

$$\frac{1}{s-z} = \frac{1}{s} + \frac{z}{s^2} + \cdots + \frac{z^N}{(s-z)s^N} \tag{7.35a}$$

and in the integrand of the second integral where $|z| > |s|$ expand

$$-\frac{1}{s-z} = \frac{1}{z} + \frac{s}{z^2} + \cdots + \frac{s^N}{(z-s)z^N}\,. \tag{7.35b}$$

$$\therefore\; f(z) = a_0 + a_1 z + \cdots + \mathcal{R}_N(z) + \frac{b_1}{z} + \frac{b_2}{z^2} + \cdots + \mathcal{S}_N(z) \tag{7.36a}$$

where

$$a_n = \frac{1}{2\pi i}\oint_{C_2} \frac{f(s)}{s^{n+1}}\,ds = \frac{1}{2\pi i}\oint_{C} \frac{f(s)}{s^{n+1}}\,ds \tag{7.36b}$$

$$b_n = \frac{1}{2\pi i}\oint_{C_1} \frac{f(s)}{s^{-n+1}}\,ds = \frac{1}{2\pi i}\oint_{C} \frac{f(s)}{s^{-n+1}}\,ds \tag{7.36c}$$

$$\mathcal{R}_N(z) = \frac{z^N}{2\pi i}\oint_{C_2} \frac{f(s)}{(s-z)s^N}\,ds \tag{7.36d}$$

$$\mathcal{S}_N(z) = \frac{1}{2\pi i z^N}\oint_{C_1} \frac{s^N f(s)}{z-s}\,ds\,. \tag{7.36e}$$

Now, if M_1 is the maximum value of $|f(s)|$ on C_1 and M_2 is the maximum value of $|f(s)|$ on C_2,

$$|\mathcal{R}_N(z)| \leq \frac{M_2 r_2}{r_2 - r}\left(\frac{r}{r_2}\right)^N \tag{7.36f}$$

$$\to 0 \text{ as } N \to \infty \text{ since } r_2 > r \tag{7.36g}$$

$$|\mathcal{S}_N(z)| \leq \frac{M_1 r_1}{r - r_1}\left(\frac{r_1}{r}\right)^N \tag{7.36h}$$

$$\to 0 \text{ as } N \to \infty \text{ since } r_1 < r\,. \tag{7.36i}$$

□

A power series has the following properties:

- If a power series $\sum_{n=0}^{\infty} a_n z^n$ converges when $z = z_1$ $(z_1 \neq 0)$ then it is absolutely convergent in the open disk $|z| < |z_1|$.

  Thus the series will converge only in a disk out to radius $R_0 = |z_0|$ where z_0 is the nearest point for which the series diverges, i.e., where the function that the series corresponds to fails to be analytic.

  E.g.,

$$f(z) = \frac{1}{1-z} \text{ is analytic for } z \neq 1$$

$$\implies \quad \sum_{n=0}^{\infty} z^n \text{ converges in the disk } |z| < 1 \text{ but not beyond.}$$

- The power series $S(z) = \sum_{n=0}^{\infty} a_n z^n$ is analytic within its circle of convergence. It can be term-by-term integrated and differentiated.

- If a series $\sum_{n=-\infty}^{\infty} c_n (z - z_0)^n$ converges to $f(z)$ at all points in some annular domain about z_0 then it is the unique Laurent series expansion for f in powers of $z - z_0$ for that domain.

Residues

If a function f is analytic throughout a deleted neighborhood $0 < |z - z_0| < \epsilon$ of a singular point z_0 then z_0 is an **isolated singular point**. E.g., $1/z$ has an isolated singular point $z_0 = 0$ but the origin is *not* isolated for $\operatorname{Log} z$.

If z_0 is an isolated singular point of f then the function can be written as a Laurent series:

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n + \frac{b_1}{z - z_0} + \frac{b_2}{(z - z_0)^2} + \cdots, \quad 0 < |z - z_0| < R_2 \tag{7.37}$$

where R_2 is some positive number. Here in particular

$$\oint_C f(z)\, dz = 2\pi i b_1 \tag{7.38}$$

where C is a positively-oriented simple closed contour around z_0 lying in the domain $0 < |z - z_0| < R_2$. Call b_1 the **residue**: $b_1 = \operatorname{Res}_{z=z_0} f(z)$.

Tricks to find the residue:

- Suppose $\phi(z)$ is analytic at $z = z_0$ and $\phi(z_0) \neq 0$, then

$$\operatorname*{Res}_{z=z_0} \frac{\phi(z)}{z - z_0} = \phi(z_0)\,. \tag{7.39}$$

- Suppose $p(z)$ and $q(z)$ are both analytic at z_0 and $p(z_0) \neq 0$, $q(z_0) = 0$, $q'(z_0) \neq 0$, then

$$\operatorname*{Res}_{z=z_0} \frac{p(z)}{q(z)} = \frac{p(z_0)}{q'(z_0)}\,. \tag{7.40}$$

Ex. 7.4. For $f(z) = \dfrac{z+1}{z^2+9}$ find $\operatorname*{Res}_{z=3i} f(z)$.

Write $f(z) = \dfrac{\phi(z)}{z - 3i}$ where $\phi(z) = \dfrac{z+1}{z+3i}$

$$\therefore \operatorname*{Res}_{z=3i} f(z) = \phi(3i) = \frac{3-i}{6}\,.$$

Ex. 7.5. $f(z) = \cot z = \dfrac{\cos z}{\sin z}$.

Let $p(z) = \cos z$, $q(z) = \sin z$, $q'(z) = \cos z$. The zeros of $q(z)$ are the points $z = n\pi$, $n = 0, \pm 1, \pm 2, \ldots$.

$$\therefore \operatorname*{Res}_{z=n\pi} f(z) = \frac{p(n\pi)}{q'(n\pi)} = 1\,.$$

- If

$$f(z) = \sum_{n=0}^{\infty} a_n (z-z_0)^n + \underbrace{\frac{b_1}{z-z_0} + \frac{b_2}{(z-z_0)^2} + \cdots + \frac{b_m}{(z-z_0)^m}}_{\textbf{principal part}} \tag{7.41}$$

for $0 < |z-z_0| < R_2$ where $b_m \neq 0$ then the isolated singular point z_0 is called a **pole of order *m***.

If $m = 1$ then it is a **simple pole**.

Ex. 7.6.

$$\frac{\sinh z}{z^4} = \frac{1}{z^4}\left\{z + \frac{z^3}{3!} + \frac{z^5}{5!} + \cdots\right\} = \frac{1}{z^3} + \frac{1}{3!}\frac{1}{z} + \frac{z}{5!} + \cdots \tag{7.42}$$

has a pole of order 3 at $z = 0$ with residue 1/6.

- If the principal part has an infinite number of terms then the singular point is an **essential singular point**.

Ex. 7.7.

$$e^{1/z} = \sum_{n=0}^{\infty} \frac{1}{n!}\frac{1}{z^n}, \quad 0 < |z| < \infty \tag{7.43}$$

has an essential singular point at $z = 0$ with residue 1.

- When all b_m are zero at an isolated singular point z_0 then z_0 is a **removable singular point**.

Ex. 7.8.

$$f(z) = \frac{e^z - 1}{z} = \frac{1}{z}\left\{z + \frac{1}{2!}z^2 + \cdots\right\} = 1 + \frac{z}{2!} + \frac{z^2}{3!} + \cdots, \quad 0 < |z| < \infty \tag{7.44}$$

has a removable singular point at $z = 0$. If we write $f(0) = 1$ then the function is entire.

Residue Theorem

Theorem 4 (Residue)**.** If C is a positively oriented simple closed contour within and on which a function f is analytic except for a finite number of singular points z_k $(k = 1, 2, \ldots, n)$ interior to C, then

$$\boxed{\oint_C f(z)\,dz = 2\pi i \sum_{k=1}^{n} \operatorname*{Res}_{z=z_k} f(z)\,.} \tag{7.45}$$

Ex. 7.9. Evaluate

$$\oint_C \frac{5z-2}{z(z-1)}\,dz \tag{7.46}$$

for C the circle $|z| = 2$ described counterclockwise.

For the domain $0 < |z| < 1$,

$$\frac{5z-2}{z(z-1)} = \frac{2-5z}{z}\frac{1}{1-z} = \left(\frac{2}{z} - 5\right)\left(1 + z + z^2 + \cdots\right) \tag{7.47a}$$

$$= \frac{2}{z} - 3 - 3z - \cdots \tag{7.47b}$$

so the residue at $z = 0$ is 2. Also, for the domain $0 < |z-1| < 1$,

$$\frac{5z-2}{z(z-1)} = \frac{5(z-1)+3}{z-1}\frac{1}{1+(z-1)} \tag{7.47c}$$

$$= \left(5 + \frac{3}{z-1}\right)\left(1 - (z-1) + (z-1)^2 - \cdots\right) \tag{7.47d}$$

$$= \frac{3}{z-1} + 2 - 2(z-1) + \cdots \tag{7.47e}$$

so the residue at $z = 1$ is 3.

$$\therefore \oint_C \frac{5z-2}{z(z-1)}\,dz = 2\pi i(2+3) = 10\pi i\,. \tag{7.48}$$

Theorem 5. If f is analytic throughout a domain D and $f(z) = 0$ at each point z of a domain or arc interior to D then $f(z) = 0$ everywhere in D.

Proof. Since $f(z) = 0$ along some arc we know that the coefficients $a_n = f^{(n)}(z_0)/n!$ must be zero since the derivatives must all be zero. This means that $f(z) = 0$ for all z for which the Taylor series is valid. □

Corollary. Suppose $f(z)$ and $g(z)$ are analytic in a domain D and $f(z) = g(z)$ along some arc or in some sub-domain. Then $f(z) = g(z)$ everywhere in D.

Proof. Consider $h(z) = f(z) - g(z) = 0$ along the arc; Theorem 5 then requires $h(z) = 0$ within D. □

Analytic Continuation

Consider two intersecting domains D_1 and D_2.

Suppose f_1 is analytic in D_1. There may be a function f_2 that is analytic in D_2 such that

$$f_2(z) = f_1(z) \quad \forall z \in D_1 \cap D_2 \,. \tag{7.49}$$

If such a function exists, then it is called the **analytic continuation** of f_1 into D_2.

When such a function exists, it is unique. The function

$$F(z) = \begin{cases} f_1(z), & z \in D_1 \\ f_2(z), & z \in D_2 \end{cases} \tag{7.50}$$

is analytic in $D_1 \cup D_2$.

However, suppose there are three domains as shown in Fig. 7.6 and

$$f_1(z) = f_2(z) \quad \forall z \in D_1 \cap D_2 \tag{7.51}$$
$$f_1(z) = f_3(z) \quad \forall z \in D_1 \cap D_3 \tag{7.52}$$

it is not necessarily true that

$$f_2(z) = f_3(z) \quad \forall z \in D_1 \cap D_3 \,. \tag{7.53}$$

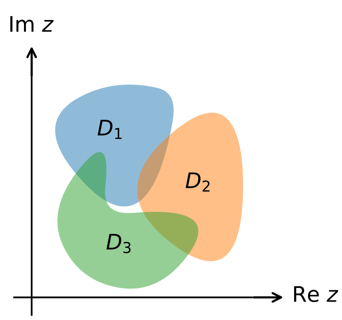


Figure 7.6: Intersecting Domains

Ex. 7.10. Consider

$$f_1(z) = \sum_{n=0}^{\infty} z^n\,, \qquad |z| < 1\,. \tag{7.54}$$

The function

$$f_2(z) = \frac{1}{1-z}\,, \qquad |z| \neq 1 \tag{7.55}$$

satisfies $f_2(z) = f_1(z)$ for $|z| < 1$. Therefore, f_2 is the analytic continuation of f_1 to the entire complex plane except $z = 1$.

Ex. 7.11. Consider the branch of $z^{1/2}$ with $-\pi < \arg z < \pi$ and define:

$$f_1(z) = \sqrt{r}e^{i\theta/2}\,, \quad r > 0,\ -\pi/2 < \theta < \pi\,. \tag{7.56}$$

This is defined in Quadrants I, II, and IV of the complex plane.

Analytically continue this across the negative real axis into Quadrant III:

$$f_2(z) = \sqrt{r}e^{i\theta/2}\,, \quad r > 0,\ \pi/2 < \theta < 3\pi/2\,. \tag{7.57}$$

This is defined in Quadrants II and III of the complex plane. Note that $f_2(z) = f_1(z)$ in the overlapping domain of Quadrant II: $r > 0$, $\pi/2 < \theta < \pi$.

Now analytically continue this across the negative imaginary axis:

$$f_3(z) = \sqrt{r}e^{i\theta/2}\,, \quad r > 0,\ \pi < \theta < 5\pi/2\,. \tag{7.58}$$

This is defined in Quadrants I, III, and IV of the complex plane. Note that $f_3(z) = f_2(z)$ in the overlapping domain of Quadrant III: $r > 0$, $\pi < \theta < 3\pi/2$.

However, $f_3(z) \neq f_1(z)$ in their overlapping domains of Quadrants I and IV; in fact, $f_3(z) = -f_1(z)$. E.g.,

$$f_1(1) = \sqrt{1}e^{i0/2} = 1 \tag{7.59}$$

but

$$f_3(1) = \sqrt{1}e^{i(2\pi)/2} = -1\,. \tag{7.60}$$

8 Example: Gamma Function

The Euler representation of the **gamma function** (see Fig. 8.1) is

$$\boxed{\Gamma(z) = \int_0^\infty e^{-t} t^{z-1}\, dt\,.} \tag{8.1}$$

Note: as $t \to 0$ the integrand behaves like t^{z-1} and so the integral behaves like $t^z/z = z^{-1} e^{z \ln t}$; therefore this definition of the gamma function is only valid for $\operatorname{Re} z > 0$.

We can integrate by parts:

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1}\, dt \tag{8.2a}$$

$$= \int_0^\infty u\, dv \qquad \textit{let } u = e^{-t},\ du = -e^{-t}\, dt \tag{8.2b}$$

$$dv = t^{z-1}\, dt,\ v = t^z/z \quad (z \neq 0)$$

$$v \to 0 \text{ as } t \to 0 \quad (\operatorname{Re} z > 0)$$

$$u \to 0 \text{ as } t \to \infty$$

$$= uv\Big|_0^\infty - \int_0^\infty v\, du \tag{8.2c}$$

$$= \int_0^\infty e^{-t} \frac{t^z}{z}\, dt \tag{8.2d}$$

$$= \frac{\Gamma(z+1)}{z}, \qquad \operatorname{Re} z > 0 \tag{8.2e}$$

Thus,

$$\boxed{\Gamma(z+1) = z\,\Gamma(z), \qquad \operatorname{Re} z > 0\,.} \tag{8.3}$$

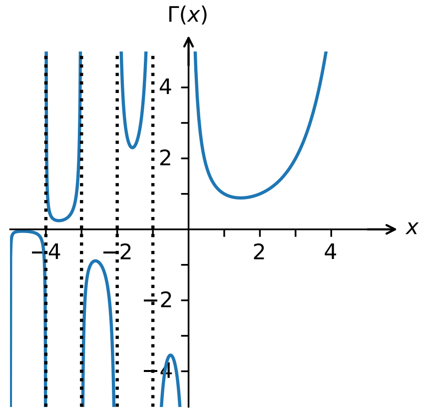


Figure 8.1: Gamma Function

Note: when $z = n$, $n > 0$,

$$\Gamma(n+1) = n\Gamma(n) \tag{8.4a}$$

and

$$\Gamma(1) = \int_0^\infty e^{-t}\,dt = 1\,. \tag{8.4b}$$

Therefore, write

$$\boxed{n! = \Gamma(n+1)\,, \quad n = 0, 1, 2, \dots\,.} \tag{8.5}$$

Use the relation $\Gamma(z+1) = z\,\Gamma(z)$ to analytically continue into the left-half of the complex plaine:

$$\Gamma(z) = \frac{\Gamma(z+1)}{z}\,, \qquad \operatorname{Re} z > -1,\ z \neq 0\,. \tag{8.6}$$

For example,

$$\Gamma(-\tfrac{1}{2}) = \frac{\Gamma(-\frac{1}{2}+1)}{-\frac{1}{2}} = -2\Gamma(\tfrac{1}{2})\,. \tag{8.7}$$

With repeated applications, can extend over (almost) all of the complex plane.

However, there is a singularity at $z = 0$ which prevents us from obtaining $\Gamma(0)$, $\Gamma(-1)$, $\Gamma(-2)$, ..., but other than this, the Gamma function has been extended over the entire complex plane.

Weirstrass Representation of the Gamma Function

Begin with the Euler representation:

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1}\, dt \tag{8.8a}$$

$$= \int_0^\alpha e^{-t} t^{z-1}\, dt + \int_\alpha^\infty e^{-t} t^{z-1}\, dt \tag{8.8b}$$

$$= \int_0^\alpha \left\{ \sum_{n=0}^\infty \frac{(-1)^n}{n!} t^n \right\} t^{z-1}\, dt + \int_\alpha^\infty e^{-t} t^{z-1}\, dt \tag{8.8c}$$

$$= \sum_{n=0}^\infty \frac{(-1)^n}{n!} \int_0^\alpha t^{n+z-1}\, dt + \int_\alpha^\infty e^{-t} t^{z-1}\, dt \tag{8.8d}$$

$$= \underbrace{\sum_{n=0}^\infty \frac{(-1)^n}{n!} \frac{\alpha^{n+z}}{z+n}}_{\substack{\text{simple poles at} \\ z = 0, -1, -2, \ldots}} + \underbrace{\int_\alpha^\infty e^{-t} t^{z-1}\, dt}_{\substack{\text{well-defined even} \\ \text{when } \operatorname{Re} z < 0 \\ \text{provided } \alpha > 0}} . \tag{8.8e}$$

Therefore this form is valid everywhere on the complex plane, with simple poles at $z = 0, -1, -2, \ldots$.

Note: the choice of $\alpha > 0$ does not matter; the Weirstrass representation of the gamma function is when $\alpha = 1$:

$$\boxed{\Gamma(z) = \sum_{n=0}^\infty \frac{(-1)^n}{n!} \frac{1}{z+n} + \int_1^\infty e^{-t} t^{z-1}\, dt.} \tag{8.9}$$

Euler Reflection Formula

For $0 < x < 1$,

$$\Gamma(x)\Gamma(1-x) = \int_0^\infty e^{-s} s^{x-1}\, ds \int_0^\infty e^{-t} t^{(1-x)-1}\, dt \tag{8.10a}$$

$$= \int_{s=0}^\infty \int_{t=0}^\infty e^{-(s+t)} s^{x-1} t^{-x}\, dt\, ds \tag{8.10b}$$

let $s = u - t$

$$= \int_{u=0}^\infty \int_{t=0}^u e^{-u} (u-t)^{x-1} t^{-x}\, dt\, du \tag{8.10c}$$

let $t = uv$

$$= \int_{u=0}^\infty \int_{v=0}^1 e^{-u} u^{x-1} (1-v)^{x-1} u^{-x} v^{-x} u\, dv\, du \tag{8.10d}$$

$$= \int_0^\infty e^{-u}\, du \int_0^1 \frac{(1-v)^{x-1}}{v^x}\, dv \tag{8.10e}$$

$$= \int_0^1 \frac{(1-v)^{x-1}}{v^x}\, dv \tag{8.10f}$$

let $v \to 1 - v$

$$= \int_0^1 \frac{v^{x-1}}{(1-v)^x}\, dv \tag{8.10g}$$

let $v = t/(1+t)$
$dv = dt/(1+t)^2$

$$= \int_0^\infty t^{x-1} (1-t)^{-x+1} \left(1 - \frac{t}{1+t}\right)^{-x} \frac{dt}{(1+t)^2} \tag{8.10h}$$

$$= \int_0^\infty t^{x-1} (1-t)^{-x+1} (1+t)^x (1+t)^{-2}\, dt \tag{8.10i}$$

$$= \int_0^\infty \frac{t^{x-1}}{1+t}\, dt\,, \qquad 0 < x < 1\,. \tag{8.10j}$$

We need to evaluate this integral.

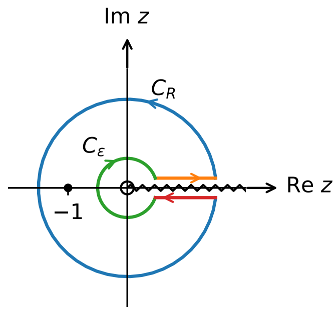


Figure 8.2: Contour for Integral in Euler Reflection Formula

Let

$$f(z) = \frac{z^{-a}}{z+1} \qquad |z| > 0,\ 0 < \arg z < 2\pi \tag{8.11}$$

where $a = 1 - x$, $0 < a < 1$. The function has a simple pole at $z = -1$ and a branch cut along the positive real axis.

Consider the contour shown in Fig. 8.2. The function is piecewise continuous (even though it is multivalued) so $\int_{C_\epsilon} f(z)\,dz$ and $\int_{C_R} f(z)\,dz$ exist.

For the linear parts of the contour above and below the branch cut write

$$f(z) = \frac{e^{-a\log z}}{z+1} = \frac{e^{-a(\ln r + i\theta)}}{re^{i\theta}+1} \quad \text{with} \quad z = re^{i\theta} \tag{8.12a}$$

so

$$f(z) = \begin{cases} \dfrac{r^{-a}}{r+1} & \text{for } z = re^{i0} \text{ (above the cut);} \\ \dfrac{r^{-a}}{r+1} e^{-i2a\pi} & \text{for } z = re^{i2\pi} \text{ (below the cut).} \end{cases} \tag{8.12b}$$

Now,

$$\begin{aligned} &\int_\epsilon^R \frac{r^a}{r+1}\,dr + \int_{C_R} f(z)\,dz - \int_\epsilon^R \frac{r^a}{r+1} e^{-i2\pi a}\,dr + \int_{C_\epsilon} f(z)\,dz \\ &\quad = 2\pi i \operatorname*{Res}_{z=-1} f(z) = 2\pi i(-1)^{-a} = 2\pi i (e^{i\pi})^{-a} &\text{(8.13a)} \\ &\quad = 2\pi i e^{-ia\pi}, &\text{(8.13b)} \end{aligned}$$

therefore

$$\int_{C_R} f(z)\,dz + \int_{C_\epsilon} f(z)\,dz = 2\pi i e^{-ia\pi} + (e^{-i2a\pi} - 1)\int_\epsilon^R \frac{r^a}{r+1}\,dr. \tag{8.14}$$

Since $a < 1$,

$$\left|\int_{C_\epsilon} f(z)\,dz\right| \le \frac{\epsilon^{-a}}{1-\epsilon} 2\pi\epsilon = \frac{2\pi}{1-\epsilon}\epsilon^{1-a} \tag{8.15a}$$

$$\to 0 \text{ as } \epsilon \to 0\,. \tag{8.15b}$$

Also, since $a > 0$,

$$\left|\int_{C_R} f(z)\,dz\right| \le \frac{R^{-a}}{R-1} 2\pi R = \frac{2\pi}{1-1/R}\frac{1}{R^a} \tag{8.16a}$$

$$\to 0 \text{ as } R \to \infty\,. \tag{8.16b}$$

Therefore, taking $\epsilon \to 0$ and $R \to \infty$,

$$\int_0^\infty \frac{r^a}{r+1}\,dr = 2\pi i \frac{e^{-ia\pi}}{1-e^{-i2a\pi}} = \pi\frac{2i}{e^{ia\pi}-e^{-ia\pi}} = \frac{\pi}{\sin a\pi}\,. \tag{8.17}$$

Thus (with $a = 1 - x$) we have

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin \pi x}\,, \qquad 0 < x < 1\,. \tag{8.18}$$

Now use analytic continuation to extend to the entire complex plane; the result is **Euler's reflection formula**:

$$\boxed{\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}\,,} \qquad z \ne 0, \pm 1, \pm 2, \ldots\,. \tag{8.19}$$

Note:

- $\Gamma(z)\Gamma(1-z)\sin\pi z = \pi$ is clearly entire;
- $\Gamma(z)$ has singularities at $z = 0, -1, -2, \ldots$;
- $\Gamma(1-z)$ has singularities at $z = 1, 2, 3, \ldots$;
- $\sin \pi z$ has zeros at $z = 0, \pm 1, \pm 2, \ldots$ that "cancel" the singularities;

thus we conclude

$$\frac{1}{\Gamma(z)} \quad \text{is entire.} \tag{8.20}$$

Useful results:

- When $z = \frac{1}{2}$,

$$\underbrace{\Gamma(\tfrac{1}{2})\Gamma(1-\tfrac{1}{2})}_{[\Gamma(\frac{1}{2})]^2} = \frac{\pi}{\sin\pi/2} = \pi \tag{8.21}$$

  so

$$\boxed{\Gamma(\tfrac{1}{2}) = \sqrt{\pi}\,.} \tag{8.22}$$

- Can then show:

$$\boxed{\Gamma(m+\tfrac{1}{2}) = \frac{1\cdot 3\cdot 5\cdot\cdots\cdot(2m-1)}{2^m}\sqrt{\pi}\,.} \tag{8.23}$$

  Therefore, define

$$\boxed{(2m-1)!! = 1\cdot 3\cdot 5\cdot\cdots\cdot(2m-1) = \frac{2^m\Gamma(m+\frac{1}{2})}{\sqrt{\pi}}} \tag{8.24}$$

  and

$$\boxed{(2m)!! = 2\cdot 4\cdot 6\cdot\cdots\cdot(2m) = \frac{(2m)!}{(2m-1)!!} = \frac{\sqrt{\pi}}{2^m}\frac{\Gamma(2m+1)}{\Gamma(m+\frac{1}{2})}} \tag{8.25}$$

  but note also that $(2m)!! = 2^m m!$ so

$$\boxed{\Gamma(2m+1) = \frac{2^{2m}}{\sqrt{\pi}}\,\Gamma(m+\tfrac{1}{2})\Gamma(m+1)\,.} \tag{8.26}$$

- This last result can be generalized to give **Legendre's duplication formula**

$$\boxed{\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}}\,\Gamma(z)\Gamma(z+\tfrac{1}{2})\,.} \tag{8.27}$$

- The binomial coefficient, Eq. (3.2), can be expressed in terms of the Gamma function as

$$\boxed{\binom{x}{y} = \frac{\Gamma(x+1)}{\Gamma(y+1)\Gamma(x-y+1)}\,.} \tag{8.28}$$

Problems

Problem 4.

Show that

a) $(1+i)^i = e^{-\pi/4}e^{2n\pi}\left[\cos(\frac{1}{2}\ln 2) + i\sin(\frac{1}{2}\ln 2)\right]$ where $n = 0, \pm 1, \pm 2, \ldots.$

b) $(-1)^{1/\pi} = \cos(2n+1) + i\sin(2n+1)$ where $n = 0, \pm 1, \pm 2, \ldots.$

Problem 5.

Derive the Cauchy-Riemann equations in polar coordinates

$$\frac{\partial u}{\partial r} = \frac{1}{r}\frac{\partial v}{\partial \theta} \qquad \text{and} \qquad \frac{1}{r}\frac{\partial u}{\partial \theta} = -\frac{\partial v}{\partial r}$$

and use these to show that if $f(z) = u(r,\theta) + iv(r,\theta)$ is analytic in some domain D that does not contain the origin then throughout D the function $u(r,\theta)$ satisfies the polar form of Laplace's equation:

$$r^2\frac{\partial^2 u}{\partial r^2} + r\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial \theta^2} = 0.$$

Verify that $u(r,\theta) = \ln r$ is harmonic in $r > 0$, $0 < \theta < 2\pi$ and show that $v(r,\theta) = \theta$ is its harmonic conjugate.

Problem 6.

Use the Cauchy-Riemann equations to determine which of the following are analytic functions of the complex variable z:

a) $|z|$;

b) $\mathrm{Re}\, z$;

c) $e^{\sin z}$.

Problem 7.

Let C denote the circle $|z-z_0| = R$ taken counterclockwise. Use the parametric representation $z = z_0 + Re^{i\theta}$, $-\pi \le \theta \le \pi$, for C to derive the following integral formulas:

a) $\displaystyle\oint_C \frac{dz}{z-z_0} = 2\pi i$;

b) $\displaystyle\oint_C (z-z_0)^{n-1}\, dz = 0 \quad \text{where} \quad n = \pm 1, \pm 2, \ldots$;

c) $\displaystyle\left|\oint_C \frac{\mathrm{Log}(z-z_0)}{(z-z_0)^2}\, dz\right| < 2\pi\left(\frac{\pi + \ln R}{R}\right) \to 0$ as $R \to \infty$.

Problem 8.

Represent the function $(z+1)/(z-1)$ by

a) its Maclaurin series, and give the region of validity for the reprensentation;

b) its Laurent series for the domain $1 < |z| < \infty$.

Problem 9.

Use residues to evaluate these integrals where the contour C is the circle $|z| = 3$ taken in the positive sense:

a) $\displaystyle\oint_C \frac{\exp(-z)}{z^2}\, dz$;

b) $\displaystyle\oint_C z^2 \exp\left(\frac{1}{z}\right) dz$;

c) $\displaystyle\oint_C \frac{z+1}{z^2-2z}\, dz.$

Module III

Evaluation of Integrals

Motivation

Let's face it: integration can be a pain in the neck. Nowadays you can use computer algebra packages such as Maple or Mathematica or WolframAlpha to do integrals for you; more traditionally one would use tables of integrals. But it is still useful to be able to do elementary integrals, and some useful tricks are reviewed here. We also explore contour integration further and touch on topics such as asymptotic series (useful for evaluating functions at large arguments) and saddle-point methods (which can give approximate solutions to integrals).

9 Elementary Methods of Integration

- Introduce a complex variable.

Ex. 9.1. Evaluate

$$I = \int_0^\infty e^{-ax} \cos bx \, dx \tag{9.1a}$$

$$= \mathrm{Re} \int_0^\infty e^{-ax} e^{ibx} \, dx \tag{9.1b}$$

$$= \mathrm{Re} \frac{1}{a - ib} \tag{9.1c}$$

$$= \frac{a}{a^2 + b^2} . \tag{9.1d}$$

Similarly

$$I = \int_0^\infty e^{-ax} \sin bx \, dx \tag{9.2a}$$

$$= \mathrm{Im} \int_0^\infty e^{-ax} e^{ibx} \, dx \tag{9.2b}$$

$$= \mathrm{Im} \frac{1}{a - ib} \tag{9.2c}$$

$$= \frac{b}{a^2 + b^2} . \tag{9.2d}$$

- Differentiation or integration with respect to a parameter.

Ex. 9.2. Evaluate

$$I = \int_0^\infty x\, e^{-ax} \cos bx\, dx\,. \tag{9.3}$$

Let

$$I(a) = \int_0^\infty e^{-ax} \cos bx\, dx = \frac{a}{a^2+b^2}\,; \tag{9.4}$$

then

$$I = -\frac{d}{da} I(a) = \frac{d}{da}\frac{a}{a^2+b^2} = \frac{a^2-b^2}{(a^2+b^2)^2}\,. \tag{9.5}$$

Ex. 9.3. Evaluate

$$I = \int_0^\infty \frac{\sin x}{x}\, dx\,. \tag{9.6}$$

Let

$$I(a) = \int_0^\infty \frac{e^{-ax}\sin x}{x}\, dx \tag{9.7}$$

so $I = I(0)$. Now,

$$\frac{d}{da} I(a) = -\int_0^\infty e^{-ax} \sin x\, dx = -\frac{1}{a^2+1} \tag{9.8}$$

so we have

$$I(a) = -\int \frac{da}{a^2+1} = C - \arctan a \tag{9.9}$$

but since $I(\infty) = 0$, we find $C = \pi/2$; therefore

$$I(a) = \frac{\pi}{2} - \arctan a \tag{9.10}$$

and finally

$$I = I(0) = \frac{\pi}{2}\,. \tag{9.11}$$

- Be clever.

Ex. 9.4. Evaluate

$$I = \int_{-\infty}^{\infty} e^{-x^2}\,dx\,. \tag{9.12}$$

Consider

$$\begin{aligned}
I^2 &= \int_{-\infty}^{\infty} e^{-x^2}\,dx \int_{-\infty}^{\infty} e^{-y^2}\,dy && (9.13a)\\
&= \iint_{-\infty}^{\infty} e^{-(x^2+y^2)}\,dx\,dy && (9.13b)\\
&\quad \text{change to polar coordinates } r^2 = x^2+y^2;\ dx\,dy = r\,d\theta\,dr\\
&= \int_0^{2\pi} d\theta \int_0^{\infty} e^{-r^2}\,r\,dr && (9.13c)\\
&\quad \text{let } u = r^2;\ du = 2r\,dr\\
&= 2\pi \cdot \frac{1}{2}\int_0^{\infty} e^{-u}\,du && (9.13d)\\
&= \pi\,. && (9.13e)
\end{aligned}$$

Therefore,

$$I = \sqrt{\pi}\,. \tag{9.14}$$

10 Contour Integration

Improper Real Integrals

Types:

- $$\int_0^{\infty} f(x)\,dx = \lim_{R\to\infty} \int_0^R f(x)\,dx\,. \tag{10.1}$$
- $$\int_{-\infty}^{\infty} f(x)\,dx = \lim_{R_1\to\infty} \int_{-R_1}^{0} f(x)\,dx + \lim_{R_2\to\infty} \int_0^{R_2} f(x)\,dx\,. \tag{10.2}$$
- $$⨍_{-\infty}^{\infty} f(x)\,dx = \lim_{R\to\infty} \int_{-R}^{R} f(x)\,dx\,. \tag{10.3}$$

The third is known as the **Cauchy principal value**.

If $\int_{-\infty}^{\infty} f(x)\,dx$ converges then its value is the same as $⨍_{-\infty}^{\infty} f(x)\,dx$.

However, note that $⨍_{-\infty}^{\infty} x\,dx = 0$ while $\int_{-\infty}^{\infty} x\,dx$ diverges.

If $f(x)$ is an *even* function then

$$\frac{1}{2} ⨍_{-\infty}^{\infty} f(x)\,dx = \frac{1}{2} \int_{-\infty}^{\infty} f(x)\,dx = \int_0^{\infty} f(x)\,dx\,. \tag{10.4}$$

Evaluation of improper real integrals can often be done easily using the Cauchy principal value and residues.

Ex. 10.1. Evaluate:

$$\int_0^\infty \frac{2x^2-1}{x^4+5x^2+4}\,dx = \frac{1}{2}\int_{-\infty}^{\infty} \frac{2x^2-1}{x^4+5x^2+4}\,dx\,. \tag{10.5}$$

Let

$$f(z) = \frac{2z^2-1}{z^4+5z^2+4} = \frac{2z^2-1}{(z^2+1)(z^2+4)}\,. \tag{10.6}$$

This function has isolated simple poles at $z = \pm i$, $z = \pm 2i$.

Consider the contour $C = L_R + C_R$, $R > 2$, as shown in Fig. 10.1.

We have:

$$\int_{-R}^{R} f(x)\,dx + \int_{C_R} f(z)\,dz = 2\pi i\left[\operatorname*{Res}_{z=i} f(z) + \operatorname*{Res}_{z=2i} f(z)\right]. \tag{10.7}$$

Note:

- $f(z) = \dfrac{\phi_1(z)}{z-i}$ where $\phi_1(z) = \dfrac{2z^2-1}{(z+i)(z^2+4)}$

$$\implies \operatorname*{Res}_{z=i} f(z) = \phi_1(i) = \frac{-3}{(2i)(3)} = -\frac{1}{2i}\,. \tag{10.8a}$$

- $f(z) = \dfrac{\phi_2(z)}{z-2i}$ where $\phi_2(z) = \dfrac{2z^2-1}{(z^2+1)(z+2i)}$

$$\implies \operatorname*{Res}_{z=2i} f(z) = \phi_2(2i) = \frac{-9}{(-3)(4i)} = \frac{3}{4i}\,. \tag{10.8b}$$

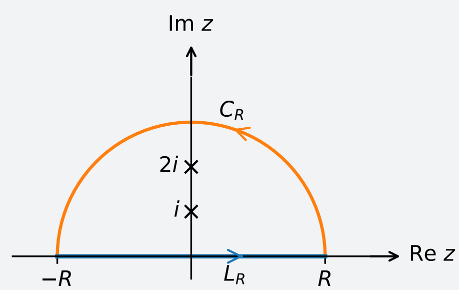


Figure 10.1: Contour for Ex. 10.1

Therefore

$$\int_{-R}^{R} f(x)\,dx = 2\pi i\left[\operatorname*{Res}_{z=i} f(z) + \operatorname*{Res}_{z=2i} f(z)\right] - \int_{C_R} f(z)\,dz \tag{10.9a}$$

$$= 2\pi i\left(-\frac{1}{2i} + \frac{3}{4i}\right) - \int_{C_R} f(z)\,dz \tag{10.9b}$$

$$= \frac{\pi}{2} - \int_{C_R} f(z)\,dz\,. \tag{10.9c}$$

We need to figure out what $\int_{C_R} f(z)\,dz$ is as $R \to \infty$.

Note: when $|z| = R$,

$$|2z^2 - 1| \le 2|z|^2 + 1 = 2R^2 + 1 \tag{10.10a}$$

$$|z^4 + 5z^2 + 4| = |z^2 + 1||z^2 + 4|$$
$$\ge \left||z|^2 - 1\right|\left||z^2| - 4\right| = (R^2 - 1)(R^2 - 4) \tag{10.10b}$$

$$\implies |f(z)| \le M_R \quad \text{where} \quad M_R = \frac{2R^2 + 1}{(R^2 - 1)(R^2 - 4)} \tag{10.10c}$$

and so,

$$\left|\int_{C_R} f(z)\,dz\right| \le M_R \pi R = \frac{\pi R(2R^2 + 1)}{(R^2 - 1)(R^2 - 4)} \tag{10.11a}$$

$$\to 0 \text{ as } R \to \infty\,. \tag{10.11b}$$

Thus,

$$⨍_{-\infty}^{\infty} \frac{2x^2 - 1}{x^4 + 5x^2 + 4}\,dx = \lim_{R\to\infty} \int_{-R}^{R} \frac{2x^2 - 1}{x^4 + 5x^2 + 4}\,dx = \frac{\pi}{2} \tag{10.12}$$

and therefore

$$\int_{0}^{\infty} \frac{2x^2 - 1}{x^4 + 5x^2 + 4}\,dx = \frac{\pi}{4}\,. \tag{10.13}$$

To evaluate integrals of the form

$$\int_{-\infty}^{\infty} f(x) \sin ax \, dx \quad (a > 0) \qquad \text{or} \qquad \int_{-\infty}^{\infty} f(x) \cos ax \, dx \tag{10.14}$$

try

$$\int_{-R}^{R} f(x) \cos ax \, dx + i \int_{-R}^{R} f(x) \sin ax \, dx = \int_{-R}^{R} f(x) e^{iax} \, dx \tag{10.15}$$

and use the fact that $|e^{iaz}| = e^{-ay}$ is bounded in the upper-half plane $y \geq 0$.

Ex. 10.2. Compute

$$\fint_{-\infty}^{\infty} \frac{x \sin x}{x^2 + 2x + 2} \, dx . \tag{10.16}$$

Let

$$f(z) = \frac{z}{z^2 + 2z + 2} = \frac{z}{(z - z_1)(z - z_1^*)} \quad \text{where} \quad z_1 = -1 + i . \tag{10.17}$$

Note: z_1 is a simple pole of $f(z)e^{iz}$ in the upper-half plane with residue

$$b_1 = \operatorname*{Res}_{z=z_1} f(z)e^{iz} = \frac{z_1 e^{iz_1}}{z_1 - z_1^*} . \tag{10.18}$$

Use the contour $C = L_R + C_R$ shown in Fig. 10.2. We see

$$\int_{-R}^{R} \frac{x e^{ix}}{x^2 + 2x + 2} \, dx = 2\pi i b_1 - \underbrace{\int_{C_R} f(z) e^{iz} \, dz}_{\text{want to bound this}} . \tag{10.19}$$

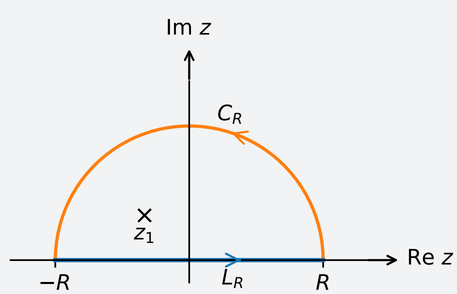


Figure 10.2: Contour for Ex. 10.2

Note: $|f(z)| \leq M_R$ where $M_R = R/(R-\sqrt{2})^2$ and $|e^{iz}| = e^{-y} \leq 1$ so

$$\left|\int_{C_R} f(z)e^{iz}\,dz\right| \leq M_R \pi R = \frac{\pi R^2}{(R-\sqrt{2})^2} \tag{10.20}$$

but this does *not* go to zero as $R \to \infty$.

We need to be more careful:

$$\int_{C_R} f(z)e^{iz}\,dz = \int_0^{\pi} f(Re^{i\theta})e^{iRe^{i\theta}}\,iRe^{i\theta}\,d\theta\,. \tag{10.21}$$

Now $|f(Re^{i\theta})| \leq M_R$ and $|e^{iRe^{i\theta}}| \leq e^{-R\sin\theta}$ so

$$\left|\int_{C_R} f(z)e^{iz}\,dz\right| \leq M_R R \int_0^{\pi} e^{-R\sin\theta}\,d\theta\,. \tag{10.22}$$

We use **Jordan's inequality** to bound the integral: since $\sin\theta \leq 2\theta/\pi$ for $0 \leq \theta \leq \pi/2$ (see Fig. 10.3),

$$\int_0^{\pi} e^{-R\sin\theta}\,d\theta \leq 2\int_0^{\pi/2} e^{-2R\theta/\pi} = 2\frac{\pi}{2R}(1-e^{-R}) \tag{10.23a}$$

$$< \frac{\pi}{R}\,. \tag{10.23b}$$

Thus,

$$\left|\int_{C_R} f(z)e^{iz}\,dz\right| < M_R R\frac{\pi}{R} = \pi M_R \tag{10.24a}$$

$$\to 0 \text{ as } R \to \infty \tag{10.24b}$$

and therefore

$$⨍_{-\infty}^{\infty} \frac{x\sin x}{x^2+2x+2}\,dx = \operatorname{Im}(2\pi i b_1) = \frac{\pi}{e}(\sin 1 + \cos 1)\,. \tag{10.25}$$

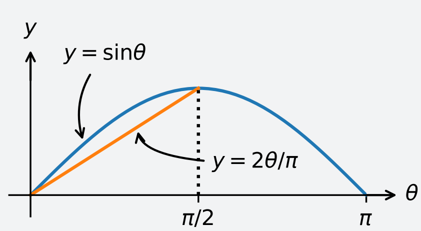


Figure 10.3: Jordan's Inequality

Definite Integrals Involving Sines and Cosines

For integrals of the form

$$I = \int_0^{2\pi} F(\sin\theta, \cos\theta)\, d\theta \tag{10.26}$$

use the following trick: Let $z = e^{i\theta}$, $0 \le \theta \le 2\pi$ and substitute:

$$\sin\theta = \frac{z - z^{-1}}{2i}, \qquad \cos\theta = \frac{z + z^{-1}}{2}, \qquad d\theta = \frac{dz}{iz}. \tag{10.27}$$

Then

$$I = \oint_C F\left(\frac{z - z^{-1}}{2i}, \frac{z + z^{-1}}{2}\right)\frac{dz}{iz} \tag{10.28}$$

where C is the unit circle about the origin evaluated in the positive direction.

Ex. 10.3. Compute

$$I = \int_0^{2\pi} \frac{d\theta}{1 + a\sin\theta}, \quad -1 < a < 1,\ a \neq 0. \tag{10.29}$$

Perform the suggested substitutions:

$$I = \oint_C \frac{1}{1 + a\dfrac{z - z^{-1}}{2i}}\frac{dz}{iz} = \oint_C \frac{2/a}{z^2 + (2i/a)z - 1}\, dz. \tag{10.30}$$

The integrand is

$$f(z) = \frac{2/a}{(z - z_1)(z - z_2)} \tag{10.31a}$$

with

$$z_1 = \left(\frac{-1 + \sqrt{1 - a^2}}{a}\right)i \quad \text{and} \quad z_2 = \left(\frac{-1 - \sqrt{1 - a^2}}{a}\right)i. \tag{10.31b}$$

Note: because $|a| < 1$, $|z_2| = (1 + \sqrt{1 - a^2})/|a| > 1$ and since $|z_1 z_2| = 1$, $|z_1| < 1$.
Therefore only z_1 is contained within C, and its residue is

$$\operatorname*{Res}_{z=z_1} f(z) = \frac{2/a}{z_1 - z_2} = \frac{1}{i\sqrt{1 - a^2}} \tag{10.32}$$

and thus

$$I = 2\pi i \operatorname*{Res}_{z=z_1} f(z) = \frac{2\pi}{\sqrt{1 - a^2}}, \quad -1 < a < 1 \tag{10.33}$$

(the case $a = 0$ is obvious).

11 Approximate Expansions of Integrals

The idea is to expand the integrand in a series.

Ex. 11.1 (Error function)**.** The **error function** is (see Fig. 11.1)

$$\boxed{\operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt\,.} \tag{11.1}$$

Expand the integrand in a power series and integrate term-by-term:

$$\operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_0^x \left\{ 1 - t^2 + \frac{t^4}{2!} - \frac{t^6}{3!} + \cdots \right\} dt \tag{11.2a}$$

$$= \frac{2}{\sqrt{\pi}} \left\{ x - \frac{x^3}{3} + \frac{x^5}{5 \cdot 2!} - \frac{x^7}{7 \cdot 3!} + \cdots \right\}. \tag{11.2b}$$

This converges for all x but it is only really useful for small x.
We would like a large-x expansion.

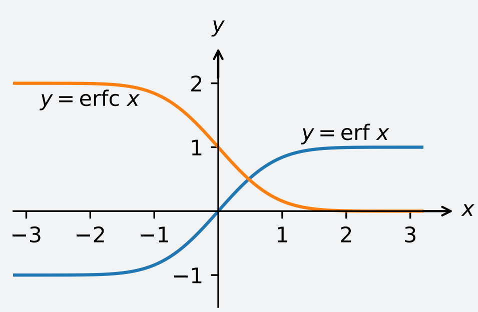


Figure 11.1: Error Function and Complementary Error Function

As $x \to \infty$, erf $x \to 1$ so compute the **complementary error function** (see Fig. 11.1)

$$\operatorname{erfc} x = 1 - \operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2}\, dt \tag{11.3a}$$

integrate by parts:
$u = 1/t$, $du = -dt/t^2$
$dv = te^{-t^2}dt$, $v = -\frac{1}{2}e^{-t^2}$

$$= \frac{2}{\sqrt{\pi}}\left[\frac{1}{2}\frac{e^{-x^2}}{x} - \int_x^\infty \frac{1}{2}\frac{e^{-t^2}}{t^2}\, dt\right] \tag{11.3b}$$

by parts again:
$u = 1/t^3$, $dv = te^{-t^2}dt$

$$= \frac{2}{\sqrt{\pi}}\left[\frac{1}{2}\frac{e^{-x^2}}{x} - \frac{1}{2^2}\frac{e^{-x^2}}{x^3} + \int_x^\infty \frac{1}{2}\frac{3}{2}\frac{e^{-t^2}}{t^4}\, dt\right] \tag{11.3c}$$

and so on.... After n times,

$$\begin{aligned}\operatorname{erfc} x = \frac{2}{\sqrt{\pi}} e^{-x^2}\Bigg\{&\frac{1}{2x} - \frac{1}{2^2x^3} + \frac{1\cdot 3}{2^3x^5} - \frac{1\cdot 3\cdot 5}{2^4x^7} + \cdots \\ &+(-1)^{n-1}\frac{1\cdot 3\cdot 5\cdots(2n-3)}{2^n x^{2n-1}}\Bigg\} \\ &+(-1)^n \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^n}\frac{2}{\sqrt{\pi}}\int_x^\infty \frac{e^{-t^2}}{t^{2n}}\, dt.\end{aligned} \tag{11.3d}$$

Consider the series with terms

$$a_n = (-1)^{n-1}\frac{(2n-3)!!}{2^n x^{2n-1}}. \tag{11.4}$$

Apply the ratio test:

$$\left|\frac{a_{n+1}}{a_n}\right| = \frac{(2n-1)!!}{(2n-3)!!}\frac{2^n}{2^{n+1}}\frac{x^{2n-1}}{x^{2n+1}} = \frac{2n-1}{2}\frac{1}{x^2} \tag{11.5a}$$

$$\sim \frac{n}{x^2} \quad \text{for large } n. \tag{11.5b}$$

For large n, we can always find an n larger than x^2 and so the ratio test indicates this series will not converge.

However, the terms are getting smaller until term $n \approx x^2$.
The error is smallest if we truncate the series here.

Asymptotic Series

The series

$$S(z) = c_0 + \frac{c_1}{z} + \frac{c_2}{z^2} + \cdots \tag{11.6}$$

is an **asymptotic series** expansion of some function $f(z)$ provided that for any n the error involved in terminating the series with the term $c_n z^{-n}$ goes to zero faster than z^{-n} as $|z| \to \infty$ (for some range of $\arg z$):

$$\lim_{|z|\to\infty} z^n [f(z) - S_n(z)| = 0 \qquad (\arg z \text{ in some range}) \tag{11.7a}$$

where

$$S_n(z) = c_0 + \frac{c_1}{z} + \frac{c_2}{z^2} + \cdots + \frac{c_n}{z^n}\,. \tag{11.7b}$$

Write: $f(z) \sim S(z)$ where "$\sim$" means "asymptically equal to."

Ex. 11.1 (continued)**.** Returning to the complementary error function,

$$\operatorname{erfc} x - \begin{pmatrix} \text{asymptotic} \\ \text{series} \end{pmatrix} = \begin{pmatrix} \text{remainder} \\ \text{integral} \end{pmatrix} \tag{11.8a}$$

where

$$\begin{pmatrix} \text{asymptotic} \\ \text{series} \end{pmatrix} = \frac{2}{\sqrt{\pi}} e^{-x^2} \left\{ \frac{1}{2x} - \frac{1}{2^2 x^3} + \cdots + (-1)^n \frac{(2n-3)!!}{2^n x^{2n-1}} \right\} \tag{11.8b}$$

and

$$\begin{pmatrix} \text{remainder} \\ \text{integral} \end{pmatrix} = (-1)^n \frac{(2n-1)!!}{2^n} \frac{2}{\sqrt{\pi}} \int_x^\infty \frac{e^{-t^2}}{t^{2n}} \, dt \tag{11.8c}$$

Note: the series is in steps of x^2.

To show the asymptotic series truly is an asymptotic series, consider

$$\begin{aligned} x^{2n} \left[\operatorname{erfc} x - \begin{pmatrix} \text{asymptotic} \\ \text{series} \end{pmatrix} \right] &= (-1)^n \frac{(2n-1)!!}{2^n} \frac{2}{\sqrt{\pi}} x^{2n} \int_x^\infty \frac{e^{-t^2}}{t^{2n}} \, dt && (11.9a) \\ &< (-1)^n \frac{(2n-1)!!}{2^n} \frac{2}{\sqrt{\pi}} \cancel{x^{2n}} \int_x^\infty \frac{e^{-t^2}}{\cancel{x^{2n}}} \, dt && (11.9b) \\ &= (-1)^n \frac{(2n-1)!!}{2^n} \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} \, dt && (11.9c) \\ &\to 0 \text{ as } x \to \infty. && (11.9d) \end{aligned}$$

Therefore we see that the asymptotic series is indeed an asymptotic series.

Ex. 11.2 (Exponential integral)**.** The **exponential integral** (see Fig. 11.2) is

$$\boxed{\operatorname{Ei} x = \int_{-\infty}^{x} \frac{e^t}{t}\, dt\,.} \tag{11.10}$$

We seek an asymptotic series for $x \to -\infty$.

Consider

$$\begin{aligned}
\operatorname{Ei}(-x) &= \int_{-\infty}^{-x} \frac{e^t}{t}\, dt && \text{(11.11a)}\\
&= \int_{\infty}^{x} \frac{e^{-t}}{t}\, dt && \text{(11.11b)}\\
&= -\frac{e^{-x}}{x} - \int_{\infty}^{x} \frac{e^{-t}}{t^2}\, dt && \text{(11.11c)}\\
&= -\frac{e^{-x}}{x} + \frac{e^{-x}}{x^2} + 2\int_{\infty}^{x} \frac{e^{-t}}{t^2}\, dt && \text{(11.11d)}
\end{aligned}$$

integrate by parts
$u = 1/t,\ du = -dt/t^2$
$dv = e^{-t}dt,\ v = -e^{-t}$

by parts again

and so on. After n times,

$$\begin{aligned}
-\operatorname{Ei}(-x) = \frac{e^{-x}}{x}\left\{1 - \frac{1}{x} + \frac{2!}{x^2} - \frac{3!}{x^3} + \cdots + (-1)^n \frac{n!}{x^n}\right\}\\
+ (-1)^n (n+1)! \int_{\infty}^{x} \frac{e^{-t}}{t^{n+2}}\, dt\,.
\end{aligned} \tag{11.12}$$

- Asymptotic series for $\operatorname{Ei}(-x)$:

$$-\operatorname{Ei}(-x) = \frac{e^{-x}}{x}\left(1 - \frac{1}{x} + \frac{2!}{x^2} - \frac{3!}{x^3} + \cdots\right). \tag{11.13}$$

- Identity for remainder term:

$$\int_{x}^{\infty} \frac{e^{-t}}{t^n}\, dt = \frac{(-1)^n}{(n-1)!}\left\{\operatorname{Ei}(-x) + \frac{e^{-x}}{x}\left[1 - \frac{1}{x} + \frac{2!}{x^2} - \cdots + (-1)^n \frac{(n-2)!}{x^{n-2}}\right]\right\}. \tag{11.14}$$

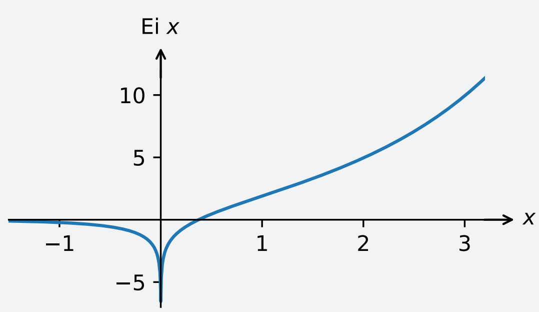


Figure 11.2: Exponential Integral

12 Saddle-Point Methods

Method of Steepest Descent

For sharply peaked integrands, the integral is dominated by the region near the peak of the integrand.

Ex. 12.1. Obtain an approximation of $\Gamma(x+1)$ for $x \gg 1$.

Recall the Euler representation of the gamma function:

$$\Gamma(x+1) = \int_0^\infty t^x e^{-t}\, dt\,. \tag{12.1}$$

The integrand is shown in Fig. 12.1.
It is peaked at the value t_0 where

$$0 = \frac{d}{dt}(t^x e^{-t})\Big|_{t=t_0} \tag{12.2a}$$

$$= e^{-t_0}\left(-t_0^x + x t_0^{x-1}\right) \tag{12.2b}$$

and so

$$t_0 = x\,. \tag{12.2c}$$

The integrand of the gamma function is sharply peaked for large x.

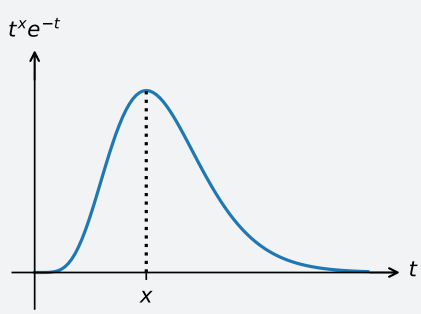


Figure 12.1: Integrand of the Gamma Function

Write integrand as $e^{f(t)} = e^{x\ln t - t}$ and expand $f(t)$ in a Taylor series about $t = t_0 = x$:

$$f(t) = x\ln t - t \quad \Longrightarrow \quad f(x) = x\ln x - x \tag{12.3a}$$

$$f'(t) = \frac{x}{t} - 1 \quad \Longrightarrow \quad f'(x) = 0 \tag{12.3b}$$

$$f''(t) = -\frac{x}{t^2} \quad \Longrightarrow \quad f''(x) = -\frac{1}{x} \tag{12.3c}$$

and so

$$f(t) = f(x) + f'(x)(t-x) + \frac{1}{2!}f''(x)(t-x)^2 + \cdots \tag{12.3d}$$

$$\approx x\ln x - x - \frac{1}{2x}(t-x)^2 . \tag{12.3e}$$

Therefore we have

$$\Gamma(x+1) \approx \int_0^\infty \exp\left[x\ln x - x - \frac{1}{2x}(t-x)^2\right] dt \tag{12.4a}$$

extend integration domain

$$\approx \int_{-\infty}^\infty \exp\left[x\ln x - x - \frac{1}{2x}(t-x)^2\right] dt \tag{12.4b}$$

$$= e^{x\ln x - x}\int_{-\infty}^\infty e^{-(t-x)^2/2x}\, dt \tag{12.4c}$$

$$= \sqrt{2\pi x}\, x^x e^{-x} . \tag{12.4d}$$

This is the first term of **Stirling's formula**.

In general, the idea is to evaluate integrals of the form

$$I(\alpha) = \int_C e^{\alpha f(z)}\, dz \qquad (\alpha \text{ large and positive}) \tag{12.5}$$

by deforming the contour so as to concentrate most of the integral near where $\mathrm{Re}\, f(z)$ is largest.

Let $z = x + iy$ and $f(z) = u(x,y) + iv(x,y)$. When $f(z)$ is analytic (not at a singularity)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \qquad \text{(harmonic)} \tag{12.6}$$

so any flat spot $\partial u/\partial x = \partial u/\partial y = 0$ is neither a maximum or a minimum since $\partial^2 u/\partial x^2 = -\partial^2 u/\partial y^2$. Therefore all such points are saddle points, and, by the Cauchy-Riemann condition, they are saddle points of v as well and at the saddle point $f'(z_0) = 0$.

Therefore

$$f(z) \approx f(z_0) + \frac{1}{2} f''(z_0)(z - z_0)^2 \tag{12.7}$$

where z_0 is a saddle point.

Let $f''(z_0) = \rho e^{i\phi}$ and let $z - z_0 = s e^{i\psi}$. Then,

$$u \approx u(x_0, y_0) + \frac{1}{2}\rho s^2 \cos(\phi + 2\psi) \tag{12.8a}$$

$$v \approx v(x_0, y_0) + \frac{1}{2}\rho s^2 \sin(\phi + 2\psi)\,. \tag{12.8b}$$

The path of steepest descent from the saddle point is when

$$\cos(\phi + 2\psi) = -1\,. \tag{12.9}$$

In this direction, $\sin(\phi + 2\psi) = 0$, so v is constant.

Deform the contour to go along the path of steepest descent:

$$I(\alpha) \approx e^{\alpha f(z_0)} \int_{-\infty}^{\infty} e^{-\alpha\rho s^2/2} e^{i\psi}\, ds \tag{12.10a}$$

where

$$\psi = -\frac{\phi}{2} \pm \frac{\pi}{2} \tag{12.10b}$$

and the sign depends on which we travel over the saddle.

Therefore

$$I(\alpha) \approx \sqrt{\frac{2\pi}{\alpha\rho}}\, e^{\alpha f(z_0)} e^{i\psi}\,. \tag{12.11}$$

Ex. 12.2. Steepest descent approximation for $\Gamma(z+1)$:

$$\Gamma(z+1) = \int_0^\infty e^{-t+z\ln t}\,dt = \int_0^\infty e^{rf(t)}dt \tag{12.12a}$$

where $r = |z|$ (assume r is large) and

$$f(t) = \frac{1}{r}(-t + z\log t). \tag{12.12b}$$

Let $z = re^{i\theta}$. Then

$$f(t) = \left(\log t - \frac{t}{z}\right)e^{i\theta} \tag{12.13a}$$

$$f'(t) = \left(\frac{1}{t} - \frac{1}{z}\right)e^{i\theta} \quad \Longrightarrow \quad f'(t_0) = 0 \text{ for } t_0 = z \tag{12.13b}$$

$$f''(t) = -\frac{1}{t^2}e^{i\theta} \tag{12.13c}$$

so

$$f(t_0) = (\log z - 1)e^{i\theta} \tag{12.14a}$$

$$f''(t_0) = \rho e^{i\phi} = -\frac{e^{i\theta}}{z^2} = -\frac{1}{r^2}e^{-i\theta} \quad \Longrightarrow \quad \rho = \frac{1}{r^2} \text{ and } \phi = \pi - \theta. \tag{12.14b}$$

Deform the contour to go through $t_0 = z$ at an angle ψ for which $\cos(\phi + 2\psi) = -1$, so

$$\psi = \frac{\theta}{2} \qquad \text{or} \qquad \psi = \frac{\theta}{2} - \pi. \tag{12.15}$$

To figure out which one of these to choose, we need to look at the topography of the surface $u(t) = \operatorname{Re} f(t)$ for a particular choice of z.
For example, when $z = 3e^{i\pi/4}$ so $r = 3$ and $\theta = \pi/4$, have

$$\operatorname{Re} f(t) = \operatorname{Re}\left(e^{i\pi/4}\log t - \frac{t}{3}\right). \tag{12.16}$$

In Fig. 12.2 this function is plotted and it is seen that the correct direction to traverse the saddle is with $\psi = \theta/2 = \pi/8$ rather than $\psi = \theta/2 - \pi = -7\pi/8$. Thus,

$$\Gamma(z+1) = \int_C e^{rf(t)}\,dt \tag{12.17a}$$

$$\approx \sqrt{\frac{2\pi}{r\rho}}\,e^{rf(z)}e^{i\psi} \tag{12.17b}$$

$$\Big\downarrow \ \rho = 1/r^2 \textit{ and } \psi = \theta/2$$

$$= \sqrt{2\pi r}\,e^{z\log z - z}\,e^{i\theta/2} \tag{12.17c}$$

$$\Big\downarrow \ \sqrt{r}e^{i\theta/2} = z^{1/2}$$

$$= \sqrt{2\pi}\,z^{z+1/2}e^{-z} \tag{12.17d}$$

This is the first term in an asymptotic series.

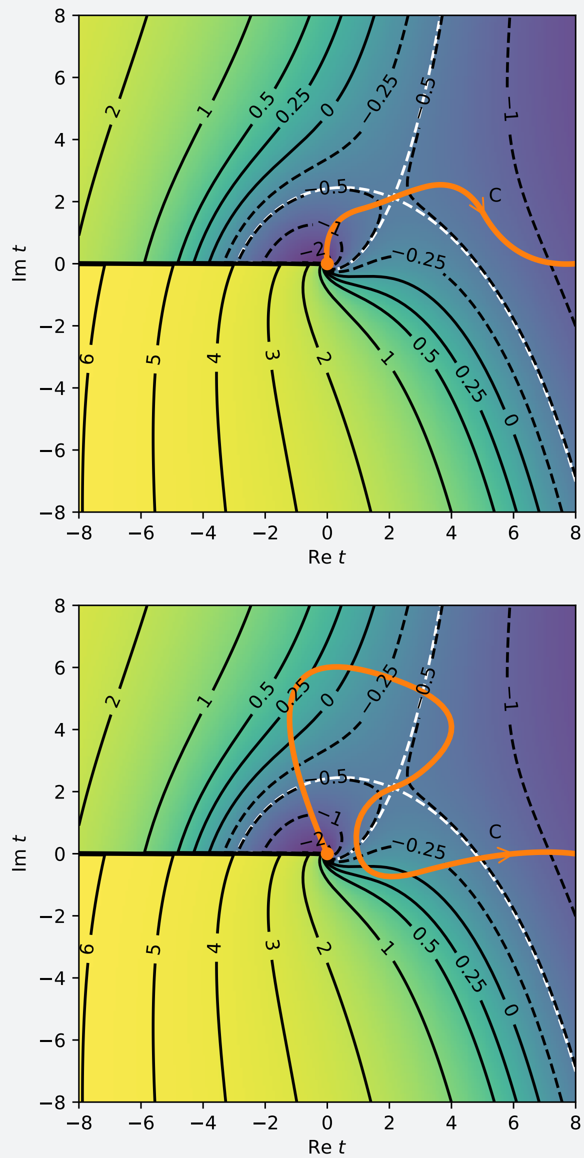


Figure 12.2: Topography of the surface $\mathrm{Re}(e^{i\pi/4}\log t - t/3)$. The saddle point is at the intersection of the white contour lines. Top: the contour is deformed so that it correctly goes over the saddle point $t_0 = 3e^{i\pi/4}$. Bottom: the contour is incorrectly deformed and goes over the ridge three times.

Since

$$\Gamma(z) = \frac{1}{z}\Gamma(z+1) \approx \sqrt{2\pi} z^{z-1/2} e^{-z} \tag{12.18}$$

write an asymptotic series:

$$\Gamma(z) \sim \sqrt{2\pi} z^{z-1/2} e^{-z} \left\{1 + \frac{A}{z} + \frac{B}{z^2} + \frac{C}{z^3} + \cdots\right\} \tag{12.19}$$

and use the recurrence $\Gamma(z+1) = z\Gamma(z)$ to find $A, B, C, \ldots$ as follows:

$$\Gamma(z+1) \sim \sqrt{2\pi} \underbrace{(z+1)^{(z+1)-1/2} e^{-(z+1)}}_{\text{consider this first}} \underbrace{\left\{1 + \frac{A}{z+1} + \frac{B}{(z+1)^2} + \frac{C}{(z+1)^3} + \cdots\right\}}_{\text{and this second}}. \tag{12.20}$$

First:

$$\begin{aligned}
&\exp\left[\left(z+\frac{1}{2}\right)\log(z+1) - z - 1\right] \\
&\quad = \exp\left[\left(z+\frac{1}{2}\right)\log z + \left(z+\frac{1}{2}\right)\log\left(1+\frac{1}{z}\right) - z - 1\right] && (12.21\text{a}) \\
&\quad = \exp\left[\left(z+\frac{1}{2}\right)\log z - z - 1 + \left(z+\frac{1}{2}\right)\left(\frac{1}{z} - \frac{1}{2z^2} + \frac{1}{3z^3} - \frac{1}{4z^4} + \cdots\right)\right] && (12.21\text{b}) \\
&\quad = \exp\left[\left(z+\frac{1}{2}\right)\log z - z - \cancel{1} + \left(\cancel{1} - \cancel{\frac{1}{2z}} + \frac{1}{3z^2} - \frac{1}{4z^3} + \cdots\right)\right. && (12.21\text{c}) \\
&\qquad\qquad \left. + \left(\cancel{\frac{1}{2z}} - \frac{1}{4z^2} + \frac{1}{6z^3} - \cdots\right)\right] \\
&\quad = \exp\left[\left(z+\frac{1}{2}\right)\log z - z + \left(\frac{1}{12z^2} - \frac{1}{12z^3} + \cdots\right)\right] && (12.21\text{d}) \\
&\quad = z^{z+1/2} e^{-z}\left(1 + \frac{1}{12z^2} - \frac{1}{12z^3} + \cdots\right) && (12.21\text{e})
\end{aligned}$$

Second:

$$\begin{aligned}
&1 + \frac{A}{z+1} + \frac{B}{(z+1)^2} + \frac{C}{(z+1)^3} \\
&\quad = 1 + \frac{A}{z}(1+1/z)^{-1} + \frac{B}{z^2}(1+1/z)^{-2} + \frac{C}{z^3}(1+1/z)^{-3} && (12.22\text{a}) \\
&\quad = 1 + \frac{A}{z}\left(1 - \frac{1}{z} + \frac{1}{z^2} - \cdots\right) + \frac{B}{z^2}\left(1 - \frac{2}{z} + \cdots\right) + \frac{C}{z^3}(1 - \cdots) && (12.22\text{b}) \\
&\quad = 1 + \frac{A}{z} + \frac{B-A}{z^2} + \frac{C-2B+A}{z^3} + \cdots. && (12.22\text{c})
\end{aligned}$$

Therefore,

$$\Gamma(z+1) \sim \sqrt{2\pi}z^{z+1/2}e^{-z}\left\{1+\frac{A}{z}+\left(B-A+\frac{1}{12}\right)\frac{1}{z^2} + \left(C-2B+A+\frac{A}{12}-\frac{1}{12}\right)\frac{1}{z^3}\cdots\right\} \tag{12.23}$$

and compare this to

$$\Gamma(z+1) = z\Gamma(z) \sim \sqrt{2\pi}z^{z+1/2}e^{-z}\left\{1+\frac{A}{z}+\frac{B}{z^2}+\frac{C}{z^3}+\cdots\right\} \tag{12.24}$$

and equate like powers:

$$A = A \quad \text{(not illuminating)} \tag{12.25a}$$

$$B = B - A + \frac{1}{12} \qquad \Longrightarrow \qquad A = \frac{1}{12} \tag{12.25b}$$

$$C = C - 2B + A + \frac{A}{12} - \frac{1}{12} \qquad \Longrightarrow \qquad B = \frac{1}{288}\,. \tag{12.25c}$$

Thus we have

$$\boxed{\Gamma(z) \sim \sqrt{2\pi}z^{z-1/2}e^{-z}\left\{1+\frac{1}{12z}+\frac{1}{288z^2}+\cdots\right\}.} \tag{12.26}$$

Now recall

$$n! = \Gamma(n+1) = n\Gamma(n) \sim \sqrt{2\pi}n^{n+1/2}e^{-n}\left\{1+\frac{1}{12n}+\frac{1}{288n^2}+\cdots\right\} \tag{12.27}$$

so

$$\boxed{n! \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n\left(1+\frac{1}{12n}+\frac{1}{288n^2}+\cdots\right).} \tag{12.28}$$

This is **Stirling's formula**.

Problems

Problem 10.

Establish the following integration formulae with the aid of residues:

a) $\displaystyle\int_0^{\infty} \frac{dx}{x^2+1} = \frac{\pi}{2}\,;$

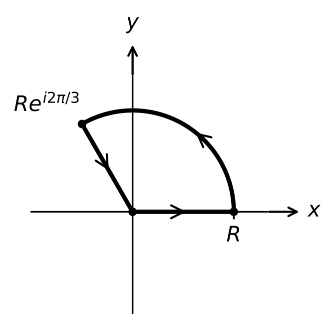
b) $\displaystyle\int_0^{\infty} \frac{dx}{x^4+1} = \frac{\pi}{2\sqrt{2}}\,;$

c) $\displaystyle\int_0^{\infty} \frac{\cos(ax)}{x^2+1}\,dx = \frac{\pi}{2}e^{-a} \quad (a \geq 0).$

Problem 11.

a) Use residues and the contour shown to establish the integral formula

$$\int_0^{\infty} \frac{dx}{x^3+1} = \frac{2\pi}{3\sqrt{3}}.$$



b) Generalize your result in (a) to evaluate

$$\int_0^{\infty} \frac{x^n}{x^m+1}\,dx$$

where $n = 0, 1, 2, \ldots$ and $m > n+1$.

Problem 12.

Use residues to show:

a) $\displaystyle\int_0^{2\pi} \frac{d\theta}{1 + a\cos\theta} = \frac{2\pi}{\sqrt{1-a^2}} \quad (-1 < a < 1)\,;$

b) $\displaystyle\int_0^{\pi} \sin^{2n}\theta\, d\theta = \frac{(2n)!}{2^{2n}(n!)^2}\,\pi.$

Problem 13.

By appropriate use of power series expansions, evaluate

a) $\displaystyle I = \int_0^1 \ln\left(\frac{1+x}{1-x}\right)\frac{dx}{x}\,;$

b) $\displaystyle I(n) = \int_0^1 \frac{\ln(1-x^n)}{x}\,dx\,.$

Problem 14.

Obtain two expansions of the *sine integral*

$$\operatorname{Si} x = \int_0^x \frac{\sin t}{t}\,dt\,,$$

one useful for small x and one useful for large x.

Problem 15.

Evaluate

$$I(x) = \int_0^{\infty} e^{xt - e^t}\,dt$$

approximately for large positive x.

Module IV

Integral Transforms

Motivation

Integral transforms — in particular the Fourier transform — are ubiquitous in physics. Whether in quantum mechanics, or X-ray diffraction, or signal analysis, we often use integral transforms to go from space or time variables to wave-number or frequency variables. Integral transforms can be used to change differential equations into algebraic equations which are often easier to solve. We focus mostly on the Fourier series and Fourier transform, but we also mention a few other transforms that are sometimes encountered. (The Hilbert transform, for example, is encountered in the Kramers-Kronig relations.)

13 Fourier Series

Consider a function $f(\theta)$, $-\pi < \theta \leq \pi$. We seek an expansion in the form:

$$f(\theta) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta)\,. \tag{13.1}$$

This series expansion for $f(\theta)$ is known as a **Fourier series**.

To find the coefficients, multiply both sides by $\cos n\theta$ or $\sin n\theta$ and integrate from $-\pi$ to π. For example, if $n \neq 0$, then

$$\int_{-\pi}^{\pi} f(\theta) \cos n\theta \, d\theta \tag{13.2a}$$

$$= \int_{-\pi}^{\pi} \left\{ \frac{a_0}{2} + \sum_{m=1}^{\infty} (a_m \cos m\theta + b_m \sin m\theta) \right\} \cos n\theta \, d\theta \tag{13.2b}$$

$$= \frac{a_0}{2} \underbrace{\int_{-\pi}^{\pi} \cos n\theta \, d\theta}_{0 \text{ for } n \neq 0} \tag{13.2c}$$

$$+ \sum_{\substack{m=1 \\ m \neq n}}^{\infty} a_m \underbrace{\int_{-\pi}^{\pi} \cos m\theta \cos n\theta \, d\theta}_{0} + a_n \int_{-\pi}^{\pi} \cos^2 n\theta \, d\theta$$

$$+ \sum_{m=1}^{\infty} b_m \underbrace{\int_{-\pi}^{\pi} \sin m\theta \cos n\theta \, d\theta}_{0}$$

$$= a_n \int_{-\pi}^{\pi} \cos^2 n\theta \, d\theta \tag{13.2d}$$

$$= a_n \int_{-\pi}^{\pi} (\tfrac{1}{2} + \underbrace{\tfrac{1}{2} \cos 2n\theta}_{0}) \, d\theta \tag{13.2e}$$

$$= \pi a_n \tag{13.2f}$$

Therefore

$$\boxed{a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(\theta)\cos n\theta\, d\theta \qquad n = 1, 2, 3, \ldots |:.} \tag{13.3}$$

Similarly

$$\boxed{a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} f(\theta)\, d\theta} \tag{13.4}$$

$$\boxed{b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(\theta)\sin n\theta\, d\theta \qquad n = 1, 2, 3, \ldots .} \tag{13.5}$$

The Fourier series converges at all points in $-\pi < \theta \leq \pi$ to[1] $f(\theta)$ provided that $f(\theta)$ is sufficiently nice.

- The Fourier series is periodic: it repeats itself in $\pi < \theta \leq 3\pi$, etc. That is, $f(\theta + 2\pi) = f(\theta)$.
- For even functions, $f(-\theta) = f(\theta)$ or $f(2\pi - \theta) = f(\theta)$, only cosine terms occur, i.e., $b_n = 0\ \forall n$.
- For odd functions, $f(-\theta) = -f(\theta)$, only sine terms occur, i.e., $a_n = 0\ \forall n$.

[1] actually, to $\frac{1}{2}[f(\theta^+) + f(\theta^-)]$

Ex. 13.1. The step function:

$$f(\theta) = \begin{cases} -1 & -\pi < \theta < 0 \\ +1 & 0 \le \theta \le \pi \end{cases} \tag{13.6}$$

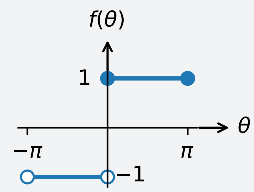


Figure 13.1: Step Function

This is an odd function so there will be no cosine terms.

$$b_n = -\frac{1}{\pi}\int_{-\pi}^{0} \sin n\theta \, d\theta + \frac{1}{\pi}\int_{0}^{\pi} \sin n\theta \, d\theta \tag{13.7a}$$

$$= \frac{2}{\pi}\int_{0}^{\pi} \sin n\theta \, d\theta \tag{13.7b}$$

$$= -\frac{2}{n\pi}\left[(-1)^n - 1\right] \tag{13.7c}$$

$$= \begin{cases} \dfrac{4}{n\pi} & n \text{ odd} \\ 0 & n \text{ even.} \end{cases} \tag{13.7d}$$

Therefore

$$f(\theta) = \frac{4}{\pi}\left\{\sin\theta + \frac{\sin 3\theta}{3} + \frac{\sin 5\theta}{5} + \cdots\right\}. \tag{13.8}$$

Aside: set $\theta = \pi/2$ to get

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots . \tag{13.9}$$

This is known as ***Gregory's series****.*
(This can also be obtained from $\arctan x = x - x^3/3 + x^5/5 - \cdots$ *with* $x = 1$.*)*

The series for $f(\theta)$ has non-uniform convergence, as seen in Fig. 13.2. The overshoot near $\theta = 0$ and $\theta = \pm\pi$ is known as **Gibbs's phenomenon**. Even in the limit of an infinite number of terms the overshoot is finite — approximately by 0.18.

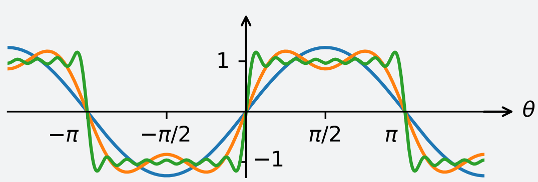


Figure 13.2: Gibbs's phenomenon: shown is the series solution truncated at $n = 1$, $n = 3$, and $n = 18$.

Ex. 13.2. Consider

$$f(\theta) = \cos k\theta\,, \qquad -\pi < \theta \le \pi\,. \tag{13.10}$$

This is an even function so only cosine terms are present.

$$a_n = \frac{2}{\pi}\int_0^\pi \cos k\theta \cos n\theta \, d\theta \tag{13.11a}$$

$$= \frac{1}{\pi}\int_0^\pi \{\cos[(k-n)\theta] + \cos[(k+n)\theta]\}\, d\theta \tag{13.11b}$$

$$= \frac{1}{\pi}\frac{\sin[(k-n)\pi]}{k-n} + \frac{1}{\pi}\frac{\sin[(k+n)\pi]}{k+n} \tag{13.11c}$$

$$= \frac{1}{\pi}\frac{(-1)^n \sin k\pi}{k-n} + \frac{1}{\pi}\frac{(-1)^n \sin k\pi}{k+n} \tag{13.11d}$$

$$= (-1)^n \frac{2k \sin k\pi}{\pi(k^2-n^2)}\,. \tag{13.11e}$$

Therefore,

$$\cos k\theta = \frac{2k\sin k\pi}{\pi}\left\{\frac{1}{2k^2} - \frac{\cos\theta}{k^2-1} + \frac{\cos 2\theta}{k^2-4} - \cdots\right\}. \tag{13.12}$$

(We used this result earlier in Ex. 4.4.)

Suppose $f(x)$ is periodic with some period L rather than 2π. Let

$$x = \frac{L}{2\pi}\theta \,. \tag{13.13}$$

Then we have

$$\boxed{f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty}\left(a_n \cos\frac{2\pi n x}{L} + b_n \sin\frac{2\pi n x}{L}\right)} \tag{13.14a}$$

where

$$\boxed{a_n = \frac{2}{L}\int_{-L/2}^{L/2} f(x)\cos\frac{2\pi n x}{L}\,dx\,, \qquad n = 0, 1, 2, \ldots} \tag{13.14b}$$

$$\boxed{b_n = \frac{2}{L}\int_{-L/2}^{L/2} f(x)\sin\frac{2\pi n x}{L}\,dx\,, \qquad n = 1, 2, 3, \ldots\,.} \tag{13.14c}$$

We can also define the Fourier series in complex form:

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi n x/L} \,. \tag{13.15}$$

Observe:

$$\begin{aligned}
&\int_{-L/2}^{L/2} e^{i2\pi m x/L} e^{-i2\pi n x/L}\,dx \\
&\qquad = \int_{-L/2}^{L/2} e^{i2\pi(m-n)x/L}\,dx && (13.16a)\\
&\qquad = \begin{cases} L & n = m \\ \dfrac{L}{i2\pi(n-m)}\; e^{i2\pi(m-n)x/L}\Big|_{-L/2}^{L/2} & n \neq m \end{cases} && (13.16b)\\
&\qquad = \begin{cases} L & n = m \\ \dfrac{L}{i2\pi(m-n)}\left[e^{i\pi(m-n)} - e^{-i\pi(m-n)}\right] & n \neq m \end{cases} && (13.16c)\\
&\qquad = L\begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases} && (13.16d)\\
&\qquad = L\delta_{mn} && (13.16e)
\end{aligned}$$

where δ_{mn} is the **Kronecker delta**.

Therefore

$$\frac{1}{L}\int_{-L/2}^{L/2} f(x)e^{-i2\pi nx/L}\,dx = \frac{1}{L}\sum_{m=-\infty}^{\infty} c_m \int_{-L/2}^{L/2} e^{i2\pi mx/L}e^{-i2\pi nx/L}\,dx \quad (13.17a)$$

$$= \sum_{m=-\infty}^{\infty} c_m\delta_{mn} \quad (13.17b)$$

$$= c_n \quad (13.17c)$$

and thus

$$\boxed{f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi nx/L}} \quad (13.18a)$$

where

$$\boxed{c_n = \frac{1}{L}\int_{-L/2}^{L/2} f(x)e^{-i2\pi nx/L}\,dx\,.} \quad (13.18b)$$

Parseval's Identity

Consider:

$$\frac{1}{L}\int_{-L/2}^{L/2} |f(x)|^2\,dx = \frac{1}{L}\int_{-L/2}^{L/2}\left(\sum_{m=-\infty}^{\infty} c_m e^{i2\pi mx/L}\right)\left(\sum_{n=-\infty}^{\infty} c_n^* e^{-i2\pi nx/L}\right)dx \quad (13.19a)$$

$$= \frac{1}{L}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} c_m c_n^* \int_{-L/2}^{L/2} e^{i2\pi mx/L}e^{-i2\pi nx/L}\,dx \quad (13.19b)$$

$$= \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} c_m c_n^* \delta_{mn} \quad (13.19c)$$

$$= \sum_{n=-\infty}^{\infty} |c_n|^2\,. \quad (13.19d)$$

Thus we have **Parseval's identity**:

$$\boxed{\frac{1}{L}\int_{-L/2}^{L/2} |f(x)|^2\,dx = \sum_{n=-\infty}^{\infty} |c_n|^2\,.} \quad (13.20)$$

14 Fourier Transforms

Recall the complex Fourier series:

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi nx/L} \quad \text{where} \quad Lc_n = \int_{-L/2}^{L/2} f(x) e^{-i2\pi nx/L}\, dx\,. \tag{14.1}$$

Consider the case $L \to \infty$. Define

$$y_n = \frac{2\pi n}{L} \qquad \text{and} \qquad Lc_n = g(y_n) \tag{14.2}$$

and note

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi nx/L} \tag{14.3a}$$

$$= \sum_{n=-\infty}^{\infty} \frac{g(y_n)}{L} e^{ixy_n} \tag{14.3b}$$

let $\Delta y = 2\pi/L$

$$= \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} g(y_n) e^{ixy_n}\, \Delta y \tag{14.3c}$$

as $L \to \infty$, $\Delta y \to 0$
this is a Riemann sum

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} g(y) e^{ixy}\, dy\,. \tag{14.3d}$$

We thus have the **Fourier transform** pairs:

$$\boxed{f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} g(y) e^{ixy}\, dy \quad \Longleftrightarrow \quad g(y) = \int_{-\infty}^{\infty} f(x) e^{-ixy}\, dx\,.} \tag{14.4}$$

We say that $g(y)$ is the Fourier transform of $f(x)$
and $f(x)$ is the inverse Fourier transform of $g(y)$.

Note: the factor of $\frac{1}{2\pi}$ is sometimes rearranged between these two equations.

Substitute $g(y)$ into the $f(x)$ equation:

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} f(x')e^{-ix'y}\,dx'\right]e^{ixy}\,dy \tag{14.5a}$$

$$= \int_{-\infty}^{\infty} f(x')\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(x-x')y}\,dy\right]dx' \tag{14.5b}$$

which holds for any function f. Thus,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(x-x')y}\,dy \tag{14.6}$$

is the continuous generalization of the Kronecker delta.

Define the **Dirac delta function** by

$$\boxed{\delta(x) = 0 \text{ for } x \neq 0\,, \qquad \int_{-a}^{+b}\delta(x)\,dx = 1 \text{ for } a, b > 0\,.} \tag{14.7}$$

Then

$$\boxed{\int f(x')\delta(x-x')\,dx' = f(x)} \tag{14.8}$$

if the domain of integration contains x.

One representation of the Dirac delta function is therefore

$$\boxed{\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ixy}\,dy\,.} \tag{14.9}$$

Using a change of variables, one can show the following identity

$$\boxed{\begin{array}{l}\displaystyle\int_a^b f(x)\delta(g(x))\,dx = \sum_n \frac{f(x_n)}{|g'(x_n)|} \\ \text{where } x_n \text{ are roots of } g(x) \text{ in } a < x_n < b.\end{array}} \tag{14.10}$$

Theorem 6 (Parseval's)**.** If $f(x)$ and $g(y)$ are Fourier transform pairs then **Parseval's identity** states

$$\boxed{\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} |g(y)|^2 \, dy} \tag{14.11}$$

Proof.

$$\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{-\infty}^{\infty} \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} g^*(y) e^{-ixy} \, dy \right] \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} g(y') e^{ixy'} \, dy' \right] dx \tag{14.12a}$$

$$= \frac{1}{2\pi} \int_{y=-\infty}^{\infty} g^*(y) \int_{y'=-\infty}^{\infty} g(y') \underbrace{\left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(y'-y)x} \, dx \right]}_{\delta(y'-y)} dy' dy \tag{14.12b}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} g^*(y) \left[\int_{-\infty}^{\infty} g(y') \delta(y' - y) \, dy' \right] dy \tag{14.12c}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} g^*(y) g(y) \, dy \,. \tag{14.12d}$$

□

Fourier Cosine Transform

Suppose $f(x)$ is an even function. Then,

$$g(y) = \int_0^\infty f(x)e^{-ixy}\,dx + \int_{-\infty}^0 f(x)e^{-ixy}\,dx \tag{14.13a}$$

$$= \int_0^\infty f(x)(e^{ixy} + e^{-ixy})\,dx \tag{14.13b}$$

$$= 2\int_0^\infty f(x)\cos(xy)\,dx\,. \tag{14.13c}$$

Note: $g(y)$ is also an even function so

$$f(x) = \frac{1}{\pi}\int_0^\infty g(y)\cos(xy)\,dy\,. \tag{14.14}$$

Therefore, $f(x)$ and $g(y)$ need only be defined for positive x and y. They are **Fourier cosine transform** pairs.

Similarly, if $f(x)$ is an odd function,

$$f(x) = \frac{1}{\pi}\int_0^\infty g(y)\sin(xy)\,dy \quad \Longleftrightarrow \quad g(y) = 2\int_0^\infty f(x)\sin(xy)\,dx \tag{14.15}$$

are **Fourier sine transform** pairs.

Ex. 14.1. Damped harmonic oscillator.

$$f(t) = \begin{cases} 0 & t < 0 \\ e^{-t/T} \sin \omega_0 t & t > 0\,. \end{cases} \tag{14.16}$$

This might describe, e.g., the current in a radiating antenna.

The Fourier transform of this function is

$$g(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t}\, dt \tag{14.17a}$$

$$= \int_0^{\infty} e^{-t/T} \frac{e^{i\omega_0 t} - e^{-i\omega_0 t}}{2i} e^{-i\omega t}\, dt \tag{14.17b}$$

$$= \frac{1}{2i} \int_0^{\infty} \exp\left\{-\left[\frac{1}{T} + i(\omega - \omega_0)\right] t\right\} dt - \frac{1}{2i} \int_0^{\infty} \exp\left\{-\left[\frac{1}{T} + i(\omega + \omega_0)\right] t\right\} dt \tag{14.17c}$$

$$= \frac{1}{2i} \frac{1}{i(\omega - \omega_0) + 1/T} - \frac{1}{2i} \frac{1}{i(\omega + \omega_0) + 1/T} \tag{14.17d}$$

$$= \frac{1}{2} \left[\frac{1}{(\omega + \omega_0) - i/T} - \frac{1}{(\omega - \omega_0) - i/T} \right]. \tag{14.17e}$$

Note: if $T \gg 1/\omega_0$, $g(\omega)$ is sharply peaked around $\omega = \pm\omega_0$. Near $\omega = \omega_0$,

$$g(\omega) \approx -\frac{1}{2} \frac{1}{(\omega - \omega_0) - i/T} \quad \implies \quad |g(\omega)| \approx \frac{1}{2} \frac{1}{\sqrt{(\omega - \omega_0)^2 + 1/T^2}}\,. \tag{14.18}$$

The energy radiated by the antenna is proportional to

$$\int_{-\infty}^{\infty} |f(t)|^2\, dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} |g(\omega)|^2\, d\omega \tag{14.19}$$

so we interpret $|g(\omega)|^2$ as the radiated power spectrum. The power spectrum peaks at frequency ω_0 and the full width at half maximum frequency band is $\Gamma = 2/T$ (see Fig. 14.1).

Note the uncertainty principle: the decay time T is inversely proportional to the width of the power spectrum.

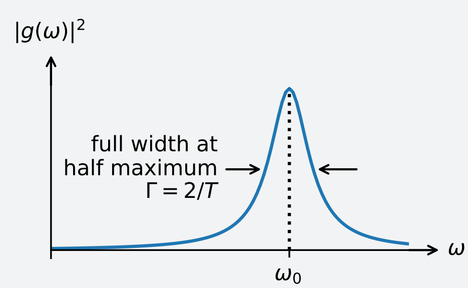


Figure 14.1: Damped Oscillator Power Spectrum

Generalization to Higher Dimensions

For example, in 3 dimensions:

$$\boxed{\varphi(\mathbf{k}) = \iiint f(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}\,dx\,dy\,dz} \tag{14.20a}$$

and

$$\boxed{f(\mathbf{x}) = \frac{1}{(2\pi)^3}\iiint \varphi(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}\,dk_x\,dk_y\,dk_z} \tag{14.20b}$$

are Fourier transform pairs.

We can deduce the 3-dimensional delta function

$$\boxed{\delta(\mathbf{x}) = \frac{1}{(2\pi)^3}\iiint e^{i\mathbf{k}\cdot\mathbf{x}}\,dk_x\,dk_y\,dk_z} \tag{14.21}$$

which has the properties

- $$\delta(\mathbf{x}) = 0 \qquad \text{for } \mathbf{x} \neq 0; \tag{14.22}$$
- $$\iiint \delta(\mathbf{x})\,dx\,dy\,dz = 1 \tag{14.23}$$

  provided the origin is in the domain of integration;
- $$\iiint f(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}_0)\,dx\,dy\,dz = f(\mathbf{x}_0) \tag{14.24}$$

  provided the $\mathbf{x}_0$ is in the domain of integration.

Ex. 14.2. Wave function for Gaussian wave packet.

$$f(\mathbf{x}) = \left(\frac{2}{\pi a^2}\right)^{3/4} e^{-r^2/a^2} = N e^{-r^2/a^2} \tag{14.25}$$

where $r = \|\mathbf{x}\|$. Note the probability distribution $|f(\mathbf{x})|^2$ is normalized: $\iiint |f(\mathbf{x})|^2\, dx\, dy\, dz = 1$.

$$\varphi(\mathbf{k}) = N \iiint e^{-r^2/a^2} e^{-i\mathbf{k}\cdot\mathbf{x}}\, dx\, dy\, dz \tag{14.26a}$$

introduce polar coordinates with z-axis along **k***; let $\mu = \cos\theta$, $k = \|\mathbf{k}\|$*

$$= N \int_{\phi=0}^{2\pi} \int_{\mu=-1}^{1} \int_{r=0}^{\infty} r^2 e^{-r^2/a^2} e^{-ikr\mu}\, dr\, d\mu\, d\phi \tag{14.26b}$$

$$= 2\pi N \int_{r=0}^{\infty} r^2 e^{-r^2/a^2} \int_{\mu=-1}^{1} e^{-ikr\mu}\, d\mu\, dr \tag{14.26c}$$

$$= 2\pi N \int_{0}^{\infty} r^2 e^{-r^2/a^2} \left[\frac{1}{-ikr} e^{-ikr\mu}\right]_{-1}^{1} dr \tag{14.26d}$$

$$= 2\pi N \int_{0}^{\infty} r e^{-r^2/a^2} \frac{1}{ik}(e^{ikr} - e^{-ikr})\, dr \tag{14.26e}$$

change lower limit of integration

$$= \frac{2\pi}{ik} N \int_{-\infty}^{\infty} r e^{-r^2/a^2} e^{ikr}\, dr \tag{14.26f}$$

complete the square

$$= \frac{2\pi}{ik} N \int_{-\infty}^{\infty} r e^{-(r^2/a^2 - ikr - k^2a^2/4) - k^2a^2/4}\, dr \tag{14.26g}$$

$$= \frac{2\pi}{ik} N e^{-k^2a^2/4} \int_{-\infty}^{\infty} r e^{-(r - ika^2/2)^2/a^2}\, dr \tag{14.26h}$$

let $y = r - ika^2/2$

$$= \frac{2\pi}{ik} N e^{-k^2a^2/4} \int_{-\infty}^{\infty} \left(y + \frac{ika^2}{2}\right) e^{-y^2/a^2}\, dy \tag{14.26i}$$

$\int_{-\infty}^{\infty} y e^{-y^2/a^2}\, dy = 0$ (odd integrand)

$$= \frac{\cancel{2}\pi}{\cancel{ik}} N e^{-k^2a^2/4} \frac{\cancel{ik}a^2}{\cancel{2}} a\sqrt{\pi} \tag{14.26j}$$

recall $N = (2/\pi a)^{3/4}$

$$= \pi \left(\frac{2}{\pi a^2}\right)^{3/4} a^3 \sqrt{\pi} e^{-k^2a^2/4} \tag{14.26k}$$

$$= (2\pi a^2)^{3/4} e^{-k^2a^2/4}. \tag{14.26l}$$

We seen that the Fourier transform of a Gaussian distribution is a Gaussian distribution.

The width of the Gaussian probability distribution $|f(\mathbf{x})|^2$ is $\Delta x = a/2$ while the width of the Gaussian probability distribution of the Fourier transform $|\varphi(\mathbf{k})|^2$ is $\Delta k = 1/a$. Thus we have

$$\Delta x \, \Delta k = \frac{1}{2} \,. \tag{14.27}$$

In quantum mechanics, $\mathbf{p} = \hbar \mathbf{k}$ so

$$\Delta x \, \Delta p = \frac{\hbar}{2} \tag{14.28}$$

for Gaussian wave packets.

15 Other Transform Pairs

- **Laplace transform**: for $f(t)$ with $f(t)=0$ for $t<0$,

$$\boxed{F(s)=\int_0^\infty f(t)e^{-st}\,dt\,.} \tag{15.1a}$$

The inverse Laplace transform is given by the **Browmwich integral**

$$\boxed{f(t)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} F(s)e^{st}\,ds\,, \quad t>0} \tag{15.1b}$$

where the integral is along the line $\operatorname{Re} s=c$, $c>0$, such that all singularities are to the left of the contour.

- **Fourier-Bessel transform** or **Hankel transform**:

$$\boxed{g(k)=\int_0^\infty f(x)J_m(x)x\,dx \quad\Longleftrightarrow\quad f(x)=\int_0^\infty g(k)J_m(k)k\,dk} \tag{15.2}$$

where $J_m(x)$ is a Bessel function (see later).

- **Mellin transformation**:

$$\boxed{\varphi(z)=\int_0^\infty f(t)t^{z-1}\,dt \quad\Longleftrightarrow\quad f(t)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\varphi(z)t^{-z}\,dz\,.} \tag{15.3}$$

- **Hilbert transformation**:

$$\boxed{g(y)=\frac{1}{\pi}⨍_{-\infty}^{\infty}\frac{f(x)}{x-y}\,dx \quad\Longleftrightarrow\quad f(x)=\frac{1}{\pi}⨍_{-\infty}^{\infty}\frac{g(y)}{y-x}\,dy\,.} \tag{15.4}$$

16 Applications of the Fourier Transform

Properties of the Fourier Transform

We adopt the following notation for the Fourier transform and its inverse:

$$\mathcal{F}[f(x);y] = \int_{-\infty}^{\infty} f(x)e^{-ixy}\,dx \tag{16.1a}$$

$$\mathcal{F}^{-1}[g(y);x] = \frac{1}{2\pi}\int_{-\infty}^{\infty} g(y)e^{ixy}\,dy\,. \tag{16.1b}$$

The Fourier transform has the following properties:

- ***Linearity.***

$$\mathcal{F}[\alpha f(x)+\beta g(x);y] = \alpha\mathcal{F}[f(x);y]+\beta\mathcal{F}[g(x);y]\,. \tag{16.2}$$

- ***Derivatives.***

$$\mathcal{F}[f'(x);y] = \int_{-\infty}^{\infty} f'(x)e^{-ixy}\,dx \tag{16.3a}$$

integrate by parts with $u = e^{-ixy}$, $dv = f'(x)\,dx$

$$= f(x)e^{-ixy}\Big|_{-\infty}^{\infty} + iy\int_{-\infty}^{\infty} f(x)e^{-ixy}\,dx \tag{16.3b}$$

assume $f(x)\to 0$ for $x\to\pm\infty$

$$= iy\mathcal{F}[f(x);y]\,. \tag{16.3c}$$

- ***Integrals.*** Similarly,

$$\mathcal{F}\left[\int f(x)\,dx;y\right] = \frac{\mathcal{F}[f(x);y]}{iy} + C\,\delta(y) \tag{16.4}$$

  where C is an arbitrary constant of integration; note $\mathcal{F}[C;y] = 2\pi C\,\delta(y)$.

- ***Translation.***

$$\mathcal{F}[f(x+a);y] = \int_{-\infty}^{\infty} f(x+a)e^{-ixy}\,dx \tag{16.5a}$$
$$= \int_{-\infty}^{\infty} f(x)e^{-i(x-a)y}\,dx \tag{16.5b}$$
$$= e^{iay}\mathcal{F}[f(x);y]\,. \tag{16.5c}$$

- ***Multiplication by an exponential.***

$$\mathcal{F}[e^{ax}f(x);y] = \mathcal{F}[f(x);y+ia] \tag{16.6}$$

(cf. translation property).

- ***Multiplication by a power of x.***

$$\mathcal{F}[xf(x);y] = i\frac{d}{dy}\mathcal{F}[f(x);y] \tag{16.7}$$

(cf. derivative property).

- ***Convolution.*** Define the **convolution** of two functions, $f(x)$ and $g(x)$, as

$$\boxed{h(x) = (f*g)(x) = \int_{-\infty}^{\infty} f(t)g(x-t)\,dt\,.} \tag{16.8}$$

Then the **convolution theorem** states

$$\boxed{\mathcal{F}[h(x);y] = \mathcal{F}[f(x);y]\cdot\mathcal{F}[g(x);y]\,.} \tag{16.9}$$

Ex. 16.1. Damped driven harmonic oscillator.

The equation of motion is

$$\left[\frac{d^2}{dx^2} + 2\zeta\omega_0\frac{d}{dt} + \omega_0^2\right]x(t) = s(t) \tag{16.10}$$

where ω_0 is the natural frequency, ζ is the damping ratio, and $s(t)$ is the source driving function.

Let $X(\omega) = \mathcal{F}[x(t);\omega]$ and $S(\omega) = \mathcal{F}[s(t);\omega]$. Then, using the derivative property,

$$[-\omega^2 + 2i\zeta\omega_0\omega + \omega_0^2]X(\omega) = S(\omega) \tag{16.11}$$

and so

$$X(\omega) = \frac{S(\omega)}{\omega_0^2 - \omega^2 + 2i\zeta\omega_0\omega} = G(\omega)S(\omega) \tag{16.12}$$

where $G(\omega)$ is the **transfer function**. By the convolution theorem, $x(t) = (g * s)(t)$ where $g(t) = \mathcal{F}^{-1}[G(\omega); t]$.

The power spectrum of the harmonic motion is

$$|X(\omega)|^2 = \frac{|S(\omega)|^2}{(\omega_0^2 - \omega^2)^2 + 4\zeta^2\omega_0^2\omega^2}\,. \tag{16.13}$$

Take the inverse Fourier transform of $X(\omega)$ to find the motion $x(t)$.
For example, suppose $s(t) = a\delta(t)$ (an impulse). Then,

$$S(\omega) = \int_{-\infty}^{\infty} a\delta(t)e^{-i\omega t}\,dt = a\,. \tag{16.14}$$

Therefore,

$$X(\omega) = -\frac{a}{\omega^2 - 2i\zeta\omega_0\omega - \omega_0^2} \tag{16.15a}$$

$$= -\frac{a}{(\omega - \omega_1 - i\zeta\omega_0)(\omega + \omega_1 - i\zeta\omega_0)} \quad \text{with} \quad \omega_1 = \omega_0\sqrt{1-\zeta^2}\,. \tag{16.15b}$$

Now perform the inverse Fourier transform:

$$x(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} X(\omega)e^{i\omega t}\,d\omega \tag{16.16a}$$

$$= -\frac{a}{2\pi}\int_{-\infty}^{\infty}\frac{e^{i\omega t}\,d\omega}{(\omega - \omega_1 - i\zeta\omega_0)(\omega + \omega_1 - i\zeta\omega_0)}\,. \tag{16.16b}$$

Do this integral using contour integration.

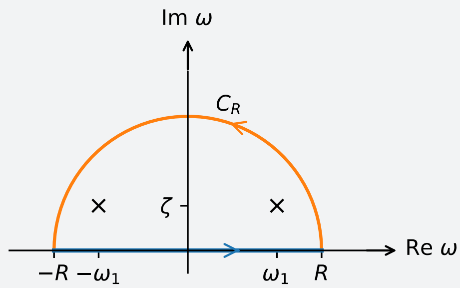


Figure 16.1: Contour for Damped Driven Harmonic Oscillator

We close the contour in the upper-half plane as shown in Fig. 16.1: C_R is the curve $\omega = Re^{i\theta}$, $0 \le \theta \le \pi$. Note that, on C_R,

$$e^{i\omega t} = e^{iRte^{i\theta}} = e^{iRt\cos\theta}e^{-Rt\sin\theta} \to 0 \text{ as } R \to \infty \text{ for } t > 0 \tag{16.17}$$

so

$$\int_{C_R} \frac{e^{i\omega t}\,d\omega}{(\omega - \omega_1 - i\zeta\omega_0)(\omega + \omega_1 - i\zeta\omega_0)} \to 0 \text{ as } R \to \infty \text{ when } t > 0\,. \tag{16.18}$$

Thus,

$$\begin{aligned}&\fint_{-\infty}^{\infty} \frac{e^{i\omega t}\,d\omega}{(\omega - \omega_1 - i\zeta\omega_0)(\omega + \omega_1 - i\zeta\omega_0)} \\ &\qquad + \underbrace{\lim_{R\to\infty} \int_{C_R} \frac{e^{i\omega t}\,d\omega}{(\omega - \omega_1 - i\zeta\omega_0)(\omega + \omega_1 - i\zeta\omega_0)}}_{\to 0} = 2\pi i \sum_{\text{Res}}\,.\end{aligned} \tag{16.19}$$

There are two simple poles in the upper-half plane with residues

$$\operatorname*{Res}_{\omega=\omega_1+i\zeta\omega_0} = \frac{e^{i\omega_1 t}e^{-\zeta\omega_0 t}}{2\omega_1} \quad \text{and} \quad \operatorname*{Res}_{\omega=-\omega_1+i\zeta\omega_0} = \frac{e^{-i\omega_1 t}e^{-\zeta\omega_0 t}}{-2\omega_1}\,. \tag{16.20}$$

Therefore

$$x(t) = -\frac{a}{2\pi}2\pi i\left(\frac{e^{i\omega_1 t}e^{-\zeta\omega_0 t}}{2\omega_1} - \frac{e^{-i\omega_1 t}e^{-\zeta\omega_0 t}}{2\omega_1}\right), \qquad t > 0 \tag{16.21a}$$

$$= -\frac{i}{2}\frac{a}{\omega_1}(e^{i\omega_1 t} - e^{-i\omega_1 t})e^{-\zeta\omega_0 t}, \qquad t > 0 \tag{16.21b}$$

$$= -\frac{i}{2}\frac{a}{\omega_1}(2i\sin\omega_1 t)e^{-\zeta\omega_0 t}, \qquad t > 0 \tag{16.21c}$$

$$= \frac{a}{\omega_1}e^{-\zeta\omega_0 t}\sin\omega_1 t, \qquad t > 0\,. \tag{16.21d}$$

For $t < 0$ we need to close the contour in the lower-half plane instead so that $\int_{C_R} \cdots \to 0$ as $R \to \infty$, but there are no poles in the lower-half plane so we find

$$x(t) = 0 \text{ for } t < 0 \quad \text{(causality!)} \tag{16.22}$$

and therefore

$$x(t) = \begin{cases} 0 & t < 0 \\ \dfrac{a}{\omega_1} e^{-\zeta\omega_0 t} \sin \omega_1 t & t > 0 \end{cases} \tag{16.23a}$$

with

$$\omega_1 = \omega_0 \sqrt{1 - \zeta^2}. \tag{16.23b}$$

This example shows that causality imposes the requirement that $X(\omega)$ has singularities only in the upper-half plane and is analytic everywhere in the lower-half plane.

Problems

Problem 16.

Expand the following functions in a Fourier series of the form

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left\{ a_n \cos\left(\frac{2\pi n x}{L}\right) + b_n \sin\left(\frac{2\pi n x}{L}\right) \right\},$$

(i.e., determine the Fourier coefficients a_0, a_n, and b_n, $n = 1, 2, 3, \ldots$):

a) the triangular function

$$f(x) = \begin{cases} 1 + 2x/L & -\frac{1}{2}L \le x \le 0 \\ 1 - 2x/L & 0 < x \le \frac{1}{2}L; \end{cases}$$

b) the function $f(x) = e^x$ for $-\frac{1}{2}L \le x \le \frac{1}{2}L$.

Problem 17.

Find the Fourier transform, $\varphi(\mathbf{k})$, of the wave function for a $2p$ electron in hydrogen:

$$f(\mathbf{x}) = \frac{1}{\sqrt{32\pi a_0^5}}\, z e^{-r/2a_0}$$

where $\mathbf{x} = (x, y, z)$, $r^2 = x^2 + y^2 + z^2$, and a_0 is the radius of the first Bohr orbit. (Hint: let $f(\mathbf{x}) = \mathbf{e}_z \cdot \mathbf{g}(\mathbf{x})$ and use symmetry to argue that $\mathcal{F}[\mathbf{g}(\mathbf{x}); \mathbf{k}] \propto \mathbf{k}$.)

Problem 18.

Prove the **Wiener-Khinchin theorem**, which relates the **autocorrelation** and the Fourier transform: Let $\mathcal{F}[f(x); y] = g(y)$; then:

$$\mathcal{F}^{-1}[|g(y)|^2; x] = \int_{-\infty}^{\infty} f^*(t) f(x+t)\, dt$$

where $\mathcal{F}^{-1}$ is the inverse Fourier transform.

Module V

Ordinary Differential Equations

Motivation

Ordinary differential equations are *even more of a pain in the neck* to solve than integrals. But, of course, physical laws are formulated in terms of differential equations, and the solutions require integrating them, so it is important to know how to do that. Here we present some common techniques for solving ordinary differential equations. We will also encounter some commonly occurring special functions.

Terminology

Consider:

$$\frac{d^3y}{dx^3} + x\sqrt{\frac{dy}{dx}} + x^2 y = 0\,.$$

Rationalize this:

$$\begin{aligned} x^2\frac{dy}{dx} &= \left(\frac{d^3y}{dx^3} + x^2 y\right)^2 \\ &= \underbrace{\left(\frac{d^3y}{dx^3}\right)^2}_{\text{this is the highest order derivative term}} + 2x^2 y\left(\frac{d^3y}{dx^3}\right) + x^4 y^2\,. \end{aligned}$$

We say this ordinary differential equation (ODE) is *third order* and *second degree*.

17 First Order ODEs

Separable Equations

If we can write the equation in the form

$$A(x)\,dx + B(y)\,dy = 0 \tag{17.1}$$

then the equation is **separable** and the solution is obtained by integration.

Ex. 17.1. Consider

$$\frac{dy}{dx} + \sqrt{\frac{1-y^2}{1-x^2}} = 0\,. \tag{17.2}$$

Then

$$\underbrace{\frac{1}{\sqrt{1-y^2}}}_{B(y)}\,dy + \underbrace{\frac{1}{\sqrt{1-x^2}}}_{A(x)}\,dx = 0\,. \tag{17.3}$$

Integrate:

$$\arcsin y + \arcsin x = c \tag{17.4a}$$
$$\Longrightarrow \quad \sin(\arcsin y + \arcsin x) = \sin c = C \tag{17.4b}$$
$$\Longrightarrow \quad \sin(\arcsin y)\cos(\arcsin x) + \cos(\arcsin y)\sin(\arcsin x) = C \tag{17.4c}$$
$$\Longrightarrow \quad y\sqrt{1-x^2} + x\sqrt{1-y^2} = C\,. \tag{17.4d}$$

Exact Equations

More generally,

$$\underbrace{A(x,y)\,dx + B(x,y)\,dy}_{\substack{\text{if this is the differential } du \\ \text{of some function } u(x,y) \\ \text{then integrate to get} \\ u(x,y)=c; \\ \text{in this case, the equation is an} \\ \textbf{exact equation}}} = 0\,. \tag{17.5}$$

Note: for an exact equation,

$$du = \underbrace{\frac{\partial u}{\partial x}}_{A(x,y)}\,dx + \underbrace{\frac{\partial u}{\partial y}}_{B(x,y)}\,dy \tag{17.6}$$

but since $\dfrac{\partial^2 u}{\partial x \partial y} = \dfrac{\partial^2 u}{\partial y \partial x}$, a *necessary* condition is

$$\boxed{\frac{\partial A}{\partial y} = \frac{\partial B}{\partial x}\,.} \tag{17.7}$$

This is also a *sufficient* condition.

Ex. 17.2. Consider

$$\underbrace{(x+y)}_{A(x,y)}\,dx + \underbrace{x}_{B(x,y)}\,dy = 0\,. \tag{17.8}$$

Note: $\dfrac{\partial A}{\partial y} = \dfrac{\partial B}{\partial x} = 1$ so this equation is exact.

Therefore

$$\frac{\partial u}{\partial x} = x + y \qquad \text{and} \qquad \frac{\partial u}{\partial y} = x \tag{17.9}$$

and so

$$u(x,y) = \tfrac{1}{2}x^2 + xy + c\,. \tag{17.10}$$

Integrating Factors

If $A\,dx + B\,dy$ is not exact, try to find a function $\lambda(x, y)$ such that

$$\lambda(A\,dx + B\,dy) = 0 \tag{17.11}$$

is exact. Then we can integrate as before. Such a function is known as an **integrating factor**.

Such a factor always exists for a first-order equation, but there is not a general method for finding it.

However for a *linear* first-order equation

$$\frac{dy}{dx} + f(x)\,y = g(x) \tag{17.12}$$

we *can* obtain λ. Multiply by $\lambda(x)$:

$$\underbrace{\lambda(x)[dy + f(x)\,y\,dx]}_{\substack{\text{this is exact iff} \\ \frac{d\lambda}{dx} = \lambda(x)f(x)}} = \underbrace{\lambda(x)g(x)\,dx}_{\text{this is integrable}} \tag{17.13}$$

so the integrating factor we seek is

$$\boxed{\lambda(x) = \exp\left[\int f(x)\,dx\right].} \tag{17.14}$$

Ex. 17.3. Consider

$$xy' + (1+x)y = e^x\,. \tag{17.15}$$

Write this in the form

$$y' + \underbrace{\left(\frac{1+x}{x}\right)}_{f(x)} y = \underbrace{\frac{e^x}{x}}_{g(x)} \tag{17.16}$$

so we see this is a linear, first-order equation.

The integrating factor is

$$\lambda(x) = \exp\left[\int f(x)\,dx\right] = \exp\left(\int \frac{1+x}{x}\,dx\right) = \exp(x + \ln x) \tag{17.17a}$$

$$= xe^x\,. \tag{17.17b}$$

Multiply the original equation by the integrating factor:

$$xe^x\left[xy' + \left(\frac{1+x}{x}\right)y\right] = e^{2x}\,. \tag{17.18}$$

We see this equation is exact:

$$\underbrace{xe^x}_{B(x)}\,dy + \underbrace{(1+x)e^x y}_{A(x,y)}\,dx = e^{2x}\,dx \tag{17.19}$$

and we verify

$$\frac{\partial B}{\partial x} = e^x + xe^x \qquad \text{and} \qquad \frac{\partial A}{\partial y} = (1+x)e^x = \frac{\partial B}{\partial x} \quad \checkmark \tag{17.20}$$

thus

$$\frac{\partial u}{\partial x} = A(x,y) = (1+x)e^x y \qquad \text{and} \qquad \frac{\partial u}{\partial y} = B(x) = xe^x \tag{17.21}$$

which implies

$$u(x,y) = xe^x y\,. \tag{17.22}$$

Therefore, integrating $du = e^{2x}\,dx$, we find

$$xe^x y = \int e^{2x}\,dx = \tfrac{1}{2}e^{2x} + c \tag{17.23}$$

or

$$y = \frac{1}{2x}e^x + \frac{c}{x}e^{-x}\,. \tag{17.24}$$

Ex. 17.4. Thermodynamics.

The integrating factor plays a fundamental role in thermodynamics.

Suppose a system has state variables:

$$\underbrace{X_1, X_2, \dots, X_n}_{\substack{\text{extensive variables,}\\ \text{i.e., displacements,}\\ \text{e.g., volume}}} \qquad \text{and} \qquad \underbrace{Y_1, Y_2, \dots, Y_n}_{\substack{\text{intensive variables,}\\ \text{i.e., forces,}\\ \text{e.g., pressure}}}$$

and an internal energy function $U = U(X_1, \dots, X_n, Y_1, \dots, Y_n)$.

For a quasistatic process, the first law of thermodynamics (conservation of energy) is

$$\underbrace{đQ}_{\text{heat flow}} = \underbrace{dU}_{\substack{\text{change in}\\ \text{internal energy}}} + \underbrace{Y_1\,dX_1 + \dots + Y_n\,dX_n}_{\text{work terms}}\,. \tag{17.25}$$

The use of $đ$ (rather than d) for the heat flow reminds us that the right hand side cannot generally be written as an exact differential so the equation cannot generally be integrated. Therefore there is no 'heat' of the system, $Q = Q(X_1, \dots, X_n, Y_1, \dots, Y_n)$.

If $n = 1$ we have claimed an integrating factor can always be found for an equation of this form, but for $n > 1$ this cannot be integrated in general with the aid of an integrating factor...

but....

Kelvin-Planck statement of the second law of thermodynamics:

> It is impossible to construct an engine which, operating in a cycle, will produce no other effect than the extraction of heat from a reservoir and the performance of an equivalent amount of work.

Reminder: an adiabatic process has $đQ = 0$.

Suppose that you can reach a point $\mathcal{P}$ in state-space by two different adiabatic processes, i.e., two adiabatic curves intersect at $\mathcal{P}$ as shown in Fig. 17.1.
Consider the cycle: $\mathcal{P} \to \mathcal{Q} \to \mathcal{R} \to \mathcal{P}$.

- Work is done by the system in $\mathcal{P} \to \mathcal{Q}$ and $\mathcal{R} \to \mathcal{P}$ but no heat is gained or lost.
- No work is done in $\mathcal{Q} \to \mathcal{R}$ but heat is gained.

The net effect is conversion of heat into an equivalent amount of work.

Therefore, adiabatic processes *cannot* intersect.

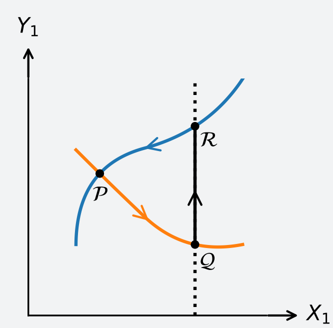


Figure 17.1: Intersecting Adiabats

Since adiabatic surfaces do not intersect, we can label them, 1, 2, 3, ..., as seen in Fig. 17.2. Thus there exists a function of state variables,

$$S = S(X_1, \ldots, X_n, Y_1, \ldots, Y_n)$$

which is constant for adiabatic processes:

$$dS = 0 \quad \text{when} \quad đQ = 0\,.$$

This implies that there must exist an integrating factor

$$\lambda = \lambda(X_1, \ldots, X_n, Y_1, \ldots, Y_n)$$

so that the adiabatic surfaces are

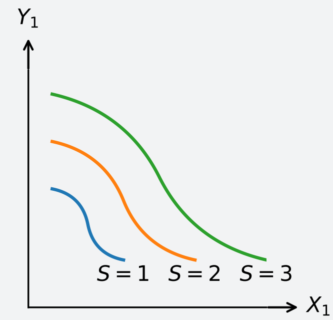


Figure 17.2: Non-intersecting Adiabats

$$0 = dS = \lambda\, đQ = \underbrace{\lambda(dU + Y_1\, dX_1 + \cdots + Y_n\, dX_n)}_{\text{exact}} \tag{17.26}$$

We recognize S as the entropy and $\lambda = 1/T$ where T is the temperature:

$$đQ = T\, dS\,. \tag{17.27}$$

This is the mathematical restatement of the second law of thermodynamics.

Change of Variables

Changing variables can often help.

Ex. 17.5. Consider an equation of the form

$$y' = f(ax + by + c) \tag{17.28}$$

which can be re-expressed as

$$dy = f(ax + by + c)\,dx\,. \tag{17.29}$$

Let

$$v = ax + by + c \tag{17.30a}$$

so

$$dv = a\,dx + b\,dy \qquad \text{or} \qquad a\,dx = dv - b\,dy\,. \tag{17.30b}$$

Then

$$a\,dy = f(v)(dv - b\,dy) \tag{17.31a}$$
$$\implies [a + bf(v)]\,dy = f(v)\,dv \tag{17.31b}$$
$$\implies dy = \frac{f(v)}{a + bf(v)}\,dv\,. \tag{17.31c}$$

The equation is now separated and we can integrate directly.

Ex. 17.6. Bernoulli equation

$$y' + f(x)\,y = g(x)\,y^n\,. \tag{17.32}$$

Divide by y^n:

$$\underbrace{\frac{1}{y^n}\frac{dy}{dx}}_{\frac{1}{1-n}\frac{d}{dx}y^{1-n}} + f(x)\,y^{1-n} = g(x)\,. \tag{17.33}$$

Thus we let $v = y^{1-n}$ to obtain

$$\frac{dv}{dx} + (1-n)f(x)v = (1-n)g(x)\,. \tag{17.34}$$

This is now a linear first-order equation that has an integrating factor:

$$\lambda(x) = e^{(1-n)\int^x f(x')\,dx'}\,. \tag{17.35}$$

Multiply by the integrating factor:

$$\underbrace{e^{(1-n)\int^x f(x')\,dx'}\frac{dv}{dx} + (1-n)f(x)ve^{(1-n)\int^x f(x')\,dx'}}_{\frac{d}{dx}\left[ve^{(1-n)\int^x f(x')\,dx'}\right]} = (1-n)g(x)e^{(1-n)\int^x f(x')\,dx'} \tag{17.36}$$

and therefore

$$ve^{(1-n)\int^x f(x')\,dx'} = \int (1-n)g(x)e^{(1-n)\int^x f(x')\,dx'}\,dx\,. \tag{17.37}$$

Homogeneous Functions

A function $f(x, y, \ldots)$ is a **homogeneous function** of degree r in the arguments if

$$\boxed{f(ax, ay, \ldots) = a^r f(x, y, \ldots)\,.} \tag{17.38}$$

A first order ODE $A(x, y)\,dx + B(x, y)\,dy = 0$ is a **homogeneous equation** if A and B are homogeneous functions of the same degree.
Then the substitution $y = vx$ makes the equation separable.

Ex. 17.7. Consider

$$\underbrace{y}_{\substack{\text{homogeneous}\\ \text{of degree 1}}}\,dx + \underbrace{(2\sqrt{xy} - x)}_{\substack{\text{homogeneous}\\ \text{of degree 1}}}\,dy = 0\,. \tag{17.39}$$

Let $y = vx$, $dy = v\,dx + x\,dv$; then

$$vx\,dx + (2x\sqrt{v} - x)(v\,dx + x\,dv) = 0 \tag{17.40a}$$

$$\implies \quad [\cancel{vx} + vx(2\sqrt{v} - \cancel{1})]\,dx + (2\sqrt{v} - 1)x^2\,dv = 0 \tag{17.40b}$$

$$\implies \quad 2v^{3/2}x\,dx + (2\sqrt{v} - 1)x^2\,dv = 0 \tag{17.40c}$$

$$\implies \quad \frac{dx}{x} + \frac{2\sqrt{v} - 1}{2v^{3/2}}\,dv = 0 \tag{17.40d}$$

which is now separated!

Why did this work?

Suppose x and y both had the same dimensions, say meters.
Homogeneity means that the ODE is dimensionally consistent.
The substitution $y = vx$ introduces a *dimensionless* variable v.
We then have to be able to write the ODE in the form

$$f(v)\,dv + g(v)\,\frac{dx}{x} = 0 \tag{17.41}$$

in order for the dimensions to work out.

(Obviously, dimensional consistency of equations of motion is an important thing in physics, so this device occurs frequently.)

Generalization: suppose that

$$(\text{dimensions of } y) = (\text{dimensions of } x)^m \tag{17.42}$$

for some power m, and that

$$A(ax, a^m y) = a^r A(x,y) \qquad \text{and} \qquad B(ax, a^m y) = a^{r-m+1} B(x,y) \tag{17.43}$$

so that the ODE $A(x,y)\,dx + B(x,y)\,dy = 0$ is dimensionally correct.
Then the substitution $y = vx^m$ reduces the equation to a separable one.

Such an equation is called an **isobaric equation**.

Ex. 17.8. Consider

$$xy^2(3y\,dx + x\,dy) - (2y\,dx - x\,dy) = 0\,. \tag{17.44}$$

Test if this is isobaric: suppose x has units of s and suppose y has units of s^m. Then the dimensions of terms of the equation are

$$\mathrm{s}\mathrm{s}^{2m}(\mathrm{s}^m\mathrm{s} \quad \& \quad \mathrm{s}\mathrm{s}^m) \quad \& \quad (\mathrm{s}^m\mathrm{s} \quad \& \quad \mathrm{s}\mathrm{s}^m) \tag{17.45a}$$

$$\implies \quad \mathrm{s}^2\mathrm{s}^{3m} \quad \& \quad \mathrm{s}\mathrm{s}^m \tag{17.45b}$$

so the equation is dimensionally consistent if $2+3m = 1+m$ or $m = -\frac{1}{2}$.

We are told to introduce v by $y = vx^{-1/2}$ or $v = y\sqrt{x}$ which is dimensionless.
Actually, it is more convenient to let $v = y^2 x$ so $x = v/y^2$ and $dx = \dfrac{dv}{y^2} - \dfrac{2v\,dy}{y^3}$. Then

$$v\left(3y\frac{dv}{y^2} - 3y\frac{2v\,dy}{y^3} + \frac{v}{y^2}\,dy\right) - \left(2y\frac{dv}{y^2} - 2y\frac{2v\,dy}{y^3} - \frac{v}{y^2}\,dy\right) = 0\,. \tag{17.46a}$$

Multiply by y^2:

$$v(3y\,dv - 6v\,dy + v\,dy) - (2y\,dv - 4v\,dy - v\,dy) = 0 \tag{17.46b}$$

$$\implies \quad (3v-2)y\,dv + 5v(1-v)\,dy = 0 \tag{17.46c}$$

which is separable.

18 Higher Order ODEs

Linear Equations with Constant Coefficients

These are equations of the form

$$a_n y^{(n)} + a_{n-1} y^{(n-1)} + \cdots + a_2 y'' + a_1 y' + a_0 y = f(x)\,. \tag{18.1}$$

- If $f(x) = 0$, the equation is a **homogeneous equation**.
- Otherwise, the equation is an **inhomogeneous equation**.

The general solution to an inhomogeneous equation is the sum of the general solution to the homogeneous equation — the **complementary function** — and *any* solution of the inhomogeneous equation — the **particular integral**.

- To solve the homogeneous equation (where $f(x) = 0$), try $y = e^{mx}$. Then

  $$a_n m^n + a_{n-1} m^{n-1} + \cdots + a_1 m + a_0 = 0\,. \tag{18.2}$$

  The n roots of this polynomial are $m_1, m_2, \ldots, m_n$; when they are distinct, the complementary function is

  $$c_1 e^{m_1 x} + c_2 e^{m_2 x} + \cdots + c_n e^{m_n x} \tag{18.3}$$

  where $c_1, c_2, \ldots, c_n$ are arbitrary constants.

  However, suppose that some of the roots are the same, e.g., suppose $m_1 = m_2$. Now there are only $n-1$ solutions and we need another. Imagine a procedure in which $m_2 \to m_1$ (i.e., we perturb the coefficients a_0, $\ldots$, a_n to break the degeneracy). Then

  $$\frac{e^{m_2 x} - e^{m_1 x}}{m_2 - m_1} \tag{18.4}$$

  is a solution (since it is the sum of two solutions), and as $m_2 \to m_1$ (by reducing the perturbation) it becomes

  $$\left.\frac{d}{dm} e^{mx}\right|_{m=m_1} = x e^{m_1 x} \tag{18.5}$$

  and this is the additional solution we need.

  If three roots are equal, $m_1 = m_2 = m_3$, then the solutions are $e^{m_1 x}$, $x e^{m_1 x}$, and $x^2 e^{m_1 x}$ (and so on).

- Finding a particular solution can be tricky....

  Try the **method of undetermined coefficients**:

  If $f(x)$ has only a finite number of linearly independent derivatives, e.g., x^n, $e^{\alpha x}$, $\sin kx$, $\cos kx$, $x^n e^{\alpha x} \cos kx$, ...
  then take as a trial $y(x)$ to be a linear combination of $f(x)$ and its independent derivatives.

Ex. 18.1. Solve

$$y'' + 3y' + 2y = e^x \,. \tag{18.6}$$

– Complementary function. Letting $y = e^{mx}$ results in the polynomial equation $m^2 + 3m + 2 = 0$ with roots $m = -1$ and $m = -2$. Thus

$$y = c_1 e^{-x} + c_2 e^{-2x} \,. \tag{18.7}$$

– Particular integral. Try $y = Ae^x$ and substitute into the ODE:

$$Ae^x + 3Ae^x + 2Ae^x = e^x \quad \Longrightarrow \quad 6A = 1 \quad \Longrightarrow \quad A = \tfrac{1}{6} \,. \tag{18.8}$$

Therefore, the general solution is

$$y = \tfrac{1}{6} e^x + c_1 e^{-x} + c_2 e^{-2x} \,. \tag{18.9}$$

Note: if $f(x)$ or a term in $f(x)$ is also part of the complementary function, the particular integral may contain this term and its derivatives multiplied by some power of x.

Ex. 18.2. Re-solve Ex. 18.1 $f(x) = e^{-x}$ rather than e^x.

– Try $y = Ae^{-x}$:

$$\cancel{Ae^{-x}} - \cancel{3Ae^{-x}} + \cancel{2Ae^{-x}} = e^{-x} \tag{18.10}$$

so this doesn't work (because e^{-x} is a solution to the homogeneous equation).

– Now try $y = Axe^{-x}$, $y' = Ae^x - Axe^{-x}$, $y'' = -2Ae^{-x} + Axe^{-x}$. Then

$$(-2Ae^{-x} + \cancel{Axe^{-x}}) + 3(Ae^{-x} - \cancel{Axe^{-x}}) + \cancel{2Axe^{-x}} = e^{-x} \tag{18.11a}$$
$$\Longrightarrow \quad Ae^{-x} = e^{-x} \tag{18.11b}$$
$$\Longrightarrow \quad A = 1 \,. \tag{18.11c}$$

Therefore the general solution is

$$y = xe^{-x} + c_1 e^{-x} + c_2 e^{-2x} \,. \tag{18.12}$$

Tricks for More General Problems

- If the dependent variable y is absent, let $y' = p$ be the new dependent variable. This lowers the order by one.
- If the equation is homogeneous in y, let $v = \ln y$ be a new dependent variable. The resulting equation will not contain v and the substitution $v' = p$ will reduce the order by one.
- If the equation is isobaric when x is given weight 1 and y is given weight m, the change in dependent variable $y = vx^m$ followed by the change in the independent variable $u = \ln x$ gives an equation in which the new independent variable u is absent.
- Watch for the possibility that the equation is exact and consider the possibility of finding an integrating factor. For example,

  $$y'' = f(y) \tag{18.13}$$

  can be integrated immediately by multiplying both sides by y'.

19 Power Series Solutions

Illustrate the basic idea with an example:

Ex. 19.1. A simple non-linear equation is

$$y'' = x - y^2. \tag{19.1}$$

Try a power series solution: $y = c_0 + c_1 x + c_2 x^2 + \cdots$. We find

$$2c_2 + 6c_3 x + 12c_4 x^2 + \cdots = x - c_0^2 - 2c_0 c_1 x - (c_1^2 + 2c_0 c_2)x^2 - \cdots \tag{19.2}$$

so equating like powers we have

$$2c_2 = -c_0^2 \qquad \Longrightarrow \qquad c_2 = -\tfrac{1}{2}c_0^2 \tag{19.3a}$$

$$6c_3 = 1 - 2c_0 c_1 \qquad \Longrightarrow \qquad c_3 = \tfrac{1}{6} - \tfrac{1}{3}c_0 c_1 \tag{19.3b}$$

$$12c_4 = -c_1^2 - 2c_0 c_2 \qquad \Longrightarrow \qquad c_4 = -\tfrac{1}{12}c_1^2 + \tfrac{1}{12}c_0^3 \tag{19.3c}$$

and so on....

Note: c_n, $n > 1$ can all be expressed in terms of c_0 and c_1, which are the two free constants of integration.

If we want a solution with $y = 0$ and $y' = 1$ at $x = 0$ then $c_0 = 0$, $c_1 = 1$, and $c_2 = 0$, $c_3 = \frac{1}{6}$, $c_4 = -\frac{1}{12}, \ldots$, so

$$y = x + \tfrac{1}{6}x^3 - \tfrac{1}{12}x^4 + \cdots \tag{19.4}$$

(but we don't know if this series converges).

Linear Differential Equations

These have the form

$$\frac{d^n y}{dx^n} + f_{n-1}(x)\frac{d^{n-1}y}{dx^{n-1}} + \cdots + f_1(x)\frac{dy}{dx} + f_0(x)y = 0\,. \tag{19.5}$$

- If $f_0(x)$, $f_1(x)$, ..., $f_{n-1}(x)$ are regular at a point $x = x_0$ we call x_0 an **ordinary point** of the differential equation. The general solution can be written as a Taylor series with radius of convergence out to the nearest **singular point**:

  $$y = \sum_{m=0}^{\infty} c_m (x - x_0)^m \tag{19.6}$$

  The coefficients c_m are obtained by substitution into the differential equation (as before).

- If x_0 is not an ordinary point but

  $$(x - x_0)f_{n-1}(x)\,, \quad (x - x_0)^2 f_{n-2}(x)\,, \quad \ldots\,, \quad (x - x_0)^n f_0(x)$$

  are all regular at x_0 then x_0 is a **regular singular point**.

  Then we can always find at least one solution of the form

  $$y = (x - x_0)^s \sum_{m=0}^{\infty} c_m (x - x_0)^m\,, \quad c_0 \neq 0 \tag{19.7}$$

  (where s is not necessarily an integer) which has a radius of convergence to the nearest singularity apart from x_0.

Explore these two cases in the next two examples.

Ex. 19.2. Legendre's equation (a non-singular case) is:

$$\boxed{(1-x^2)y'' - 2xy' + n(n+1)y = 0\,.} \tag{19.8}$$

This has regular singular points at $x = \pm 1$. Expand about $x = 0$:

$$y = c_0 + c_1 x + c_2 x^2 + \cdots \tag{19.9}$$

and insert this into the differential equation to obtain

$$(1-x^2)\sum_{m=2}^{\infty}(m)(m-1)c_m x^{m-2} - 2x\sum_{m=1}^{\infty}(m)c_m x^{m-1} + n(n+1)\sum_{m=0}^{\infty} c_m x^m = 0\,. \tag{19.10a}$$

Write out the $m = 0$ and $m = 1$ terms explicitly:

$$n(n+1)(c_0 + c_1 x) - 2xc_1 + \sum_{m=2}^{\infty} c_m[m(m-1)x^{m-2} - m(m-1)x^m - 2mx^m + n(n+1)x^m] = 0 \tag{19.10b}$$

$$\implies \quad n(n+1)(c_0 + c_1 x) - 2xc_1 + \sum_{m=2}^{\infty} c_m\Big\{\underbrace{m(m-1)x^{m-2}}_{\text{consider this}} + [n(n+1) - m(m+1)]x^m\Big\} = 0\,. \tag{19.10c}$$

Note that

$$\sum_{m=2}^{\infty} c_m m(m-1)x^{m-2} = c_2(1)(2) + c_3(3)(2)x + \sum_{m=4}^{\infty} c_m m(m-1)x^{m-2} \tag{19.11a}$$

let $m = m' + 2$

$$= 2c_2 + 6c_3 x + \sum_{m'=2}^{\infty} c_{m'+2}(m'+2)(m'+1)x^{m'} \tag{19.11b}$$

so we have

$$[n(n+1)c_0 + 2c_2] + [n(n+1)c_1 - 2c_1 + 6c_3]x + \sum_{m=2}^{\infty}\Big\{c_{m+2}(m+2)(m+1) + c_m[n(n+1) - m(m+1)]x^m\Big\} = 0\,. \tag{19.12}$$

Now equate powers of x to find

$$2c_2 = -n(n+1)c_0 \qquad \Longrightarrow \qquad c_2 = -\frac{n(n+1)}{2}c_0 \tag{19.13a}$$

$$6c_3 = 2c_1 - n(n+1)c_1 \qquad \Longrightarrow \qquad c_3 = \frac{2-n(n+1)}{6}c_1 \tag{19.13b}$$

and the general recurrence relation

$$\begin{aligned}(m+1)(m+2)c_{m+2} &= -[n(n+1)-m(m+1)]c_m \\ \Longrightarrow \quad \frac{c_{m+2}}{c_m} &= \frac{m(m+1)-n(n+1)}{(m+1)(m+2)} = \frac{(m+n+1)(m-n)}{(m+1)(m+2)}.\end{aligned} \tag{19.13c}$$

Hence our solution is

$$\begin{aligned}y = & c_0\left[1 - n(n+1)\frac{x^2}{2!} + n(n+1)(n-2)(n+3)\frac{x^4}{4!} + \cdots\right] \\ & + c_1\left[x - (n-1)(n+2)\frac{x^3}{3!} + (n-1)(n+2)(n-3)(n+4)\frac{x^5}{5!} + \cdots\right].\end{aligned} \tag{19.14}$$

Note that $\frac{c_{m+2}}{c_m} \to 1$ as $m \to \infty$ so both series converge for $x^2 < 1$.

Write the general solution as

$$y = c_0 U_n(x) + c_1 V_n(x) \tag{19.15a}$$

where

$$U_n(x) = 1 - n(n+1)\frac{x^2}{2!} + n(n+1)(n-2)(n+3)\frac{x^4}{4!} + \cdots \tag{19.15b}$$

$$V_n(x) = x - (n-1)(n+2)\frac{x^3}{3!} + (n-1)(n+2)(n-3)(n+4)\frac{x^5}{5!} + \cdots \tag{19.15c}$$

are the two independent solutions, and c_0 and c_1 are the two constants of integration.

Although the series converge for $|x| < 1$, we saw in Ex. 2.4 that they diverge for $|x| = 1$; however, we normally want solutions over the domain $-1 \le x \le 1$. This can be arranged in one of two ways:

1. Let $c_1 = 0$ and choose one of $n = -1, -3, -5, \ldots$ or $n = 0, 2, 4, \ldots$.
   Then the first series $U_n(x)$ terminates and the second series $V_n(x)$ is absent.
2. Let $c_0 = 0$ and choose one of $n = -2, -4, -6, \ldots$ or $n = 1, 3, 5, \ldots$.
   Then the second series $V_n(x)$ terminates and the first series $U_n(x)$ is absent.

Therefore, to have a finite solution on $-1 \le x \le 1$, n must be an integer. The resulting solution is a polynomial which, when normalized by the condition $y(1) = 1$, is called a **Legendre polynomial**:

$$P_n(x) = \begin{cases} U_n(x)/U_n(1) & n = 0, 2, 4, \ldots \\ V_n(x)/V_n(1) & n = 1, 3, 4, \ldots . \end{cases} \tag{19.16}$$

The first few Legendre polynomials are

$$\boxed{P_0(x) = 1\,, \quad P_1(x) = x\,, \quad P_2(x) = \tfrac{1}{2}(3x^2 - 1)\,, \quad P_3(x) = \tfrac{1}{2}(5x^3 - 3x)\,, \quad \text{etc.}} \tag{19.17}$$

See Fig. 19.1.

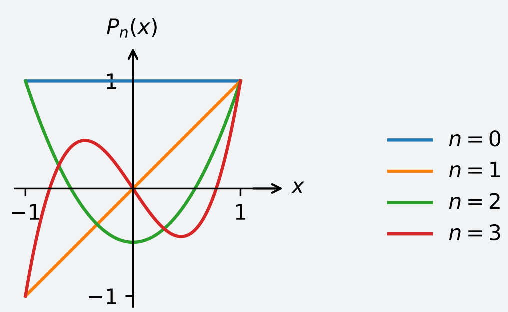


Figure 19.1: Legendre Polynomials

What about the non-terminating series for integer n?
This series diverges at $x = \pm 1$. Consider, for example, the case $n = 0$ and $c_0 = 0$:

$$y = c_1 \left[x - (-1)(2)\frac{x^3}{3!} + (-1)(2)(-3)(4)\frac{x^5}{5!} - \cdots \right]. \tag{19.18}$$

Note:

$$\frac{c_{m+2}}{c_m} = \frac{(m+n+1)(m-n)}{(m+1)(m+2)} = \frac{m}{m+2} \quad \text{since } n = 0 \tag{19.19a}$$

$$\implies \quad (m+2)c_{m+2} = m c_m \tag{19.19b}$$

$$\implies \quad c_m = \frac{c_1}{m}. \tag{19.19c}$$

Thus

$$y = c_1 \left[x + \frac{x^3}{3} + \frac{x^5}{5} + \frac{x^7}{7} + \cdots \right]. \tag{19.20}$$

We've seen this series before in Eq. (3.11): it is $\frac{1}{2}\ln\left(\frac{1+x}{1-x}\right)$ and is singular at $x = \pm 1$.

We have **Legendre functions of the second kind** of order n:

$$Q_n(x) = \begin{cases} U_n(1)V_n(x) & n = 0, 2, 4, \ldots \\ -V_n(1)U_n(x) & n = 1, 3, 5, \ldots \end{cases} \tag{19.21}$$

with

$$\boxed{Q_0(x) = \frac{1}{2}\ln\left(\frac{1+x}{1-x}\right), \quad Q_1(x) = \frac{x}{2}\ln\left(\frac{1+x}{1-x}\right) - 1, \quad \text{etc.}} \tag{19.22}$$

See Fig. 19.2.

The general solution to Legendre's equation with integer n is

$$y = AP_n(x) + BQ_n(x). \tag{19.23}$$

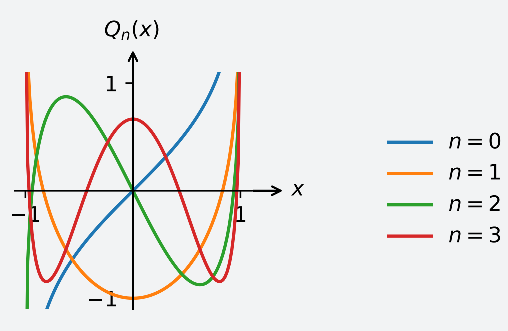


Figure 19.2: Legendre Functions of the Second Kind

Ex. 19.3. Bessel's equation (a singular case) is:

$$\boxed{x^2 y'' + xy' + (x^2 - \nu^2)y = 0\,.} \tag{19.24}$$

This has a regular singular point at $x = 0$ so the solution has the form

$$y(x,s) = x^s \sum_{n=0}^{\infty} c_n x^n\,, \qquad c_0 \neq 0\,. \tag{19.25}$$

We have

$$xy' = \sum_{n=0}^{\infty} (s+n) c_n x^{s+n} \tag{19.26a}$$

$$x^2 y'' = \sum_{n=0}^{\infty} (s+n)(s+n-1) c_n x^{s+n} \tag{19.26b}$$

so, substituting into Bessel's equation we find

$$\sum_{n=0}^{\infty} \Big\{ \underbrace{\left[(s+n)(s+n-1) + (s+n) - \nu^2\right]}_{(s+n)^2-\nu^2=(s+n+\nu)(s+n-\nu)} c_n x^{s+n} + c_n x^{s+n+2} \Big\} = 0\,. \tag{19.27}$$

Write out the first two terms explicitly:

$$(s^2 - \nu^2) c_0 x^s + [(s+1)^2 - \nu^2] c_1 x^{s+1} + \sum_{n=2}^{\infty} [(s+\nu+n)(s-\nu+n) c_n + c_{n-2}] x^{s+n} = 0\,. \tag{19.28}$$

We see that Bessel's equation is solved if

- $$s^2 = \nu^2 \tag{19.29a}$$
  which is called the **indicial equation**;
- $$c_1 [(s+1)^2 - \nu^2] = 0 \tag{19.29b}$$
  which is solved if $c_1 = 0$ or $(s+1) = \pm\nu$;
- $$\frac{c_n}{c_{n-2}} = -\frac{1}{(s+\nu+n)(s-\nu+n)} \tag{19.29c}$$
  which is the recurrence relation.

We choose to solve the second of these by setting $c_1 = 0$. Then only n even terms survive and the recurrence formula gives all c_n (n even) in terms of c_0. The solutions to the indicial equation are $s = \pm\nu$ and the two independent solutions are

$$y(x,+\nu) \qquad \text{and} \qquad y(x,-\nu)\,. \tag{19.30}$$

Aside: had we left c_1 free and instead set $(s+1) = \pm\nu$ then, with the indicial equation, we have the requirement $s = -\nu = -1/2$. It turns out that the terms that appear from this are identical to those contained in the other solution $s = +\nu = 1/2$ with $c_1 = 0$, so we can choose $c_1 = 0$ even for the $\nu = 1/2$ case.

Set $s^2 = \nu^2$ and $c_1 = 0$. Then

$$\frac{c_n}{c_{n-2}} = -\frac{1}{(s+n)^2 - s^2} = -\frac{1}{\cancel{s^2} + 2sn + n^2 - \cancel{s^2}} = -\frac{1}{n(2s+n)}\,. \tag{19.31}$$

The non-vanishing coefficients are c_{2n}:

$$c_2 = -\frac{c_0}{2(2s+2)} = -\frac{1}{4\cdot(s+1)}c_0 \tag{19.32a}$$

$$c_4 = -\frac{c_2}{4(2s+2)} = -\frac{c_2}{8(s+2)} = \frac{1}{4\cdot 8\cdot(s+1)(s+2)}c_0 \tag{19.32b}$$

$$c_6 = -\frac{c_4}{6(2s+6)} = -\frac{c_4}{12(s+3)} = \frac{1}{4\cdot 8\cdot 12\cdot(s+1)(s+2)(s+3)}c_0 \tag{19.32c}$$

$$\vdots$$

$$c_{2n} = -\frac{c_{2n-2}}{2n(2s+2n)} = -\frac{c_{2n-2}}{4n(s+n)}$$

$$= \frac{(-1)^n}{2^{2n}n!(s+1)(s+2)(s+3)\cdots(s+n)}c_0\,. \tag{19.32d}$$

But there is a problem if ν is an integer: the procedure works fine for the $s = +\nu$ solution (assume ν is positive), but the second solution with $s = -\nu$ won't work because

$$\frac{c_n}{c_{n-2}} = -\frac{1}{(s+\nu+n)(s-\nu+n)} \underset{s=-\nu}{=} -\frac{1}{n(n-2\nu)} \tag{19.33}$$

so when $n = 2\nu$, the ratio is infinite and $c_{2\nu}$ and higher are infinite!

We need a way to get a second solution, so we try this trick: don't impose the indicial relation (i.e., leave s and ν unrelated), multiply $y(x,s)$ by the factor $(s+\nu)$, then take the limit as $s \to -\nu$. The factor will cancel the infinities with this procedure.

It turns out this doesn't work… but let's try it and see why.

Before taking $s \to -\nu$, the solution will be

$$(s+\nu)y(x,s) = c_0 x^s \Big\{(s+\nu) - \frac{(s+\nu)}{(s+\nu+2)(s-\nu+2)}x^2 + \cdots \\ \pm \frac{\cancel{(s+\nu)}}{(s+\nu+2)(s-\nu+2)\cdots(s+\nu+2\nu)\underbrace{\cancel{(s-\nu+2\nu)}}_{\text{infinity is cancelled}}}x^{2\nu} \\ \mp \cdots \Big\}. \tag{19.34}$$

Now as $s \to -\nu$, the terms up to $x^{2\nu}$ vanish and we have

$$\Big[(s+\nu)y(x,s)\Big]_{s=-\nu} = c_0 x^{-\nu}\Big\{\pm \frac{1}{2\cdot(2-2\nu)\cdots(2\nu)}x^{2\nu} \mp \cdots\Big\} \tag{19.35a}$$

$$= c_0' x^{\nu}\Big\{1 - c_2' x^2 + \cdots\Big\} \tag{19.35b}$$

where

$$c_0' = \pm \frac{c_0}{2\cdot(2-2\nu)\cdots(2\nu)} \tag{19.35c}$$

and

$$\frac{c_n'}{c_{n-2}'} = \frac{c_{2\nu+n}}{c_{2\nu+n-2}} = -\frac{1}{(s+\nu+2\nu+n)(s-\nu+2\nu+n)} \tag{19.35d}$$

$$= -\frac{1}{[(s+2\nu)+\nu+n][(s+2\nu)-\nu+n]}. \tag{19.35e}$$

But note: $s+2\nu$ when $s=-\nu$ is the same as s when $s=+\nu$ so this solution is actually the *same* as the $y(x,+\nu)$ solution (up to an overall factor).
Thus it is *not* an independent solution.

Instead, substitute $[(s+\nu)y(x,s)]$ into Bessel's equation. The result will not be zero since we have not yet imposed the indicial equation:

$$\left[x^2\frac{\partial^2}{\partial x^2} + x\frac{\partial}{\partial x} + (x^2-\nu^2)\right](s+\nu)y(x,s) = (s+\nu)\underbrace{(s^2-\nu^2)}_{\substack{\text{result is proportional to}\\ \text{indicial equation}}} \\ = (s+\nu)^2(s-\nu). \tag{19.36}$$

Now take the partial derivative with respect to s:

$$\left[x^2\frac{\partial^2}{\partial x^2} + x\frac{\partial}{\partial x} + (x^2-\nu^2)\right]\frac{\partial}{\partial s}[(s+\nu)y(x,s)] = \underbrace{2(s+\nu)(s-\nu)+(s+\nu)^2}_{\text{vanishes as } s\to-\nu}. \tag{19.37}$$

Therefore our second solution is

$$\lim_{s\to-\nu}\frac{\partial}{\partial s}[(s+\nu)y(x,s)]. \tag{19.38}$$

To see how this works, consider the case $\nu = 2$:

$$y(x,s) = c_0 x^s\left\{1 - \frac{x^2}{s(s+4)} + \frac{x^4}{s(s+4)\underbrace{(s+2)}_{\substack{\text{this is what causes the}\\ \text{problem when } s=-\nu}}(s+6)} - \cdots\right\} \tag{19.39}$$

so

$$(s+2)y(x,s) = c_0 x^s\left\{(s+2) - \frac{(s+2)}{s(s+4)}x^2 + \frac{x^4}{s(s+4)(s+6)} - \frac{x^6}{s(s+4)(s+6)(s+4)(s+8)} + \cdots\right\}. \tag{19.40}$$

Now take the derivative with respect to s. Note: $\frac{\partial}{\partial s}x^s = \frac{\partial}{\partial s}e^{s\ln x} = x^s \ln x$.

$$\begin{aligned}\frac{\partial}{\partial s}[(s+\nu)y(x,s)] &= (s+2)y(x,s)\ln x \\ &\quad + c_0 x^s \frac{\partial}{\partial s}\left\{(s+2) - \frac{(s+2)}{s(s+4)}x^2 + \frac{x^4}{s(s+4)(s+6)} - \frac{x^6}{s(s+4)(s+6)(s+4)(s+8)} + \cdots\right\} &\text{(19.41a)}\\ &= (s+2)y(x,s)\ln x \\ &\quad + c_0 x^s\left\{1 - \frac{(s+2)}{s(s+4)}\left(\frac{1}{s+2} - \frac{1}{s} - \frac{1}{s+4}\right)x^2 + \frac{1}{s(s+4)(s+6)}\left(-\frac{1}{s} - \frac{1}{s+4} - \frac{1}{s+6}\right)x^4 - \cdots\right\}. &\text{(19.41b)}\end{aligned}$$

Now we set $s = -2$. Note that [cf. Eq. (19.35c)]

$$\Big[(s+2)y(x,s)\Big]_{s=-2} = \left[\frac{1}{s(s+4)(s+6)}\right]_{s=-2} y(x,+2) = -\frac{1}{16}y(x,2) \tag{19.42}$$

and therefore

$$\frac{\partial}{\partial s}[(s+2)y(x,s)] = -\frac{1}{16}y(x,2)\ln x + c_0\frac{1}{x^2}\left\{1 + \frac{x^2}{4} + \frac{x^4}{64} + \cdots\right\}. \tag{19.43}$$

This is our second independent solution. Note that it is singular at $x = 0$.

Application: Quantum Harmonic Oscillator

The stationary states of a one-dimensional quantum harmonic oscillator satisfy the time-independent Schrödinger equation

$$\frac{d^2\psi}{dx^2} + (E - x^2)\psi = 0\,. \tag{19.44}$$

Here, for convenience, we use the dimensionless variables: to restore dimensions, $x \to \sqrt{m\omega/\hbar}\,x$ and $E \to E/(\frac{1}{2}\hbar\omega)$ where ω is the angular frequency of the oscillator.

For large values of x we have

$$\frac{d^2\psi}{dx^2} - x^2\psi \approx 0 \tag{19.45}$$

and so the solutions are $\psi \sim e^{\pm x^2/2}$ as $x \to \infty$: $\psi' \sim \pm x e^{\pm x^2/2}$ and $\psi'' \sim x^2 e^{\pm x^2/2}$ (where the omitted term is higher order in the asymptotic series) so $\psi'' - x^2\psi$ vanishes at leading order in the asymptotic series.

Physical solutions must not become infinite as $x \to \infty$. This motivates the substitution

$$\psi = y e^{-x^2/2}\,. \tag{19.46}$$

(We must watch for the solutions $y \sim e^{x^2}$ that generate the unwanted $\psi \sim e^{+x^2/2}$ behavior.) We have:

$$\psi' = y' e^{-x^2/2} - xy e^{-x^2/2} \tag{19.47a}$$

$$\psi'' = y'' e^{-x^2/2} - 2xy' e^{-x^2/2} - y e^{-x^2/2} + x^2 y e^{-x^2/2} \tag{19.47b}$$

so, substituting into the Schrödinger equation, we have

$$(y'' - 2xy' - y + \cancel{x^2 y}) + Ey - \cancel{x^2 y} = 0\,. \tag{19.47c}$$

The resulting equation is the **Hermite differential equation**:

$$\boxed{y'' - 2xy' + (E-1)y = 0\,.} \tag{19.48}$$

We seek a power series solution of the form

$$y = \sum_{n=0}^{\infty} c_n x^n . \tag{19.49}$$

Substitute this into the Hermite equation:

$$0 = \sum_{n=2}^{\infty} n(n-1)c_n x^{n-2} - 2\sum_{n=1}^{\infty} n c_n x^n + (E-1)\sum_{n=0}^{\infty} c_n x^n \tag{19.50a}$$

$$\begin{aligned} &= \sum_{n=2}^{\infty} n(n-1)c_n x^{n-2} \\ &\qquad - 2c_1 x - 2\sum_{n=2}^{\infty} n c_n x^n \\ &\qquad + (E-1)c_0 + (E-1)c_1 x + (E-1)\sum_{n=2}^{\infty} c_n x^n \end{aligned} \tag{19.50b}$$

$$\begin{aligned} &= \sum_{n=0}^{\infty} (n+2)(n+1)c_{n+2} x^n \\ &\qquad - 2c_1 x + (E-1)c_0 + (E-1)c_1 x + \sum_{n=2}^{\infty} (E-1-2n)c_n x^n \end{aligned} \tag{19.50c}$$

$$\begin{aligned} &= 2c_2 + 6c_3 x + \sum_{n=2}^{\infty} (n+2)(n+1)c_{n+2} x^n \\ &\qquad - 2c_1 x + (E-1)c_0 + (E-1)c_1 x + \sum_{n=2}^{\infty} (E-1-2n)c_n x^n \end{aligned} \tag{19.50d}$$

$$\begin{aligned} &= [(E-1)c_0 + 2c_2] + [(E-3)c_1 + 6c_3]x \\ &\qquad + \sum_{n=2}^{\infty} [(n+2)(n+1)c_{n+2} - (2n+1-E)c_n] x^n . \end{aligned} \tag{19.50e}$$

Therefore

$$c_2 = \frac{1-E}{2} c_0 , \qquad c_3 = \frac{3-E}{6} c_1 , \tag{19.51a}$$

and

$$\frac{c_{n+2}}{c_n} = \frac{(2n+1)-E}{(n+1)(n+2)} , \qquad n = 2, 3, 4, \ldots . \tag{19.51b}$$

Therefore our power series solution is

$$y = c_0 \left\{ 1 + (1-E)\frac{x^2}{2!} + (1-E)(5-E)\frac{x^4}{4!} + \cdots \right\}$$
$$+ c_1 \left\{ x + (3-E)\frac{x^3}{3!} + (3-E)(7-E)\frac{x^5}{5!} + \cdots \right\}. \tag{19.52}$$

In general, for large n, $\frac{c_{n+2}}{c_n} \sim \frac{2}{n}$ as $n \to \infty$ so $c_{2n+2} \sim \frac{2}{2n} c_{2n} = \frac{c_{2n}}{n}$.
Therefore

$$c_{2(n+1)} \sim \frac{c_{2n}}{n} \sim \frac{c_{2(n-1)}}{n(n-1)} \sim \cdots \sim \frac{c_0}{n!} \text{ as } n \to \infty \tag{19.53}$$

and similarly with the odd-n coefficients.
Therefore the terms are $\sim \frac{(x^2)^n}{n!}$ as $n \to \infty$ so $y \sim e^{x^2}$ for large x as expected: this generates the $\psi \sim e^{x^2/2}$ solutions.

The bounded (as $x \to \pm\infty$) solutions are when one of the series truncates (and the coefficient of the other series is chosen to be 0). This only happens when

$$(2n+1) - E = 0 \quad \Longrightarrow \quad E = 2n+1\,. \tag{19.54}$$

Then one of the two series will truncate.

We see that the boundary conditions pose restrictions on the form of the differential equation. Acceptable values of E are

$$E = E_n = 2n+1\,, \qquad n = 0, 1, 2, \ldots\,. \tag{19.55}$$

These are **eigenvalues**. The corresponding solutions (that don't blow up) are the **eigenfunctions**

$$\psi(x) = \psi_n(x) = H_n(x)e^{-x^2/2} \tag{19.56}$$

where $H_n(x)$ are **Hermite polynomials** of order n:

$$H_0(x) = 1 \qquad \text{for} \qquad E_0 = 1 \tag{19.57a}$$
$$H_1(x) = 2x \qquad \text{for} \qquad E_1 = 3 \tag{19.57b}$$
$$H_2(x) = -2(1-2x^2) \qquad \text{for} \qquad E_2 = 5 \tag{19.57c}$$
$$H_3(x) = -12(x - \tfrac{2}{3}x^3) \qquad \text{for} \qquad E_3 = 7 \tag{19.57d}$$

etc. See Fig. 19.3.

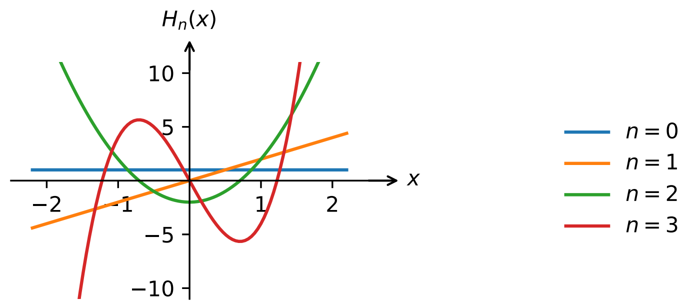


Figure 19.3: Hermite Polynomials

We say that ψ_n are the eigenfunctions of the differential operator $-d^2/dx^2 + x^2$ belonging to the eigenvalues E_n:

$$\left(-\frac{d^2}{dx^2} + x^2\right)\psi_n = E_n\psi_n\,. \tag{19.58}$$

Restoring physical units, the Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\psi_n = E_n\psi_n \tag{19.59}$$

and, we have the (suitably normalized) eigenstates

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/(2\hbar)} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right), \quad n = 0, 1, 2, \ldots \tag{19.60a}$$

belonging to the eigenenergies

$$E_n = \hbar\omega(n + \tfrac{1}{2}), \quad n = 0, 1, 2, \ldots\,. \tag{19.60b}$$

Consider a more generic quantum mechanics problem.

The time-independent Schrödinger equation is

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}[E - V(x)]\psi \tag{19.61}$$

where $V(x)$ is some arbitrary potential, e.g., like the potential shown in Fig. 19.4.

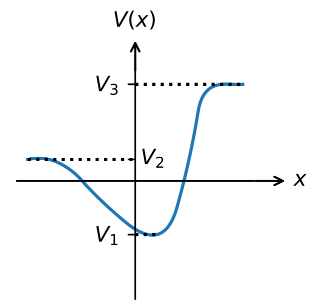


Figure 19.4: A Potential

- If $E > V(x)$, $\dfrac{\psi''}{\psi} < 0$
  $\implies$ ψ curves *toward* the x-axis
  $\implies$ sinusoidal character.
- If $E < V(x)$, $\dfrac{\psi''}{\psi} > 0$
  $\implies$ ψ curves *away from* the x-axis
  $\implies$ exponential character.

We require ψ to remain finite everywhere so unbounded exponential behavior is unacceptable. This boundary condition imposes restrictions on the solutions.

Consider these cases:

- $E > V_3$: Solutions are oscillatory everywhere
  $\implies$ always acceptable.
- $V_2 < E < V_3$: Most solutions blow up as $x \to \infty$, however we can find a unique solution (up to an overall factor) that falls off exponentially as $x \to +\infty$. This fixes the phase of the solution in the left-hand side.
- $V_1 < E < V_2$: Solutions behave exponentially at both ends $x \to \pm\infty$.
  Adjusting it so that it does not blow up on the left-hand side almost certainly means it blows up on the right-hand side and vice versa.
  Only for certain values of E can satisfactory solutions be found
  $\implies$ eigenvalues.
- $E < V_1$: No satisfactory solutions are possible.

20 The WKB Method

The **Wentzel-Kramers-Brillouin (WKB) method** obtains approximate solutions of differential equations of the form

$$-\frac{d^2y}{dx^2}+f(x)y=0 \tag{20.1}$$

where $f(x)$ is slowly-varying.

Note: for $f\approx$ const, the solution would be an exponential or a sinusoid depending on the sign of the constant. Therefore try

$$y=e^{S(x)}\,,\qquad y'=S'(x)e^{S(x)}\,,\qquad y''=S''(x)e^{S(x)}+[S'(x)]^2e^{S(x)} \tag{20.2}$$

which results in

$$-[S'(x)]^2-S''(x)+f(x)=0\,. \tag{20.3}$$

If $S''(x)$ is small then

$$S'(x)\approx\pm\sqrt{f(x)}\quad\Longrightarrow\quad S(x)\approx\pm\int\sqrt{f(x)}\,dx\,. \tag{20.4}$$

By "small" we mean (see below)

$$|S''(x)|\approx\frac{1}{2}\left|\frac{f'(x)}{\sqrt{f(x)}}\right|\ll|f(x)|\,. \tag{20.5}$$

The solution will be

$$y\approx\exp\left[\pm\int\sqrt{f(x)}\,dx\right] \tag{20.6}$$

so we can regard $1/\sqrt{f}\approx\lambdabar$ where $\lambdabar=\frac{1}{2\pi}$(wavelength) for $f<0$ or the exponential scale length for $f>0$.

The condition of validity of the approximation is

$$\begin{pmatrix}\text{fractional}\\ \text{change in } f \text{ over}\\ \text{one length scale}\end{pmatrix}=\left|\frac{\delta f}{f}\right|=\left|\frac{\lambdabar f'}{f}\right|\ll 1\quad\Longrightarrow\quad\left|\frac{f'(x)}{\sqrt{f(x)}}\right|\ll|f(x)|\,. \tag{20.7}$$

Improve the approximation by including the S'' term:

$$S'' \approx \pm \frac{1}{2} \frac{f'(x)}{\sqrt{f(x)}} \tag{20.8a}$$

$$\begin{aligned}
\Longrightarrow \quad [S'(x)]^2 &= f(x) - S''(x) \\
&\approx f(x) \mp \frac{1}{2} \frac{f'(x)}{\sqrt{f(x)}} \\
&= f(x)\left[1 \mp \frac{1}{2} \frac{f'(x)}{f^{3/2}(x)}\right] && (20.8b) \\
\Longrightarrow \quad S'(x) &\approx \pm\sqrt{f(x)}\left\{1 \mp \frac{1}{4} \frac{f'(x)}{f^{3/2}(x)} + \cdots\right\} \\
&\approx \pm\sqrt{f(x)} - \frac{1}{4} \frac{f'(x)}{f(x)} && (20.8c) \\
\Longrightarrow \quad S(x) &\approx \pm \int \sqrt{f(x)}\, dx - \frac{1}{4} \ln f(x)\,. && (20.8d)
\end{aligned}$$

Our solution is:

$$y(x) \approx \frac{1}{\sqrt[4]{f(x)}} \left\{ c_+ \exp\left[+\int \sqrt{f(x)}\, dx\right] + c_- \exp\left[-\int \sqrt{f(x)}\, dx\right]\right\}. \tag{20.9}$$

Note that there are two solutions corresponding either to exponentially growing or decaying solutions for $f > 0$ or to cosine or sine sinusoids for $f < 0$.

The method fails if $f(x)$ varies rapidly or if $f(x)$ goes through zero.

If $f(x)$ goes through zero, we need to join an oscillatory solution where $f(x) < 0$ to an exponential solution where $f(x) > 0$. In doing so, c_+ and c_- become related and the phase of oscillation is determined.

Ex. 20.1. Airy equation.

Here we take $f(x) = x$ so

$$\frac{d^2y}{dx^2} - xy = 0\,. \qquad (20.10)$$

Figure 20.1 shows two different solutions to Airy's equation, one that is exponentially decreasing in the right-hand side and one that is exponentially increasing.

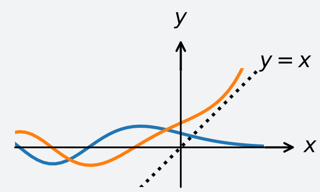


Figure 20.1: Solutions to Airy's Equation

- For $x \ll -1$:

$$\sqrt{f(x)} = \sqrt{x} = -i\sqrt{-x} \qquad \text{and} \qquad \sqrt[4]{f(x)} = \frac{\sqrt[4]{-x}}{\sqrt{i}} = \frac{(-x)^{1/4}}{e^{i\pi/4}}\,; \qquad (20.11a)$$

  also

$$\int_0^x \sqrt{f(x)}\,dx = -i\int_0^x \sqrt{-x}\,dx = i\int_0^{-x}\sqrt{x}\,dx = i\frac{2}{3}(-x)^{3/2} \qquad (20.11b)$$

  so the two solutions will have the form

$$(-x)^{-1/4}\exp\left(\pm i\frac{2}{3}(-x)^{3/2} + i\frac{\pi}{4}\right). \qquad (20.11c)$$

  Therefore,

$$y \approx A(-x)^{-1/4}\cos\left(\frac{2}{3}(-x)^{3/2} + \delta\right), \quad x \ll -1 \qquad (20.12)$$

  where A is a free amplitude constant and δ is an undetermined phase.

- For $x \gg 1$, the two solutions have the form

$$x^{-1/4}\exp\left(\pm\int\sqrt{x}\,dx\right) = x^{-1/4}\exp\left(\pm\frac{2}{3}x^{3/2}\right) \qquad (20.13)$$

  and we take the negative exponential solution which remains bounded as $x \to \infty$:

$$y \approx Bx^{-1/4}\exp\left(-\frac{2}{3}x^{3/2}\right), \quad x \gg 1 \qquad (20.14)$$

  where B is a free amplitude constant.

We now want to connect these forms at $x = 0$. This will allow us to determine the phase δ in the left-hand side that results in the exponential decay in the right-hand side.

Deduce the connection formula using Fourier transform methods: Let

$$g(k) = \int_{-\infty}^{\infty} y(x) e^{-ikx}\, dx\,. \tag{20.15}$$

Since

$$\frac{d^2y}{dx^2} - xy = 0 \tag{20.16}$$

we find

$$-k^2 g(k) - i\frac{d}{dk} g(k) = 0 \qquad \Longrightarrow \qquad g(k) = Ce^{ik^3/3} \tag{20.17}$$

where C is a constant of integration, so

$$y(x) = C\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik^3/3} e^{ikx}\, dk\,. \tag{20.18}$$

Convention: set $C = 1$; the result is the **Airy function of the first kind**, which can be written in these forms

$$\boxed{\mathrm{Ai}\, x = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\left[i\left(\frac{k^3}{3} + kx\right)\right] dk} \tag{20.19}$$

$$\boxed{\mathrm{Ai}\, x = \frac{1}{\pi}\int_{0}^{\infty} \cos\left(\frac{k^3}{3} + kx\right) dk\,.} \tag{20.20}$$

We will use the first form.

Note: the second independent solution to the Airy equation is the **Airy function of the second kind**,

$$\boxed{\mathrm{Bi}\, x = \frac{1}{\pi}\int_{0}^{\infty} \left[\exp\left(-\frac{k^3}{3} + kx\right) + \sin\left(\frac{k^3}{3} + kx\right)\right] dk\,.} \tag{20.21}$$

The functions Ai x and Bi x are shown in Fig. 20.2. We see that the function Bi x has the unwanted exponentially increasing behavior.

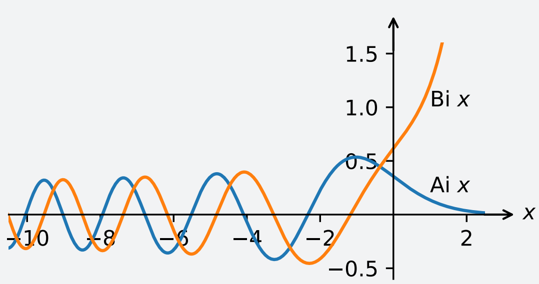


Figure 20.2: Airy Functions of the First and Second Kind

We now want to compute the asymptotic forms of the Airy integral for $x \to -\infty$ and $x \to \infty$ and compare to our WKB results in order to identify the phase δ. We will use the saddle-point method.

- For $x \to -\infty$, write the integrand of Ai x as

$$e^{(-x)f(k)} \qquad \text{with} \qquad f(k) = i\left(k + \frac{k^3}{3x}\right) \tag{20.22}$$

since $(-x)$ is large and positive. We have:

$$f'(k) = i\left(1 + \frac{k^2}{x}\right) \qquad \Longrightarrow \qquad f'(k_0) = 0 \quad \text{for} \quad k_0 = \pm\sqrt{-x} \tag{20.23a}$$

$$f''(k) = 2i\frac{k}{x} \qquad \Longrightarrow \qquad f''(k_0) = \mp 2i\frac{1}{\sqrt{-x}}\,. \tag{20.23b}$$

Note: there are two saddle points, $k_0 = \pm\sqrt{-x}$. Also

$$f(k_0) = \pm i\left(\sqrt{-x} - \frac{1}{3}\sqrt{-x}\right) = \pm\frac{2}{3}i\sqrt{-x}\,. \tag{20.23c}$$

Therefore,

$$f(k) \approx f(k_0) + \frac{1}{2}f''(k_0)(k-k_0)^2\,. \tag{20.24}$$

Write $f''(k_0) = \rho e^{i\phi}$ with $\rho = 2/\sqrt{-x}$ and $\phi = \mp\pi/2$, and $k - k_0 = se^{i\psi}$ with $\psi = -\phi/2 \pm \pi/2$. Then

$$y = \frac{1}{2\pi}\int_C e^{(-x)f(k)}\,dk \underset{x\to-\infty}{\sim} \frac{1}{2\pi}\sqrt{\frac{2\pi}{(-x)\rho}}\,e^{(-x)f(k_0)}e^{i\psi} \tag{20.25}$$

where C is a contour deformed to go over the saddle points.

To figure out how to deform the contour C to go over the saddle points appropriately we need to look at the topography of Re $f(k)$. The top panel of Fig. 20.3 shows that $\psi = +\pi/4$ for $k_0 = -\sqrt{-x}$ and $\psi = -\pi/4$ for $k_0 = +\sqrt{-x}$. We need to go over both saddle points so we need to add the two contributions

$$y \sim \frac{1}{2\pi}\sqrt{\frac{2\pi}{(-x)}\frac{\sqrt{-x}}{2}}\exp\left(\pm\frac{2}{3}i(-x)^{3/2}\right)e^{\mp i\pi/4}\,, \quad x \to -\infty \tag{20.26}$$

together to get the asymptotic form of the Airy function for $x \to -\infty$:

$$\text{Ai}\,x \sim \frac{1}{\sqrt{\pi}(-x)^{1/4}}\cos\left(\frac{2}{3}(-x)^{3/2} - \frac{\pi}{4}\right), \quad x \to -\infty\,. \tag{20.27}$$

- For $x \to +\infty$, write the integrand of $\operatorname{Ai} x$ as

$$e^{xf(k)} \qquad \text{with} \qquad f(k) = i\left(k + \frac{k^3}{3x}\right) \tag{20.28}$$

since x is large and positive. We have:

$$f'(k) = i\left(1 + \frac{k^2}{x}\right) \qquad \Longrightarrow \qquad f'(k_0) = 0 \quad \text{for} \quad k_0 = \pm i\sqrt{x} \tag{20.29a}$$

$$f''(k) = 2i\frac{k}{x} \qquad \Longrightarrow \qquad f''(k_0) = \mp 2\frac{1}{\sqrt{x}}\,. \tag{20.29b}$$

Note: there are two saddle points, $k_0 = \pm i\sqrt{x}$, but now we will only go over one. Also

$$f(k_0) = \pm i\left(\sqrt{-x} - \frac{1}{3}\sqrt{-x}\right) = \mp\frac{2}{3}\sqrt{x}\,. \tag{20.29c}$$

Write $f''(k_0) = \rho e^{i\phi}$ with $\rho = 2/\sqrt{x}$ and $\phi = 0$ or π. From the topography of $\operatorname{Re} f(x)$ shown in the bottom panel of Fig. 20.3, we see we should go over one saddle point $k_0 = +i\sqrt{x}$ with $k - k_0 = se^{i\psi}$ where $\psi = 0$. Then

$$\operatorname{Ai} x = \frac{1}{2\pi}\int_C e^{xf(k)}\,dk \underset{x\to+\infty}{\sim} \frac{1}{2\pi}\sqrt{\frac{2\pi}{x\rho}}\,e^{xf(k_0)}e^{i\psi} \tag{20.30a}$$

$$= \frac{1}{2\pi}\sqrt{\frac{2\pi}{x}\frac{\sqrt{x}}{2}}\exp\left(-\frac{2}{3}x^{3/2}\right) \tag{20.30b}$$

where C is a contour deformed to go over the desired saddle point. Thus

$$\operatorname{Ai} x \sim \frac{1}{2\sqrt{\pi}x^{1/4}}\exp\left(-\frac{2}{3}x^{3/2}\right), \quad x \to +\infty\,. \tag{20.31}$$

We therefore have:

$$\operatorname{Ai} x \sim \frac{1}{\sqrt{\pi}(-x)^{1/4}}\cos\left(\frac{2}{3}(-x)^{3/2} - \frac{\pi}{4}\right), \quad x \to -\infty \tag{20.32a}$$

$$\operatorname{Ai} x \sim \frac{1}{2\sqrt{\pi}x^{1/4}}\exp\left(-\frac{2}{3}x^{3/2}\right), \quad x \to +\infty \tag{20.32b}$$

while our WKB solution was

$$y \approx A(-x)^{-1/4}\cos\left(\frac{2}{3}(-x)^{3/2} + \delta\right), \quad x \ll -1 \tag{20.33a}$$

$$y \approx Bx^{-1/4}\exp\left(-\frac{2}{3}x^{3/2}\right), \quad x \gg 1\,. \tag{20.33b}$$

Comparison tells us $A = 2B$ and $\delta = -\pi/4$. The phase is now determined! Any other phase would have introduced an exponentially-growing term as $x \to +\infty$.

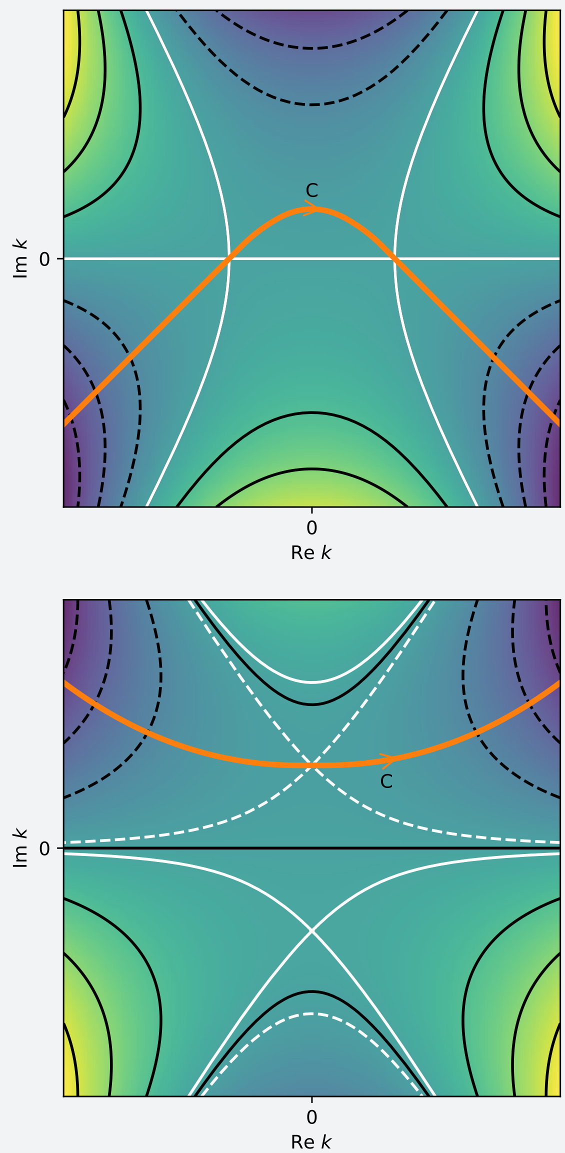


Figure 20.3: Topography of the surface $\mathrm{Re}[i(k + k^3/(3x))]$ for $x < 0$ (top) and $x > 0$ (bottom). The saddle points are at the intersection of the white contour lines. Top: the contour is deformed so that it goes over both saddle point $k_0 = \pm\sqrt{-x}$. Bottom: the contour is deformed to go over the saddle point $k_0 = i\sqrt{x}$ but not $k_0 = -i\sqrt{x}$.

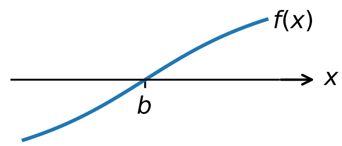
The WKB method can be used for more general $f(x)$ but we will still need to connect an osciliatory solution for the $f(x) < 0$ region to an exponential solution for the $f(x) > 0$ region.

Note that $f(x)$ is approximately linear as it passes through zero, so the undetermined phase is just that of the Airy function.

Therefore the rule is, when $f(b) = 0$, $f(x) > 0$ for $x > b$,

$$\underbrace{\frac{2}{\sqrt[4]{-f(x)}}\cos\left(\int_x^b \sqrt{-f(x)}\,dx - \frac{\pi}{4}\right)}_{f(x)<0 \text{ for } x<b} \rightleftharpoons \underbrace{\frac{1}{\sqrt[4]{f(x)}}\exp\left(-\int_b^x \sqrt{f(x)}\,dx\right)}_{f(x)>0 \text{ for } x>b}. \quad (20.34)$$

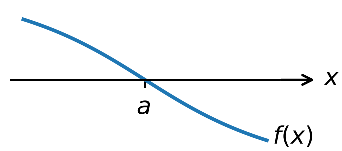
This is a **connection formula.**



solutions for $x < b$ solutions for $x > b$

$$2(-f)^{-1/4}\cos\left(\int_x^b \sqrt{-f}\,dx - \frac{\pi}{4}\right) \rightleftharpoons f^{-1/4}\exp\left(-\int_b^x \sqrt{f}\,dx\right)$$

$$(-f)^{-1/4}\sin\left(\int_x^b \sqrt{-f}\,dx - \frac{\pi}{4}\right) \rightleftharpoons -f^{-1/4}\exp\left(\int_b^x \sqrt{f}\,dx\right)$$



solutions for $x < a$ solutions for $x > a$

$$f^{-1/4}\exp\left(\int_a^x \sqrt{f}\,dx\right) \rightleftharpoons 2(-f)^{-1/4}\cos\left(\int_a^x \sqrt{-f}\,dx - \frac{\pi}{4}\right)$$

$$-f^{-1/4}\exp\left(-\int_a^x \sqrt{f}\,dx\right) \rightleftharpoons (-f)^{-1/4}\sin\left(\int_a^x \sqrt{-f}\,dx - \frac{\pi}{4}\right)$$

Figure 20.4: Connection Formulas for $-\frac{d^2y}{dx^2} + f(x)y = 0$

Ex. 20.2. Bohr-Sommerfeld quantization rule.

Time-independent Schrödinger equation:

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}[V(x) - E]\psi = 0 \qquad (20.35)$$

The potential $V(x)$ shown in Fig. 20.5 has two turning points at $x = a$ and $x = b$.
Use the WKB method with

$$f(x) = \frac{2m}{\hbar^2}[V(x) - E]. \qquad (20.36)$$

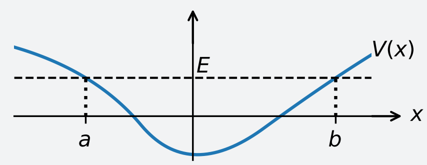


Figure 20.5: Potential for Bohr-Sommerfeld Quantization Rule

- For $x < a$, the solution is exponential. Boundedness as $x \to -\infty$ means that in $a < x < b$ we have

$$\psi(x) \approx \frac{A}{[E - V(x)]^{1/4}} \cos\left(\int_a^x \frac{\sqrt{2m[E - V(x)]}}{\hbar}\, dx - \frac{\pi}{4} \right) \qquad (20.37)$$

  (from the connection formula).
- For $x > b$, the solution is again exponential. Boundedness as $x \to +\infty$ means that in $a < x < b$ we have

$$\psi(x) \approx \frac{B}{[E - V(x)]^{1/4}} \cos\left(\int_x^b \frac{\sqrt{2m[E - V(x)]}}{\hbar}\, dx - \frac{\pi}{4} \right). \qquad (20.38)$$

These must be the same! Let

$$\eta = \int_a^b \frac{\sqrt{2m[E - V(x)]}}{\hbar}\, dx \quad \text{and} \quad \alpha = \int_x^b \frac{\sqrt{2m[E - V(x)]}}{\hbar}\, dx - \frac{\pi}{4} \qquad (20.39)$$

then we see we must have $|A| = |B|$ and

$$\begin{aligned} \cos(\eta - \alpha - \pi/2) &= \pm\cos(\alpha) \\ &= \pm\cos(-\alpha) \end{aligned} \qquad (20.40)$$

$$\Longrightarrow \qquad \eta = \frac{\pi}{2} + n\pi\,, \qquad n = 0, 1, 2, \ldots. \qquad (20.41)$$

Therefore

$$\int_a^b \sqrt{2m[E - V(x)]}\, dx = (n + \tfrac{1}{2})\pi\hbar\,, \qquad n = 0, 1, 2, \ldots. \qquad (20.42)$$

This is the **Bohr-Sommerfeld quantization rule** and the integral on the left hand side is one half of the classical action.

Problems

Problem 19.

An ideal gas in a box has internal energy $U(V, P) = \frac{3}{2}PV$ where P is the pressure of the gas and V is the volume of the box. The first law of thermodynamics for a quasistatic process is

$$\text{đ}Q = dU + P\,dV$$

where đQ is the heat flow to the system. Although the right-hand-side is not an exact integral, so there is no function $Q(V, P)$ for the "heat of the system" (hence we write đQ rather than dQ), the right-hand-side can be integrated by means of an integrating factor λ. That is, $d\sigma = \lambda \cdot (dU + P\,dV)$ *is* exact and can be integrated. Determine $\lambda(V, P)$ and the integral $\sigma(V, P)$ in terms of the state variables V and P. What are the physical significance of these quantities?

Problem 20.

Find the general solution of

a) $y' + y\cos x = \frac{1}{2}\sin 2x$;

b) $2x^3 y' = 1 + \sqrt{1 + 4x^2 y}$.

Problem 21.

Find the general solution of

a) $y''' - 2y'' - y' + 2y = \sin x$;

b) $a^2 y''^2 = (1 + y'^2)^3$.

Problem 22.

An object is dropped (from rest) from some distance r_0 from the center of the Earth and it accelerates according to Newton's law of gravity,

$$\ddot{r} = -\frac{GM_\oplus}{r^2}.$$

Determine $t(r)$ for the fall, where $t = 0$ when $r = r_0$. Find the number of days it would take an object to fall to the surface of the Earth, $r = R_\oplus$, if it were dropped from the distance of the Moon, $r_0 = 60R_\oplus$.

Use: $GM_\oplus = 398\,600\,\mathrm{km^3\,s^{-2}}$ and $R_\oplus = 6371\,\mathrm{km}$.

Problem 23.

Bessel's equation for $\nu = 0$ is

$$x^2 y'' + xy' + x^2 y = 0.$$

We have found one solution

$$J_0(x) = 1 - \frac{x^2}{4} + \frac{x^4}{64} - \cdots.$$

Show that a second solution exists of the form

$$J_0(x)\ln x + Ax^2 + Bx^4 + Cx^6 + \cdots$$

and find the first three coefficients A, B, and C.

Problem 24.

Consider the equation

$$\frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} + \left[-k^2 + \frac{2}{x} - \frac{\ell(\ell+1)}{x^2}\right]y = 0, \qquad 0 \le x \le \infty$$

where $\ell = 0, 1, 2, \ldots$. Find all values of the constant k that can give a solution that is finite on the entire range of x (including $x = \infty$). An equation like this arises in solving the Schrödinger equation for the hydrogen atom [here $r = a_0 x$, $R(r) = a_0^2 y(x)$, and $E = -k^2(e^2/2a_0)$ with $a_0 = \hbar^2/(m_e e^2)$].

(Hint: Let $y = v/x$, then "factor out" the behavior at infinity.)

Problem 25.

For what values of the constant K does the differential equation

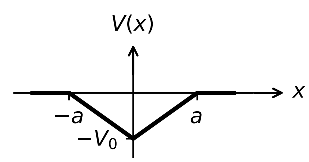
$$y'' - \left(\frac{1}{4} + \frac{K}{x}\right)y = 0 \qquad (0 < x < \infty)$$

have a nontrivial solution vanishing at $x = 0$ and $x = \infty$?

Problem 26.

Use the WKB method to find approximate negative values of the constant E for which the equation

$$\frac{d^2y}{dx^2} + [E - V(x)]y = 0$$



has a solution that is finite for all x between $x = -\infty$ and $x = +\infty$ *inclusive*.

Problem 27.

Recall Bessel's equation is:

$$x^2y'' + xy' + (x^2 - \nu^2)y = 0.$$

The first derivative term can be eliminated by making the substitution $y(x) = u(x)x^{-1/2}$. Use the WKB method to get an approximate solution for $u(x)$ for large x and thus obtain an approximate solution for $y(x)$ for $x \gg \nu$. You may assume that $\nu \gg 1/2$ and don't worry about the overall constant. Your solution should be the one that is finite at the origin.

Module VI

Eigenvalue Problems

Motivation

We've seen that when solutions to differential equations are required to satisfy specific boundary conditions then there can be restrictions on the form of the differential equation in order for it to admit such solutions. Here we will explore such **eigenvalue problems** in more detail as they commonly arise in physics problems.

We will start with some general properties of linear differential operators, eigenvalues, and eigenfunctions. We then turn to a rather general class of eigenvalue problems called Sturm-Liouville problems. Such equations occur frequently in physics applications, and we will encounter several important special functions such as Bessel functions, Legendre polynomials, and spherical harmonics. We will examine the case of degenerate eigenvalues and show how complete bases of eigenfunctions can be used to form eigenfunction expansions of other functions. Finally we'll look at inhomogeneous equations and introduce the concept of a Green function.

21 General Discussion of Eigenvalue Problems

The eigenvalue problem is

$$\mathcal{L}\, u(x) = \lambda u(x) \tag{21.1}$$

where $\mathcal{L}$ is a linear differential operator and λ is an **eigenvalue**. The solution $u(x)$ is called an **eigenfunction** of $\mathcal{L}$ belonging to λ.

In addition to the equation we also need to specify a domain Ω and boundary conditions.

$\mathcal{L}$ is a **Hermitian** differential operator if

$$\int_\Omega u^*(x)\mathcal{L}\, v(x)\, dx = \left[\int_\Omega v^*(x)\mathcal{L}\, u(x)\, dx\right]^* \tag{21.2}$$

where $u(x)$ and $v(x)$ are functions that obey the boundary conditions.

Suppose $\mathcal{L}$ is Hermitian. Then, if $u_i(x)$ and $u_j(x)$ are eigenfunctions belonging to eigenvalues λ_i and λ_j,

$$\mathcal{L}\, u_i(x) = \lambda_i u_i(x) \qquad \text{and} \qquad \mathcal{L}\, u_j(x) = \lambda_j u_j(x)\,. \tag{21.3}$$

Because $\mathcal{L}$ is Hermitian,

$$\int_\Omega u_j^*(x)\mathcal{L}\, u_i(x)\, dx = \left[\int_\Omega u_i^*(x)\mathcal{L}\, u_j(x)\, dx\right]^* \tag{21.4a}$$

$$= \left[\lambda_j \int_\Omega u_i^*(x) u_j(x)\, dx\right]^* \tag{21.4b}$$

$$= \lambda_j^* \int_\Omega u_i(x) u_j^*(x)\, dx \tag{21.4c}$$

but we also have

$$\int_\Omega u_j^*(x)\mathcal{L}\, u_i(x)\, dx = \lambda_i \int_\Omega u_j^*(x) u_i(x)\, dx \tag{21.4d}$$

so therefore

$$(\lambda_i - \lambda_j^*) \int_\Omega u_j^*(x) u_i(x)\, dx = 0\,. \tag{21.5}$$

- Case $i = j$: the eigenvalues of Hermitian operators are *real* since $\lambda_i = \lambda_i^*$.
- Case $i \neq j$: the eigenfunctions of Hermitian operators are **orthogonal** if the eigenvalues are different, where

$$(u, v) = \int_\Omega u^*(x) v(x)\, dx = 0 \tag{21.6}$$

for functions $u(x)$ and $v(x)$ that are orthogonal.

Ex. 21.1. A familiar set of orthogonal functions are the trigonometric functions associated with $\mathcal{L} = -\dfrac{d^2}{dx^2}$:

$$\frac{d^2}{dx^2} u(x) + \lambda u(x) = 0\,, \quad 0 \leq x \leq 2\pi \tag{21.7}$$

along with the periodic boundary conditions

$$u(0) = u(2\pi) \qquad \text{and} \qquad u'(0) = u'(2\pi)\,. \tag{21.8}$$

The eigenvalues are $\lambda_n = (n\pi)^2$ for integer n and the eigenfunctions are $u_n(x) \propto e^{in\pi x}$.

$\mathcal{L}$ is Hermitian with the periodic boundary conditions: if $u(x)$ and $v(x)$ are two functions that satisfy the boundary conditions then

$$-\int_0^{2\pi} u^*(x) \frac{d^2}{dx^2} v(x)\, dx = -\cancelto{0}{\left[u^* \frac{dv}{dx} \right]_0^{2\pi}} + \int_0^{2\pi} \frac{du^*}{dx} \frac{dv}{dx}\, dx \tag{21.9a}$$

$$= \cancelto{0}{\left[\frac{du^*}{dx} v \right]_0^{2\pi}} - \int_0^{2\pi} v(x) \frac{d^2}{dx^2} u^*(x)\, dx \tag{21.9b}$$

$$= \left[-\int_0^{2\pi} v^*(x) \frac{d^2}{dx^2} u(x)\, dx \right]^*. \tag{21.9c}$$

More generally, eigenvalue problems can include a weight function $\rho(x)$ with $\rho(x) \geq 0$ in the domain so that

$$\mathcal{L}\, u(x) = \lambda \rho(x) u(x) \tag{21.10}$$

in which case the orthogonality condition will be

$$(u, v) = \int_\Omega u^*(x) v(x) \rho(x)\, dx = 0\,. \tag{21.11}$$

22 Sturm-Liouville Problems

The **Sturm-Liouville differential equation** is

$$\boxed{\frac{d}{dx}\left[p(x)\frac{d}{dx}u(x)\right] - q(x)u(x) + \lambda\rho(x)u(x) = 0} \tag{22.1}$$

for $a \le x \le b$ with $u(a) = u(b) = 0$ (other boundary conditions are possible). Here, $p(x)$, $q(x)$, and $\rho(x)$ are all real-valued and $\rho(x) \ge 0$ on the domain.

We can verify that

$$\mathcal{L} = -p(x)\frac{d^2}{dx^2} - p'(x)\frac{d}{dx} + q(x) \tag{22.2}$$

is Hermitian and that the orthogonality of eigenfunctions u_i and u_j, $\lambda_i \ne \lambda_j$, is

$$(u_i, u_j) = \int_\Omega u_i^*(x)u_j(x)\rho(x)\,dx = 0\,. \tag{22.3}$$

The eigenvalues of a Sturm-Liouville problem can be arranged in order $\lambda_0 \le \lambda_1 \le \lambda_2 \le \cdots$, where λ_0 is the smallest eigenvalue and $\lambda_n \to \infty$ as $n \to \infty$ for finite domain Ω.

The eigenfunctions of a Sturm-Liouville problem form a complete set of functions in the domain with the boundary conditions.

Some examples of Sturm-Liouville problems are:

- **Legendre's equation**

$$\boxed{(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + n(n+1)y = 0\,.} \tag{22.4}$$

Here $p(x) = 1-x^2$, $q(x) = 0$, $\rho(x) = 1$, where $-1 \le x \le 1$, and $\lambda_n = n(n+1)$.

- **Hermite's equation**

$$\boxed{\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + 2ny = 0\,.} \tag{22.5}$$

Here $p(x) = e^{-x^2}$, $q(x) = 0$, $\rho(x) = e^{-x^2}$, where $-\infty \le x \le \infty$, and $\lambda_n = 2n$.

- **Bessel's equation**

$$\boxed{x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + (k^2x^2 - \nu^2)y = 0} \tag{22.6}$$

(note: we have introduced the factor k^2 now). Here $p(x) = x$, $q(x) = \nu^2/x$, $\rho(x) = x$, the domain is $0 \le x \le \infty$, and $\lambda = k^2$.

The eigenfunctions and orthogonality relations for these equations are:

- **Legendre polynomials**, $P_n(x)$:

$$\int_{-1}^{1} P_n(x)P_m(x)\,dx = 0 \quad \text{for } n \ne m. \tag{22.7}$$

- **Hermite polynomials**, $H_n(x)$:

$$\int_{-\infty}^{\infty} H_n(x)H_m(x)\,e^{-x^2}\,dx = 0 \quad \text{for } n \ne m. \tag{22.8}$$

- **Bessel function**, $J_\nu(kx)$:

$$\int_{a}^{b} J_\nu(Ax)J_\nu(Bx)\,x\,dx = 0 \tag{22.9}$$

provided $J_\nu(Ax)$ and $J_\nu(Bx)$ vanish at $x = a$ and $x = b$ respectively,
or if $J'_\nu(Ax)$ and $J'_\nu(Bx)$ vanish at $x = a$ and $x = b$ respectively,
(or various other similar conditions).

Independence of Solutions

Recall Bessel's equation with $k = 1$ has solutions $J_\nu(x)$ and $J_{-\nu}(x)$ and these are independent unless ν is an integer.

In general, two solutions, u and v, are said to be **linearly dependent** if there are values α and β ($\alpha \neq 0$, $\beta \neq 0$) such that

$$\alpha u + \beta v = 0\,. \tag{22.10a}$$

Take a derivative:

$$\alpha u' + \beta v' = 0 \tag{22.10b}$$

and multiply Eq. (22.10a) by v' and subtract Eq. (22.10b) times v:

$$\alpha \underbrace{(uv' - u'v)}_{\text{must vanish}} = 0\,. \tag{22.10c}$$

Define the **Wronskian** as

$$\boxed{W[u(x), v(x)] = u(x)v'(x) - u'(x)v(x)} \tag{22.11}$$

or sometimes just write W. Thus, linear dependence requires $W = 0$.

Furthermore, if $W \neq 0$, the solutions are **linearly independent**.

Suppose that u and v are solutions to the Sturm-Liouville equation:

$$pu'' + p'u' - qu + \lambda\rho u = 0 \tag{22.12a}$$

$$pv'' + p'v' - qv + \lambda\rho v = 0 \tag{22.12b}$$

The Wronskian is:

$$W = uv' - vu' \tag{22.13a}$$

$$\implies \quad pW = puv' - pvu' \tag{22.13b}$$

$$\implies \quad (pW)' = u\cdot[pv'' + p'v'] + \cancel{pu'v'} - v\cdot[pu'' + p'u'] - \cancel{pu'v'} \tag{22.13c}$$

$$= u\cdot[(q - \lambda\rho)v] - v\cdot[(q - \lambda\rho)u] \tag{22.13d}$$

$$= 0 \tag{22.13e}$$

and therefore

$$W[u(x), v(x)] = \frac{C}{p(x)} \tag{22.14}$$

for solutions to a Sturm-Liouville equation where C is some constant (which can be zero). Note: C depends on u and v, i.e., on the pair of solutions chosen.

Ex. 22.1. Bessel functions.

Solutions to Bessel's equation with conventional normalization are

$$\begin{aligned} J_\nu(x) &= \frac{1}{\Gamma(\nu+1)}\left(\frac{x}{2}\right)^\nu\left[1-\frac{1}{\nu+1}\left(\frac{x}{2}\right)^2+\frac{1}{(\nu+1)(\nu+2)}\frac{1}{2!}\left(\frac{x}{2}\right)^4-\cdots\right] \\ &= \sum_{k=0}^{\infty}\frac{(-1)^k}{k!\Gamma(\nu+k+1)}\left(\frac{x}{2}\right)^{\nu+2k}. \end{aligned} \tag{22.15}$$

Consider $W[J_\nu, J_{-\nu}]$. We know it must have the form

$$W = \frac{C}{p(x)} = \frac{C}{x} \tag{22.16}$$

and we want to determine C. Note that as $x \to 0$,

$$J_\nu(x) \underset{x\to 0}{\sim} \frac{1}{\Gamma(\nu+1)}\left(\frac{x}{2}\right)^\nu \qquad \text{and} \qquad J_{-\nu}(x) \underset{x\to 0}{\sim} \frac{1}{\Gamma(-\nu+1)}\left(\frac{x}{2}\right)^{-\nu} \tag{22.17}$$

so, for $x \to 0$, we have

$$W = J_\nu(x)J'_{-\nu}(x) - J'_\nu(x)J_{-\nu}(x) \tag{22.18a}$$

$$\underset{x\to 0}{\sim} \frac{1}{\Gamma(\nu+1)}\frac{1}{\Gamma(1-\nu)}\left[\left(\frac{x}{2}\right)^\nu\left(-\frac{\nu}{2}\right)\left(\frac{x}{2}\right)^{-\nu-1} - \left(\frac{\nu}{2}\right)\left(\frac{x}{2}\right)^{\nu-1}\left(\frac{x}{2}\right)^{-\nu}\right] \tag{22.18b}$$

$$= \frac{1}{\nu\Gamma(\nu)\Gamma(1-\nu)}\left[-\frac{\nu}{x}-\frac{\nu}{x}\right] \tag{22.18c}$$

recall Euler's reflection formula $\Gamma(\nu)\Gamma(1-\nu) = \dfrac{\pi}{\sin\pi\nu}$

$$= -\frac{2\sin\pi\nu}{\pi x}. \tag{22.18d}$$

Thus the constant is determined.

Therefore

$$W[J_\nu(x), J_{-\nu}(x)] = -\frac{2\sin\pi\nu}{\pi x}. \tag{22.19}$$

Note: when $\nu = n$ is an integer, $W = 0$, so $J_n(x)$ and $J_{-n}(x)$ are linearly dependent.
In fact, the normalization has been chosen so that $J_{-n}(x) = (-1)^n J_n(x)$.
Conversely, when ν is not an integer, $W \neq 0$ so $J_\nu(x)$ and $J_{-\nu}(x)$ are linearly independent.

We seek a second, linearly independent solution when $\nu = n$ is an integer.
One method to get a second solution is to use the Wronskian. Let

$$W = W[J_n, y_n] = J_n y'_n - J'_n y_n = J_n^2 \cdot \left(\frac{y_n}{J_n}\right)' \tag{22.20}$$

where $W = C/x$ and y_n is the second solution we seek. Therefore,

$$y_n(x) = CJ_n(x) \int^x \frac{dx'}{x' J_n^2(x')} . \tag{22.21}$$

For example, for $\nu = 0$,

$$J_0(x) = 1 - \frac{x^2}{4} + \frac{x^4}{64} - \cdots \qquad \text{and} \qquad J_0^{-2}(x) = 1 + \frac{x^2}{2} + \frac{5}{32}x^4 + \cdots \tag{22.22}$$

so

$$y_0(x) = CJ_0(x) \int \frac{1}{x} \left\{ 1 + \frac{x^2}{2} + \frac{5}{32}x^4 + \cdots \right\} dx . \tag{22.23}$$

For $C = 1$ we have

$$y_0(x) = J_0(x) \left\{ \ln x + \frac{x^2}{4} + \frac{5}{128}x^4 + \cdots \right\} \tag{22.24a}$$

$$= J_0(x) \ln x + \frac{1}{4}x^2 - \frac{3}{128}x^4 + \cdots . \tag{22.24b}$$

More conventionally, define the second solution to be

$$\boxed{Y_n(x) = \lim_{\nu \to n} \frac{J_\nu(x) \cos \nu\pi x - J_{-\nu}(x)}{\sin \nu\pi} .} \tag{22.25}$$

This is the **Bessel function of the second kind**.

It is straightforward to show that $W[J_\nu, Y_\nu] \neq 0$ even for integer ν.

For integer $\nu = n$, both the numerator and denominator vanish as $\nu \to n$ so Y_n must be evaluated by l'Hospital's rule... but this requires derivatives of J_ν with respect to ν, which is a nuisance since ν appears in the Γ functions in the series....

It is easiest just to look up $Y_n(x)$. The Bessel functions of the first and second kind are shown in Fig. 22.1.

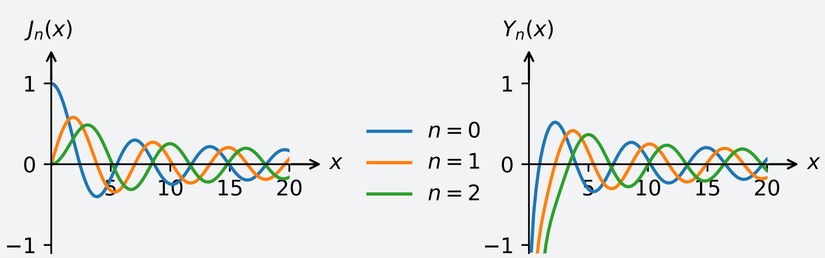


Figure 22.1: Bessel Functions of the First and Second Kind

Generating Functions

Consider a function of two variables, $g(x,t)$. We can use it to generate a set of functions $A_n(x)$ by expanding it in powers of t:

$$g(x,t) = \sum_n A_n(x) t^n \,. \tag{22.26}$$

This is a Laurent series in t. We call $g(x,t)$ a **generating function**.

The following example illustrates the use of generating functions.

Ex. 22.2. Consider

$$\boxed{g(x,t) = \exp\left[\left(\frac{x}{2}\right)\left(t - \frac{1}{t}\right)\right] .} \tag{22.27}$$

We can obtain $A_n(x)$ from the Laurent series via the contour integral

$$A_n(x) = \frac{1}{2\pi i} \oint_C \frac{g(x,t)}{t^{n+1}}\, dt \tag{22.28}$$

where C is a positively-oriented simple closed contour about the origin.

Let $t = e^{i\theta}$, $-\pi \le \theta \le \pi$:

$$A_n(x) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} \frac{g(x, e^{i\theta})}{e^{i(n+1)\theta}}\, i e^{i\theta}\, d\theta \tag{22.29a}$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{ix\sin\theta}}{e^{in\theta}}\, d\theta \tag{22.29b}$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} [\cos(x\sin\theta - n\theta) + \underbrace{i\sin(x\sin\theta - n\theta)}_{0 \text{ (odd)}}]\, d\theta \tag{22.29c}$$

so

$$\boxed{A_n(x) = \frac{1}{\pi} \int_0^{\pi} \cos(x\sin\theta - n\theta)\, d\theta \,.} \tag{22.30}$$

Recurrence relations can be obtained by taking derivatives with respect to x or t:

$$\frac{\partial g}{\partial t} = \left(\frac{x}{2}\right)\left(1+\frac{1}{t^2}\right)\exp\left[\left(\frac{x}{2}\right)\left(t-\frac{1}{t}\right)\right] \tag{22.31a}$$

$$= \left(\frac{x}{2}\right)\left(1+\frac{1}{t^2}\right)g(x,t) \tag{22.31b}$$

$$= \left(\frac{x}{2}\right)\left(1+\frac{1}{t^2}\right)\sum_{n=-\infty}^{\infty} A_n(x)t^n \tag{22.31c}$$

$$= \left(\frac{x}{2}\right)\sum_{n=-\infty}^{\infty}[A_n(x)t^n + A_n(x)t^{n-2}] \tag{22.31d}$$

$$= \left(\frac{x}{2}\right)\sum_{n=-\infty}^{\infty}[A_{n-1}(x) + A_{n+1}(x)]t^{n-1} \tag{22.31e}$$

but

$$\frac{\partial g}{\partial t} = \frac{\partial}{\partial t}\sum_{n=-\infty}^{\infty} A_n(x)t^n = \sum_{n=-\infty}^{\infty} nA_n(x)t^{n-1} \tag{22.31f}$$

so we find

$$\boxed{A_{n-1}(x) + A_{n+1}(x) = \frac{2n}{x}A_n(x).} \tag{22.32}$$

Now take a derivative with respect to x:

$$\frac{\partial g}{\partial x} = \frac{1}{2}\left(t-\frac{1}{t}\right)\exp\left[\left(\frac{x}{2}\right)\left(t-\frac{1}{t}\right)\right] \tag{22.33a}$$

$$= \frac{1}{2}\left(t-\frac{1}{t}\right)g(x,t) \tag{22.33b}$$

$$= \frac{1}{2}\left(t-\frac{1}{t}\right)\sum_{n=-\infty}^{\infty} A_n(x)t^n \tag{22.33c}$$

$$= \frac{1}{2}\sum_{n=-\infty}^{\infty}[A_n(x)t^{n+1} - A_n(x)t^{n-1}] \tag{22.33d}$$

$$= \frac{1}{2}\sum_{n=-\infty}^{\infty}[A_{n-1}(x) - A_{n+1}(x)]t^{n} \tag{22.33e}$$

but

$$\frac{\partial g}{\partial x} = \frac{\partial}{\partial x}\sum_{n=-\infty}^{\infty} A_n(x)t^n = \sum_{n=-\infty}^{\infty} A_n'(x)t^{n} \tag{22.33f}$$

so we find

$$\boxed{A_{n-1}(x) - A_{n+1}(x) = 2A_n'(x).} \tag{22.34}$$

Adding and subtracting this recurrence relation to the previous yields

$$\boxed{A_n'(x) = A_{n-1}(x) - \frac{n}{x}A_n(x)} \quad \text{and} \quad \boxed{A_n'(x) = \frac{n}{x}A_n(x) - A_{n+1}(x)} \tag{22.35}$$

Manipulate these:

$$xA_n'(x) = xA_{n-1}(x) - nA_n(x) \tag{22.36a}$$

$$[xA_n'(x)]' = A_{n-1}(x) + xA_{n-1}'(x) - nA_n'(x) \tag{22.36b}$$

$$= A_{n-1}(x) + x\left[\frac{n-1}{x}A_{n-1}(x) - A_n(x)\right] - n\left[A_{n-1}(x) - \frac{n}{x}A_n(x)\right] \tag{22.36c}$$

$$= \cancel{A_{n-1}(x)} + \cancel{(n-1)A_{n-1}(x)} - xA_n(x) - \cancel{nA_{n-1}(x)} + \frac{n^2}{x}A_n(x) \tag{22.36d}$$

$$= -xA_n(x) + \frac{n^2}{x}A_n(x) \tag{22.36e}$$

so we have

$$xA_n''(x) + A_n'(x) = -xA_n(x) + \frac{n^2}{x}A_n(x) \tag{22.36f}$$

or

$$x^2A_n''(x) + xA_n'(x) + (x^2 - n^2)A_n(x) = 0\,. \tag{22.37}$$

But this is Bessel's equation(!) so $A_n(x)$ are Bessel functions.

Now expand $g(x,t)$ in a series in t explicitly:

$$g(x,t) = \exp\left[\left(\frac{x}{2}\right)\left(t - \frac{1}{t}\right)\right] \tag{22.38a}$$

$$= \sum_{r=0}^{\infty}\frac{1}{r!}\left(\frac{x}{2}\right)^r t^r \sum_{s=0}^{\infty}\frac{1}{s!}\left(\frac{x}{2}\right)^s (-1)^s t^{-s} \tag{22.38b}$$

$$= \sum_{r=0}^{\infty}\sum_{s=0}^{\infty}\frac{1}{r!}\frac{1}{s!}(-1)^s\left(\frac{x}{2}\right)^{r+s} t^{r-s} \tag{22.38c}$$

let $n = r - s$ and note we are summing over all possible n since $r - s$ can take any value

$$= \sum_{n=-\infty}^{\infty}\underbrace{\left[\sum_{s=0}^{\infty}\frac{1}{(s+n)!}\frac{1}{s!}(-1)^s\left(\frac{x}{2}\right)^{n+2s}\right]}_{\text{this is } A_n(x)} t^n \tag{22.38d}$$

and therefore

$$\boxed{A_n(x) = \sum_{s=0}^{\infty}\frac{1}{s!}\frac{1}{(s+n)!}(-1)^s\left(\frac{x}{2}\right)^{n+2s}\,.} \tag{22.39}$$

Bessel Functions of Integer Order

In summary:

- Generating function

$$\exp\left[\left(\frac{x}{2}\right)\left(t-\frac{1}{t}\right)\right]=\sum_{n=-\infty}^{\infty}J_n(x)t^n \tag{22.40}$$

- Integral form

$$J_n(x)=\frac{1}{\pi}\int_0^{\pi}\cos(n\theta-x\sin\theta)\,d\theta \tag{22.41}$$

- Recurrence relations

$$J_{n-1}(x)+J_{n+1}(x)=\frac{2n}{x}J_n(x) \tag{22.42}$$

$$J_{n-1}(x)-J_{n+1}(x)=2J_n'(x) \tag{22.43}$$

$$J_n'(x)=J_{n-1}(x)-\frac{n}{x}J_n(x) \tag{22.44}$$

$$J_n'(x)=\frac{n}{x}J_n(x)-J_{n+1}(x) \tag{22.45}$$

- Series expansion

$$J_n(x)=\sum_{k=0}^{\infty}\frac{1}{k!}\frac{1}{(k+n)!}(-1)^k\left(\frac{x}{2}\right)^{n+2k} \tag{22.46}$$

- **Hankel functions**

$$\boxed{H_n^{(1)}(x)=J_n(x)+i\,Y_n(x)} \tag{22.47}$$

$$\boxed{H_n^{(2)}(x)=J_n(x)-i\,Y_n(x)} \tag{22.48}$$

Bessel Functions of Half-Integer Order

Consider $J_\nu(x)$ with $\nu = 1/2$. The series solution is

$$J_{1/2}(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(\frac{1}{2}+k+1)} \left(\frac{x}{2}\right)^{1/2+2k} . \tag{22.49}$$

Recall Legendre's duplication formula: $2^{2z-1}\Gamma(z)\Gamma(z+\frac{1}{2}) = \sqrt{\pi}\Gamma(2z)$
and set $z = k+1$:

$$k!\Gamma(\tfrac{1}{2}+k+1) = \sqrt{\pi}\Gamma(2k+2)2^{1-2(k+1)} = \sqrt{\pi}(2k+1)!2^{-2k-1} . \tag{22.50}$$

Thus

$$J_{1/2}(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} \frac{2}{\sqrt{\pi}} \left(\frac{x}{2}\right)^{1/2} x^{2k} \tag{22.51a}$$

$$= \left(\frac{2}{\pi x}\right)^{1/2} \underbrace{\sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} x^{2k+1}}_{\sin x} \tag{22.51b}$$

and therefore

$$\boxed{J_{1/2}(x) = \left(\frac{2}{\pi x}\right)^{1/2} \sin x .} \tag{22.52}$$

Similiarly

$$\boxed{J_{-1/2}(x) = \left(\frac{2}{\pi x}\right)^{1/2} \cos x .} \tag{22.53}$$

Use the recurrence formulas to get

$$J_{3/2}(x) = \left(\frac{2}{\pi x}\right)^{1/2} \left(\frac{1}{x}\sin x - \cos x\right) , \tag{22.54}$$

$$J_{-3/2}(x) = \left(\frac{2}{\pi x}\right)^{1/2} \left(-\frac{1}{x}\cos x - \sin x\right) , \tag{22.55}$$

etc.

Conventionally define the **spherical Bessel functions**

$$\boxed{j_\ell(x) = \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x)} \tag{22.56}$$

and

$$\boxed{y_\ell(x) = \sqrt{\frac{\pi}{2x}} Y_{\ell+1/2}(x) = (-1)^{\ell+1} \sqrt{\frac{\pi}{2x}} J_{-\ell-1/2}(x)\,.} \tag{22.57}$$

The first few spherical Bessel functions are

$$j_0(x) = \frac{\sin x}{x}\,, \qquad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}\,, \qquad \text{etc.} \tag{22.58}$$

$$y_0(x) = -\frac{\cos x}{x}\,, \qquad y_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}\,, \qquad \text{etc.} \tag{22.59}$$

These functions are shown in Fig. 22.2.

In addition, the **spherical Hankel functions** are

$$\boxed{h_\ell^{(1)}(x) = j_\ell(x) + i\, y_\ell(x)} \tag{22.60}$$

$$\boxed{h_\ell^{(2)}(x) = j_\ell(x) - i\, y_\ell(x)\,.} \tag{22.61}$$

The spherical Bessel functions are solutions to the differential equation

$$x^2 y''(x) + 2x y'(x) + [x^2 - \ell(\ell+1)] y(x) = 0\,. \tag{22.62}$$

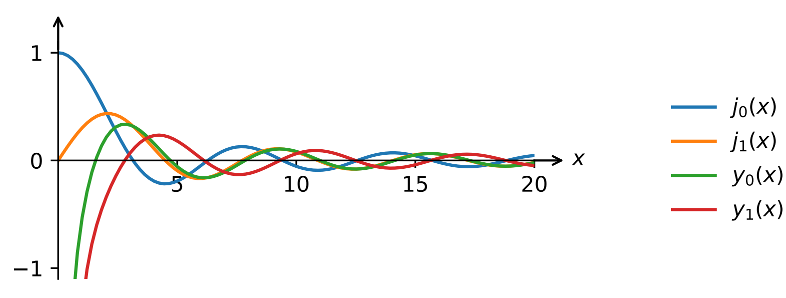


Figure 22.2: Spherical Bessel Functions

Modified Bessel Functions

The **modified Bessel functions** of the first and second kind are defined by

$$\boxed{I_n(z) = \frac{J_n(iz)}{i^n}} \tag{22.63}$$

and

$$\boxed{K_n(z) = \frac{\pi i}{2} i^n H_n^{(1)}(iz)} \tag{22.64}$$

respectively. They are shown in Fig. 22.3.

These functions are solutions to the **modified Bessel equation**

$$\boxed{x^2 y''(x) + xy'(x) - (x^2 + n^2)y(x) = 0 \quad n \geq 0\,.} \tag{22.65}$$

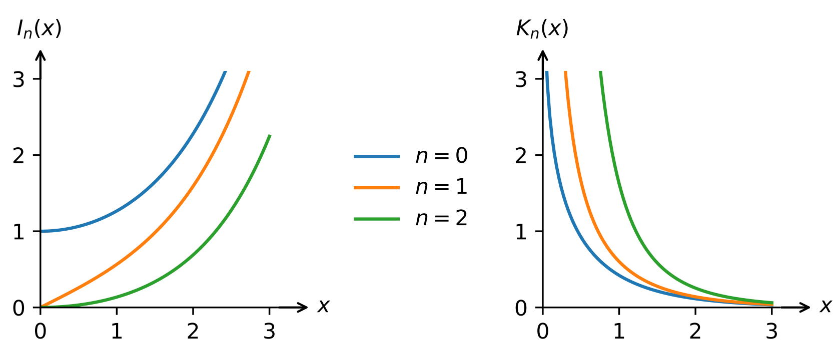


Figure 22.3: Modified Bessel Functions of the First and Second Kind

Legendre Polynomials

The generating function for the Legendre polynomials is

$$g(x,t) = \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x)t^n\,. \tag{22.66}$$

Consider:

$$\frac{\partial g}{\partial t} = -\frac{1}{2}\frac{1}{(1-2xt+t^2)^{3/2}}(-2x+2t) = \frac{x-t}{1-2xt+t^2}g(x,t) \tag{22.67a}$$

$$\implies \quad (1-2xt+t^2)\frac{\partial g}{\partial t} = (x-t)g(x,t) \tag{22.67b}$$

$$\implies \quad (1-2xt+t^2)\sum_{n=0}^{\infty} nP_n(x)t^{n-1} = (x-t)\sum_{n=0}^{\infty} P_n(x)t^n \tag{22.67c}$$

$$\begin{aligned}\implies \quad & \sum_{n=0}^{\infty}\left\{nP_n(x)t^{n-1} - 2xnP_n(x)t^n + nP_n(x)t^{n+1}\right\} \\ & \qquad = \sum_{n=0}^{\infty}\left\{xP_n(x)t^n - P_n(x)t^{n+1}\right\}\end{aligned} \tag{22.67d}$$

$$\begin{aligned}\implies \quad & \sum_{n=0}^{\infty}\left\{(n+1)P_{n+1}(x) - 2xnP_n(x) + (n-1)P_{n-1}(x)\right\}t^n \\ & \qquad = \sum_{n=0}^{\infty}\left\{xP_n(x) - P_{n-1}(x)\right\}t^n\end{aligned} \tag{22.67e}$$

and so we obtain the recurrence relation

$$\boxed{(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0\,.} \tag{22.68}$$

Now consider

$$\frac{\partial g}{\partial x} = \frac{t}{(1-2xt+t^2)^{3/2}} = \frac{t}{1-2xt+t^2}g(x,t) \tag{22.69}$$

but

$$\frac{\partial g}{\partial x} = \sum_{n=0}^{\infty} P_n'(x)t^n \tag{22.70}$$

$$\implies \quad (1-2xt+t^2)\sum_{n=0}^{\infty} P_n'(x)t^n = t\sum_{n=0}^{\infty} P_n(x)t^n \tag{22.71}$$

and so we obtain another recurrence relation

$$\boxed{P_{n+1}'(x) + P_{n-1}'(x) = 2xP_n'(x) + P_n(x)\,.} \tag{22.72}$$

By combining these two recurrence relations we obtain

$$\boxed{P'_{n+1}(x) - P'_{n-1}(x) = (2n+1)P_n(x)} \tag{22.73}$$

$$\boxed{P'_{n+1}(x) = (n+1)P_n(x) + xP'_n(x)} \tag{22.74}$$

$$\boxed{P'_{n-1}(x) = -nP_n(x) + xP'_n(x)} \tag{22.75}$$

and further manipulations yield

$$(1-x^2)P''_n(x) - 2xP'_n(x) + n(n+1)P_n(x) = 0 \tag{22.76}$$

which is Legendre's equation, so $P_n(x)$ are indeed Legendre functions.

Orthonormalization

Consider

$$[g(x,t)]^2 = \frac{1}{1-2xt+t^2} = \left[\sum_{n=0}^{\infty} P_n(x)t^n\right]^2 = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} P_m(x)P_n(x)t^{m+n}. \tag{22.77}$$

Now integrate both sides $\int_{-1}^{1} dx$:

$$\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} t^{m+n}\int_{-1}^{1} P_m(x)P_n(x)\,dx = \int_{-1}^{1}\frac{1}{1-2xt+t^2}\,dx \tag{22.78a}$$

$y = 1-2xt+t^2$
$dx = -\frac{1}{2t}dy$

$$= \frac{1}{2t}\int_{(1-t)^2}^{(1+t)^2}\frac{dy}{y} \tag{22.78b}$$

$$= \frac{1}{t}\ln\left(\frac{1+t}{1-t}\right) \tag{22.78c}$$

recall: $\frac{1}{2}\ln\left(\frac{1+x}{1-x}\right) = x + \frac{x^3}{3} + \frac{x^5}{5} + \cdots$

$$= 2\sum_{n=0}^{\infty}\frac{t^{2n}}{2n+1} \tag{22.78d}$$

so

$$\sum_{n=0}^{\infty}\frac{2t^{2n}}{2n+1} = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} t^{m+n}\underbrace{\int_{-1}^{1} P_m(x)P_n(x)\,dx}_{\text{must be }\propto\,\delta_{mn}}. \tag{22.78e}$$

Therefore

$$\boxed{\int_{-1}^{1} P_n(x)P_m(x)\,dx = \frac{2}{2n+1}\delta_{mn}.} \tag{22.79}$$

Special values

Let $x = 1$:

$$g(1,t) = \frac{1}{\sqrt{1-2t+t^2}} = \frac{1}{1-t} = \sum_{n=0}^{\infty} t^n \tag{22.80a}$$

but

$$g(1,t) = \sum_{n=0}^{\infty} P_n(1) t^n \tag{22.80b}$$

and therefore

$$\boxed{P_n(1) = 1} \tag{22.81}$$

(this is the conventional normalization for Legendre polynomials). Similarly,

$$\boxed{P_n(-1) = (-1)^n\,.} \tag{22.82}$$

Let $x = 0$ and use the binomial series

$$g(0,t) = \frac{1}{\sqrt{1+t^2}} = 1 - \frac{1}{2}t^2 + \frac{1}{2}\frac{3}{2}\frac{t^4}{2!} - \frac{1}{2}\frac{3}{2}\frac{5}{2}\frac{t^6}{3!} + \cdots \tag{22.83a}$$

$$= \sum_{n=0}^{\infty} (-1)^n \frac{(2n-1)!!}{(2n)!} t^{2n} \tag{22.83b}$$

so we find

$$\boxed{P_{2n}(0) = (-1)^n \frac{(2n-1)!!}{(2n)!} \qquad \text{and} \qquad P_{2n+1}(0) = 0\,.} \tag{22.84}$$

Finally, note that $g(-x,-t) = g(x,t)$ which yields

$$\boxed{P_n(-x) = (-1)^n P_n(x)\,.} \tag{22.85}$$

Useful identity

Let $x = \cos\theta$ and $t = r'/r$ in the generating function with $r' < r$. Then:

$$g(\cos\theta, r'/r) = \sum_{\ell=0}^{\infty} \left(\frac{r'}{r}\right)^{\ell} P_\ell(\cos\theta) = \frac{1}{\sqrt{1 - 2(r'/r)\cos\theta + (r'/r)^2}} \tag{22.86a}$$

$$= \frac{r}{\sqrt{r^2 + r'^2 - 2rr'\cos\theta}} \tag{22.86b}$$

$$= \frac{r}{\|\mathbf{x} - \mathbf{x}'\|} \tag{22.86c}$$

where $\mathbf{x}$ and $\mathbf{x}'$ are two vectors with $r = \|\mathbf{x}\|$, $r' = \|\mathbf{x}'\|$, and $\mathbf{x} \cdot \mathbf{x}' = rr'\cos\theta$. Thus

$$\frac{1}{\|\mathbf{x} - \mathbf{x}'\|} = \sum_{\ell=0}^{\infty} \frac{(r')^{\ell}}{r^{\ell+1}} P_\ell(\cos\theta), \quad r' < r. \tag{22.87}$$

If $r' > r$, exchange r' and r or else the series will not converge. Therefore

$$\boxed{\frac{1}{\|\mathbf{x} - \mathbf{x}'\|} = \sum_{\ell=0}^{\infty} \frac{r_<^{\ell}}{r_>^{\ell+1}} P_\ell(\cos\theta)} \tag{22.88}$$

where $r_< = \min(r', r)$ and $r_> = \max(r', r)$.

Second solution

The Wronskian can be used to find the second independent solution $Q_n(x)$:

$$W[P_n, Q_n] = P_n Q_n' - P_n' Q_n = P_n^2 \left(\frac{Q_n}{P_n}\right)' \tag{22.89a}$$

but

$$W[P_n, Q_n] \propto \frac{1}{1-x^2} \tag{22.89b}$$

so

$$\boxed{Q_n(x) = P_n(x) \int \frac{dx}{(1-x^2)[P_n(x)]^2}} \tag{22.90}$$

(with the conventional choice of normalization).

Explicitly:

- For $n = 0$, $P_0(x) = 1$ and

$$Q_0(x) = \int \frac{dx}{1-x^2} = \frac{1}{2} \ln\left(\frac{1+x}{1-x}\right). \tag{22.91}$$

- For $n = 1$, $P_1(x) = x$ and

$$\begin{aligned} Q_1(x) &= x \int \frac{dx}{x^2(1-x^2)} = x\left[-\frac{1}{x} + \frac{1}{2}\ln\left(\frac{1+x}{1-x}\right)\right] \\ &= \frac{x}{2}\ln\left(\frac{1+x}{1-x}\right) - 1\,. \end{aligned} \tag{22.92}$$

Associated Legendre Differential Equation

The **associated Legendre differential equation** is

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \left[n(n+1) - \frac{m^2}{1-x^2}\right]y = 0\,. \tag{22.93}$$

Note that this reduces to the Legendre equation when $m = 0$.

Non-singular solutions in the domain $-1 \le x \le 1$ exist only when n and m are integers with $0 \le |m| \le n$. If $P_n(x)$ is a solution to Legendre's equation, then

$$P_n^m(x) = (-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_n(x) \tag{22.94}$$

is a solution to the associated Legendre's equation when m is a positive integer. These are called the **associated Legendre functions**.

For $m < 0$ and m is an integer, use

$$P_n^{-m}(x) = (-1)^m\frac{(n-m)!}{(n+m)!}P_n^m(x)\,. \tag{22.95}$$

The first few associated Legendre functions are (recall $P_n^0(x) = P_n(x)$):

$$P_1^1(x) = -\sqrt{1-x^2}\,,\quad P_2^1(x) = -3x\sqrt{1-x^2}\,,\quad P_2^2(x) = 3(1-x^2)\,. \tag{22.96}$$

These are shown in Fig. 22.4.

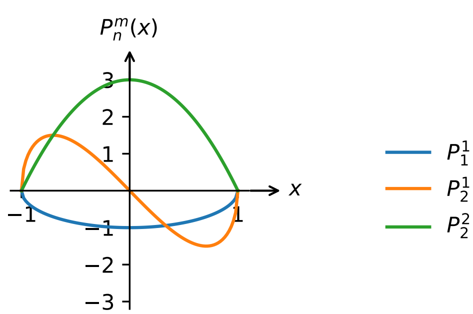


Figure 22.4: Associated Legendre Functions

Spherical Harmonics

The **spherical harmonics** are defined as

$$\boxed{Y_\ell^m(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}P_\ell^m(\cos\theta)e^{im\phi}\,.} \tag{22.97}$$

The first few spherical harmonics are

$$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}} \tag{22.98}$$

$$Y_1^0(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta \tag{22.99}$$

$$Y_1^1(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{i\phi} \tag{22.100}$$

$$Y_2^0(\theta,\phi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta-1) \tag{22.101}$$

$$Y_2^1(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta e^{i\phi} \tag{22.102}$$

$$Y_2^2(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2i\phi} \tag{22.103}$$

and, for negative integer m, use

$$\boxed{Y_\ell^{-m}(\theta,\phi) = (-1)^m[Y_\ell^m(\theta,\phi)]^*\,.} \tag{22.104}$$

A few useful identities are:

$$Y_\ell^{-\ell}(\theta,\phi) = \frac{1}{2^\ell \ell!}\sqrt{\frac{(2\ell+1)!}{4\pi}}\sin^\ell\theta e^{-i\ell\phi} \tag{22.105}$$

$$Y_\ell^0(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}}P_\ell(\cos\theta) \tag{22.106}$$

$$\sum_{m=-\ell}^{\ell}|Y_\ell^m(\theta,\phi)|^2 = \frac{2\ell+1}{4\pi} \tag{22.107}$$

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} Y_\ell^m(\theta,\phi)[Y_{\ell'}^{m'}(\theta,\phi)]^*\sin\theta\,d\theta\,d\phi = \delta_{\ell\ell'}\delta_{mm'}\,. \tag{22.108}$$

23 Degeneracy and Completeness

When two or more eigenvalues are the same they are called **degenerate**.

A linear combination of eigenfunctions belonging to a degenerate set is again an eigenfunction with the same eigenvalue.

Construct an orthogonal set of eigenfunctions by the **Gram-Schmidt** procedure demonstrated in the next example:

Ex. 23.1. Suppose u, v, and w all belong to eigenvalue λ.

- Take $u_1 = u$.
- Let $u_2 = v + \alpha u_1$ and choose α so

$$0 = \int u_1^*(x) u_2(x) \rho(x)\, dx = \int u^*(x) v(x) \rho(x)\, dx + \alpha \int u^*(x) u(x) \rho(x)\, dx \tag{23.1}$$

$$\implies \quad \alpha = -\frac{\int u^*(x) v(x) \rho(x)\, dx}{\int u^*(x) u(x) \rho(x)\, dx}. \tag{23.2}$$

- Let $u_3 = w + \beta u_1 + \gamma u_2$. Choose β so that

$$0 = \int u_1^*(x) u_3(x) \rho(x)\, dx = \int u_1^*(x) w(x) \rho(x)\, dx + \beta \int u_1^*(x) u_1(x) \rho(x)\, dx \tag{23.3}$$

$$\implies \quad \beta = -\frac{\int u_1^*(x) w(x) \rho(x)\, dx}{\int u_1^*(x) u_1(x) \rho(x)\, dx}. \tag{23.4}$$

  Similarly choose γ so that

$$0 = \int u_2^*(x) u_3(x) \rho(x)\, dx = \int u_2^*(x) w(x) \rho(x)\, dx + \gamma \int u_2^*(x) u_2(x) \rho(x)\, dx \tag{23.5}$$

$$\implies \quad \gamma = -\frac{\int u_2^*(x) w(x) \rho(x)\, dx}{\int u_2^*(x) u_2(x) \rho(x)\, dx}. \tag{23.6}$$

We now have u_1, u_2, and u_3 which are orthogonal eigenfunctions.

Therefore, even when there is a degenerate set, it is possible to get a complete set of orthogonal eigenfunctions:

$$\boxed{(u_i, u_j) = \int_\Omega u_i^*(x) u_j(x) \rho(x)\, dx = \delta_{ij}\,.} \tag{23.7}$$

(Here we've assumed that the eigenfunctions are actually orthonormal.)

Functions over the domain Ω having the required boundary conditions can be expanded in terms of this complete orthonormal set:

$$\boxed{f(x) = \sum_n c_n u_n(x) \qquad \text{with} \qquad c_n = \int_\Omega u_n^*(x) f(x) \rho(x)\, dx\,.} \tag{23.8}$$

Substitute the expression for c_n into the expansion:

$$f(x) = \sum_n u_n(x) \int_\Omega u_n^*(x') f(x') \rho(x')\, dx' \tag{23.9a}$$

$$= \int_\Omega f(x') \underbrace{\left[\rho(x') \textstyle\sum_n u_n(x) u_n^*(x')\right]}_{\text{must be } \delta(x-x')} dx' \tag{23.9b}$$

and therefore we have the **completeness relation**

$$\boxed{\rho(x') \sum_n u_n(x) u_n^*(x') = \delta(x - x')\,.} \tag{23.10}$$

Ex. 23.2. Fourier series, as we've seen in §13.

Ex. 23.3. Legendre polynomials: $\rho(x) = 1$.

- $$f(x) = A_0 P_0(x) + A_1 P_1(x) + A_2 P_2(x) + \cdots \qquad \text{for } -1 \le x \le 1 \tag{23.11}$$
- $$A_k = \frac{2k+1}{2} \int_{-1}^{1} f(x) P_k(x)\, dx \tag{23.12}$$

  where the normalization comes from $\displaystyle\int_{-1}^{1} [P_k(x)]^2\, dx = \frac{2}{2k+1}$
- $$\sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(x) P_n(x') = \delta(x - x') \tag{23.13}$$

Ex. 23.4. Spherical harmonics:

- $$f(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} c_{\ell m} Y_\ell^m(\theta, \phi) \tag{23.14}$$
- $$c_{\ell m} = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} f(\theta, \phi) [Y_\ell^m(\theta, \phi)]^* \sin\theta\, d\theta\, d\phi \tag{23.15}$$
- $$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_\ell^m(\theta, \phi) [Y_\ell^m(\theta', \phi')]^* = \frac{1}{\sin\theta} \delta(\theta - \theta') \delta(\phi - \phi') \tag{23.16}$$

24 Inhomogeneous Problems — Green Functions

Consider the inhomogeneous problem (take $\rho = 1$ for simplicity)

$$\mathcal{L}\, u(x) - \lambda u(x) = f(x) \tag{24.1}$$

where $f(x)$ is a source and seek a solution via eigenfunction expansion:

$$u(x) = \sum_n c_n u_n(x) \qquad \text{and} \qquad f(x) = \sum_n d_n u_n(x)\,. \tag{24.2}$$

Then we have

$$\sum_n c_n(\lambda_n - \lambda) u_n(x) = \sum_n d_n u_n(x) \tag{24.3a}$$

and since the eigenfunctions are linearly independent

$$c_n = \frac{d_n}{\lambda_n - \lambda} = \frac{(u_n, f)}{\lambda_n - \lambda}\,. \tag{24.3b}$$

Therefore

$$u(x) = \sum_n \frac{u_n(x)}{\lambda_n - \lambda} \int_\Omega u_n^*(x') f(x')\, dx' \tag{24.4a}$$

$$= \int_\Omega G(x, x') f(x')\, dx' \tag{24.4b}$$

where

$$G(x, x') = \sum_n \frac{u_n(x) u_n^*(x')}{\lambda_n - \lambda} \tag{24.4c}$$

is known as a **Green function**. It depends on the linear operator $\mathcal{L}$, the value λ, the domain Ω, and the boundary conditions.

Note that if $f(x) = \delta(x - x_0)$ where x_0 is in the domain then

$$u(x) = \int_\Omega G(x, x')\delta(x' - x_0)\, dx' \tag{24.5a}$$

$$= G(x, x_0) \tag{24.5b}$$

thus we have

$$\mathcal{L}\, G(x, x_0) - \lambda G(x, x_0) = \delta(x - x_0) \tag{24.6}$$

(note that the differential operator $\mathcal{L}$ acts on the x variable, not on x_0).
This is the differential equation for the Green function. Appropriate boundary conditions are sill required (and different boundary conditions result in different Green functions).

Therefore, Green functions are solutions to the inhomogeneous problems with unit point sources.

The solution for more general source distributions is obtained by linear superposition of the solutions for many point sources, as seen in Eq. (24.4b).

Ex. 24.1. A string of length ℓ vibrating with angular frequency ω with fixed ends is described by

$$\frac{d^2u}{dx^2} + k^2 u = 0\,, \qquad \underbrace{u(0) = u(\ell) = 0}_{\text{fixed ends boundary condition}} \tag{24.7}$$

where $u(x)$ is the transverse displacement of the string from its equilibrium.
Here $k = \omega/c$ where c is the speed of sound in the string.

Find the Green function for this differential equation and boundary conditions.

- Method 1.
  Let $k^2 = -\lambda$ and solve the eigenvalue problem

$$\frac{d^2u}{dx^2} = \lambda u\,, \qquad u(0) = u(\ell) = 0\,. \tag{24.8}$$

The eigenvalues are

$$\lambda_n = -\left(\frac{n\pi}{\ell}\right)^2, \quad n = 1, 2, 3, \ldots \tag{24.9}$$

and the normalized eigenfunctions are

$$u_n(x) = \sqrt{\frac{2}{\ell}}\sin\left(\frac{n\pi x}{\ell}\right), \quad n = 1, 2, 3, \ldots\,. \tag{24.10}$$

Therefore

$$G(x, x') = \sum_n \frac{u_n(x)u_n^*(x')}{\lambda_n - \lambda} \tag{24.11a}$$

$$= \frac{2}{\ell}\sum_{n=1}^{\infty} \frac{\sin(n\pi x/\ell)\sin(n\pi x'/\ell)}{k^2 - (n\pi/\ell)^2} \tag{24.11b}$$

Note: when the string vibrates at an eigenfrequency, the Green function becomes infinite.
Note also: $G(x, x') = G^*(x', x)$ so for real-valued Green functions

$$\boxed{G(x, x') = G(x', x)\,.} \tag{24.12}$$

This is a **reciprocity relation**: the response at position x to a disturbance at position x' is equal to the response at position x' to a disturbance at position x.

- Method 2.
  Solve

$$\frac{d^2G(x,x')}{dx^2} + k^2 G(x,x') = \delta(x-x')\,, \qquad G(0,x') = G(\ell,x') = 0\,. \tag{24.13}$$

Note: for $x \neq x'$, $\dfrac{d^2G}{dx^2} + k^2 G = 0$, so

$$G(x,x') = \begin{cases} a\sin kx & x < x' \\ b\sin k(x-\ell) & x > x' \end{cases} \tag{24.14}$$

where a and b are constants. This satisfies the boundary conditions at $x = 0$ and $x = \ell$ and the homogeneous equation for $x \neq x'$.
We need to match these two solutions at $x = x'$ to determine a and b.
Integrate the differential equation over x from $x' - \epsilon$ to $x' + \epsilon$:

$$\underbrace{\int_{x'-\epsilon}^{x'+\epsilon} \frac{d^2G(x,x')}{dx^2}\,dx}_{\to \frac{dG}{dx} \text{ as } \epsilon\to 0} + k^2 \underbrace{\int_{x'-\epsilon}^{x'+\epsilon} G(x,x')\,dx}_{\text{vanishes as } \epsilon\to 0} = \underbrace{\int_{x'-\epsilon}^{x'+\epsilon} \delta(x-x')\,dx}_{1} \tag{24.15}$$

so we have

$$\lim_{\epsilon\to 0}\left[\left.\frac{dG(x,x')}{dx}\right|_{x=x'+\epsilon} - \left.\frac{dG(x,x')}{dx}\right|_{x=x'-\epsilon} \right] = 1 \tag{24.16}$$

i.e., the derivative of G is discontinuous at x' and jumps by 1.
Integrate again:

$$\lim_{\epsilon\to 0} G(x,x')\Big|_{x=x'-\epsilon}^{x=x'+\epsilon} = 0 \tag{24.17}$$

i.e., G is continuous at x'.
Matching the two solutions at $x = x'$ then yields

continuous: $$a\sin kx' = b\sin k(x'-\ell) \tag{24.18a}$$
unit jump in derivative: $$ka\cos kx' + 1 = kb\cos k(x'-\ell) \tag{24.18b}$$

and we find

$$a = \frac{\sin k(x'-\ell)}{k\sin k\ell} \qquad \text{and} \qquad b = \frac{\sin kx'}{k\sin k\ell}\,. \tag{24.19}$$

Therefore

$$G(x,x') = \frac{1}{k\sin k\ell}\begin{cases} \sin kx \sin k(x'-\ell) & 0 \le x < x' \\ \sin kx' \sin k(x-\ell) & x' < x \le \ell\,. \end{cases} \tag{24.20}$$

General method

Consider the linear operator

$$\mathcal{L} = p(x)\frac{d^2}{dx^2} + p'(x)\frac{d}{dx} + q(x) \tag{24.21}$$

and the inhomogeneous equation

$$\mathcal{L}\, y(x) - f(x) = 0 \qquad \text{with} \qquad y(a) = y(b) = 0\,, \quad a \le x \le b\,. \tag{24.22}$$

Let $u(x)$ be a solution of $\mathcal{L}\, u = 0$ with $u(a) = 0$.
Let $v(x)$ be a solution of $\mathcal{L}\, v = 0$ with $v(b) = 0$.
Let

$$G(x,x') = \begin{cases} A u(x) & a \le x < x' \\ B v(x) & x' < x \le b \end{cases} \tag{24.23}$$

and enforce

$$\lim_{\epsilon\to 0}\left[G\Big|_{x=x'-\epsilon} - G\Big|_{x=x'+\epsilon}\right] = 0 \tag{24.24a}$$

and

$$\lim_{\epsilon\to 0}\left[\frac{dG}{dx}\bigg|_{x=x'-\epsilon} - \frac{dG}{dx}\bigg|_{x=x'-\epsilon}\right] = -\frac{1}{p(x')}\,. \tag{24.24b}$$

This determines

$$A = \frac{v(x')}{C} \qquad \text{and} \qquad B = \frac{u(x')}{C} \tag{24.25a}$$

where

$$W[u(x'), v(x')] = \frac{C}{p(x')}\,. \tag{24.25b}$$

Therefore

$$G(x,x') = \frac{1}{C}\begin{cases} u(x)v(x') & a \le x < x' \\ u(x')v(x) & x' < x \le b \end{cases} \tag{24.26a}$$

with

$$C = p(x')[u(x')v'(x') - u'(x')v(x')]\,. \tag{24.26b}$$

Then

$$y(x) = \int_a^b G(x,x')f(x')\,dx'\,. \tag{24.27}$$

Problems

Problem 28.

The Sturm-Liouville differential equation is

$$\mathcal{L}\, u(x) + \lambda\rho(x)u(x) = 0$$

where

$$\mathcal{L} = p(x)\frac{d^2}{dx^2} + p'(x)\frac{d}{dx} - q(x).$$

Show that $\mathcal{L}$ is Hermitian when the domain is chosen to be $a \leq x \leq b$ and the boundary conditions are taken to be $u(a) = u(b) = 0$. Show that orthogonality now means:

$$0 = (u, v) = \int_a^b u^*(x)v(x)\rho(x)\, dx.$$

The next two problems refer to Hermite's differential equation

$$y'' - 2xy' + 2ny = 0 \qquad -\infty < x < \infty.$$

The Hermite polynomials are solutions that can be obtained from the generating function

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

Problem 29.

a) Use the generating function to prove the following identities:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x),$$
$$H_n'(x) = 2nH_{n-1}(x),$$
$$H_{2n}(0) = (-1)^n \frac{(2n)!}{n!},$$
$$H_{2n+1}(0) = 0,$$

and

$$H_n(x) = (-1)^n H_n(-x).$$

b) Using the identities proven in part (a), show that $H_n(x)$ is a solution to Hermite's equation.

c) From the generating function, show that

$$H_n(x) = \sum_{s=0}^{\lfloor n/2 \rfloor} (-1)^s \frac{n!}{(n-2s)!s!}(2x)^{n-2s}$$

where $\lfloor n/2 \rfloor$ means the greatest integer less than or equal to $n/2$.

Problem 30.

a) Prove Rodrigues's formula:

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

b) By integrating the product

$$e^{-x^2} g(x,s)g(x,t)$$

over all x, show that

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x)H_n(x)\,dx = 2^n n! \sqrt{\pi}\,\delta_{mn}.$$

Problem 31. Use Gram-Schmidt orthogonalization of the set of polynomials 1, x, x^2, x^3, … on the interval $-1 \le x \le 1$ to generate the orthogonal Legendre polynomials $P_0(x)$, $P_1(x)$, $P_2(x)$, and $P_3(x)$. Note that Legendre polynomials are normalized so that $P_n(1) = 1$.

Problem 32.

Consider the differential equation

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2}\right] y(r) = 0 \qquad 0 < r < \infty$$

where $n = 1, 2, 3, \ldots$. Find two independent solutions, one which vanishes as $r \to 0$, the other that vanishes for $r \to \infty$. (Hint: let $x = \ln r$.)

Problem 33.

Given the result of problem 32 find the solution to the differential equation

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{n^2}{r^2}\right] G(r, r') = \frac{1}{r}\,\delta(r - r') \qquad 0 < r < \infty$$

with the boundary conditions that the solution vanishes as $r \to 0$ and $r \to \infty$.

Module VII

Matrices and Vectors

Motivation

We now move our general discussion beyond one dimension.

We first address solving linear systems of equations and introduce matrices and review some of their properties. Next we talk about vector spaces, linear operators, and we re-encounter eigenvalue problems which arise in quantum and classical mechanics. Then we review vector calculus and differential operators that are used to formulate fundamental physical laws, e.g., electrodynamics. In the last section we provide formulae for these differential operators in cylindrical and spherical coordinate systems which are commonly used to simplify problems.

25 Linear Algebra

A **linear system of equations** is a system of equations of the form

$$\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n &= b_2 \\
&\vdots \\
a_{m1}x_1 + a_{m2}x_2 + a_{m3}x_3 + \cdots + a_{mn}x_n &= b_m
\end{aligned} \tag{25.1}$$

where a_{ij} and b_i, $i = 1 \ldots m$, $j = 1 \ldots n$ are constants and x_j, $j = 1 \ldots n$ are unknowns. This is a system having m equations and n unknowns.

- If the number of equations is fewer than the number of unknowns, $m < n$, then the system is **underdetermined** and in general has an infinite number of solutions.
- If the number of equations is greater than the number of unknowns, $m > n$, then the system is **overdetermined**, and generally has no solution.
- In general, there is a unique solution when the number of equations equals the number of unknowns, $m = n$.

The use of the term "in general" above means that there are exceptions for certain values of the coefficients. For example, if two equations are the same up to an overall factor, e.g.,

$$2x + 3y = 4 \qquad \text{and} \qquad 6x + 9y = 12 \tag{25.2}$$

(the second equation is 3 times the first) then they are not **linearly independent** — they are the same equation, and we can drop one of them.

Another possibility is when two equations are **inconsistent**, e.g.,

$$2x + 3y = 4 \qquad \text{and} \qquad 2x + 3y = 5\,. \tag{25.3}$$

An inconsistent system of equations has no solutions.

To solve a system of n equations in n unknowns, solve the first equation for the first unknown, and substitute this in the remaining equations. Now there are $n-1$ equations in $n-1$ unknowns.

Ex. 25.1. For a system of 3 equations in 3 unknowns,

$$
\begin{aligned}
a_{11}x + a_{12}y + a_{13}z &= b_1\\
a_{21}x + a_{22}y + a_{23}z &= b_2\\
a_{31}x + a_{32}y + a_{33}z &= b_3
\end{aligned}
\tag{25.4}
$$

solve the first equation for x:

$$x = \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}}y - \frac{a_{13}}{a_{11}}z \tag{25.5}$$

and substitute this into the next two equations. Actually, it is a little neater if we multiply the other two equations by a_{11}. Then we have

$$
\begin{aligned}
(a_{11}a_{22} - a_{21}a_{12})y + (a_{11}a_{23} - a_{21}a_{13})z &= a_{11}b_2 - a_{21}b_1\\
(a_{11}a_{32} - a_{31}a_{12})y + (a_{11}a_{33} - a_{31}a_{13})z &= a_{11}b_3 - a_{31}b_2\,.
\end{aligned}
\tag{25.6}
$$

Solve the first of these for y:

$$y = \frac{1}{a_{11}a_{22} - a_{21}a_{12}}\left[a_{11}b_2 - a_{21}b_1 - (a_{11}a_{23} - a_{21}a_{13})z\right]. \tag{25.7}$$

Now multiply the last equation by $(a_{11}a_{22} - a_{21}a_{12})$ and substitute in for y:

$$
\begin{aligned}
&[(a_{11}a_{22} - a_{21}a_{12})(a_{11}a_{33} - a_{31}a_{13}) - (a_{11}a_{32} - a_{31}a_{12})(a_{11}a_{23} - a_{21}a_{13})]z\\
&\quad = (a_{11}a_{22} - a_{21}a_{12})(a_{11}b_3 - a_{31}b_1) - (a_{11}a_{32} - a_{31}a_{12})(a_{11}b_2 - a_{21}b_1)\,.
\end{aligned}
\tag{25.8}
$$

Provided the coefficient in front of z is not zero, we can now solve for z. Then substitute z into the equation for y to determine y and finally substitute the equations for z and y into the equation for x to determine x.

This is straightforward but tedious. (Fortunately we have computers.)

The solution is

$$x = \frac{(a_{22}a_{33} - a_{23}a_{32})b_1 - (a_{12}a_{33} - a_{13}a_{32})b_2 + (a_{12}a_{23} - a_{13}a_{22})b_3}{D} \tag{25.9a}$$

$$y = \frac{-(a_{21}a_{33} - a_{23}a_{31})b_1 + (a_{11}a_{33} - a_{13}a_{31})b_2 - (a_{11}a_{23} - a_{13}a_{21})b_3}{D} \tag{25.9b}$$

$$z = \frac{(a_{21}a_{32} - a_{22}a_{31})b_1 - (a_{11}a_{32} - a_{12}a_{31})b_2 + (a_{11}a_{22} - a_{12}a_{21})b_3}{D} \tag{25.9c}$$

with

$$
\begin{aligned}
D = {} & a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32}\\
& - a_{13}a_{22}a_{31} - a_{12}a_{21}a_{33} - a_{11}a_{23}a_{32}\,.
\end{aligned}
\tag{25.9d}
$$

Matrices

To express the linear system of equations more succinctly, introduce the **matrix**. First note that the linear system can be written

$$\sum_{j=1}^{n} a_{ij} x_j = b_i\,, \quad i = 1 \ldots m\,. \tag{25.10}$$

Let $\underline{A} = [a_{ij}]$ be an $m \times n$ matrix, $\underline{b} = [b_i]$ be a $m \times 1$ matrix or **column vector** and $\underline{x} = [x_i]$ be a $n \times 1$ matrix (column vector). Then our system of equations can be written concisely as

$$\underline{A}\,\underline{x} = \underline{b} \tag{25.11}$$

where

$$\underline{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix}, \quad \underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}, \quad \text{and} \quad \underline{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}. \tag{25.12}$$

Matrix multiplication is defined as follows: if $\underline{A} = [a_{ij}]$ is an $m \times n$ matrix, $\underline{B} = [b_{jk}]$ is an $n \times p$ matrix, and $\underline{C} = [c_{ik}]$ is an $m \times p$ matrix, $i = 1 \ldots m$, $j = 1 \ldots n$, $k = 1 \ldots p$, then

$$\boxed{\underline{C} = \underline{A}\,\underline{B} \quad \Longleftrightarrow \quad c_{ik} = \sum_{j=1}^{n} a_{ij} b_{jk}\,,} \quad \text{for } i = 1 \ldots m \text{ and } k = 1 \ldots p. \tag{25.13}$$

Note that matrix multiplication is only defined between a $n \times m$ matrix on the left and a $p \times q$ matrix on the right if $p = m$ and the result is a $m \times q$ matrix. Consequently, if $\underline{A}\,\underline{B}$ is defined, it does not necessarily mean that $\underline{B}\,\underline{A}$ is defined.

Even if $\underline{A}$ and $\underline{B}$ are both $n \times n$ matrixes so that $\underline{A}\,\underline{B}$ and $\underline{B}\,\underline{A}$ both exist, it does not necessarily follow that $\underline{A}\,\underline{B} = \underline{B}\,\underline{A}$.

For example: $\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 3 & 4 \\ 4 & 6 \end{bmatrix}$ but $\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 3 \\ 4 & 7 \end{bmatrix}$.

In other words, matrix multiplication does not **commute**.

In addition to matrix multiplication, matrices can be multiplied by a scalar to form a matrix of the same shape:

$$\boxed{\underline{C} = \alpha \underline{A} \quad \Longleftrightarrow \quad c_{ij} = \alpha a_{ij}} \tag{25.14}$$

and matrices of the same shape can be added:

$$\boxed{\underline{C} = \underline{A} + \underline{B} \quad \Longleftrightarrow \quad c_{ij} = a_{ij} + b_{ij}\,.} \tag{25.15}$$

It can then be verified that matrix addition is **commutative**, $\underline{A}+\underline{B} = \underline{B}+\underline{A}$, and **associative**, $(\underline{A}+\underline{B})+\underline{C} = \underline{A}+(\underline{B}+\underline{C})$, and matrix multiplication is **associative**, $(\underline{A}\,\underline{B})\underline{C} = \underline{A}(\underline{B}\,\underline{C})$ and **distributive** $\underline{A}(\underline{B}+\underline{C}) = \underline{A}\,\underline{B}+\underline{A}\,\underline{C}$.

Some special matrices are the **zero matrix** $\underline{0}$ which has zero for all elements and the **identity matrix** $\underline{1} = [\delta_{ij}]$. These have the properties $\underline{A}+\underline{0} = \underline{A}$, $\underline{A}\,\underline{0} = \underline{0}\,\underline{A} = \underline{0}$, and $\underline{A}\,\underline{1} = \underline{1}\,\underline{A} = \underline{A}$.

Some other important matrix operations are as follows.

- Complex conjugation: if $\underline{A} = [a_{ij}]$ and $\underline{C} = [c_{ij}]$ have the same shape then

$$\boxed{\underline{C} = \underline{A}^* \quad \Longleftrightarrow \quad c_{ij} = a^*_{ij}\,.} \tag{25.16}$$

- **Transpose**: if $\underline{A} = [a_{ij}]$ is an $m \times n$ matrix and $\underline{C} = [c_{k\ell}]$ is a $n \times m$ matrix then

$$\boxed{\underline{C} = \underline{A}^{\mathsf{T}} \quad \Longleftrightarrow \quad c_{k\ell} = a_{ji}\,.} \tag{25.17}$$

- **Adjoint**:

$$\boxed{\underline{A}^\dagger = (\underline{A}^{\mathsf{T}})^*\,.} \tag{25.18}$$

- **Trace**: if $\underline{A} = [a_{ij}]$ is a $n \times n$ (square) matrix then

$$\boxed{\mathrm{Tr}\,\underline{A} = \sum_{i=1}^{n} a_{ii}\,.} \tag{25.19}$$

- **Determinant**: if $\underline{A} = [a_{ij}]$ is a $n \times n$ (square) matrix then

$$\boxed{\det \underline{A} = \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \cdots \sum_{i_n=1}^{n} \epsilon_{i_1 i_2 \ldots i_n} a_{1,i_1} a_{2,i_2} \cdots a_{n,i_n}} \tag{25.20}$$

  where $\epsilon_{i_1 i_2 \ldots i_n}$ is the **Levi-Civita symbol** defined by

$$\boxed{\epsilon_{1,2,\ldots,n} = 1 \quad \text{and} \quad \epsilon_{i_1,\ldots,i_p,\ldots,i_q,\ldots,i_n} = -\epsilon_{i_1,\ldots,i_q,\ldots i_p,\ldots,i_n}} \tag{25.21}$$

  or $\epsilon_{i_1,i_2,\ldots,i_n} = +1$ if $(i_1, i_2, \ldots, i_n)$ is an even permultation of $(1, 2, \ldots, n)$; $\epsilon_{i_1,i_2,\ldots,i_n} = -1$ if $(i_1, i_2, \ldots, i_n)$ is an odd permultation of $(1, 2, \ldots, n)$; and $\epsilon_{i_1,i_2,\ldots,i_n} = 0$ otherwise.

The **minor** m_{ij} of the square matrix $\underline{A} = [a_{ij}]$ is $m_{ij} = \det([(a_{k\ell})_{k\neq i,\ell\neq j}])$ and the **cofactor matrix** is $\underline{C} = [(-1)^{i+j} m_{ij}]$. Then the **matrix inverse** of $\underline{A}$ is

$$\boxed{\underline{A}^{-1} = \frac{1}{\det \underline{A}} \underline{C}^{\mathsf{T}} .} \tag{25.22}$$

The inverse matrix has the property $\underline{A}^{-1}\underline{A} = \underline{A}\,\underline{A}^{-1} = \underline{1}$.

Some useful identities:

$$(\underline{A}\,\underline{B})^{-1} = \underline{B}^{-1}\underline{A}^{-1} \tag{25.23a}$$

$$(\underline{A}\,\underline{B})^{\mathsf{T}} = \underline{B}^{\mathsf{T}}\underline{A}^{\mathsf{T}} \tag{25.23b}$$

$$\mathrm{Tr}(\underline{A}\,\underline{B}) = \mathrm{Tr}(\underline{B}\,\underline{A}) \tag{25.23c}$$

$$\det(\underline{A}\,\underline{B}) = (\det \underline{A})(\det \underline{B}) = \det(\underline{B}\,\underline{A}) . \tag{25.23d}$$

A matrix $\underline{A}$ is a:

- **real matrix** if $\underline{A}^* = \underline{A}$, (25.24a)
- **symmetric matrix** if $\underline{A}^{\mathsf{T}} = \underline{A}$, (25.24b)
- **antisymmetric matrix** if $\underline{A}^{\mathsf{T}} = -\underline{A}$, (25.24c)
- **Hermitian matrix** if $\underline{A}^{\dagger} = \underline{A}$, (25.24d)
- **orthogonal matrix** if $\underline{A}^{-1} = \underline{A}^{\mathsf{T}}$, (25.24e)
- **unitary matrix** if $\underline{A}^{-1} = \underline{A}^{\dagger}$, (25.24f)
- **diagonal matrix** if $\underline{A} = [a_{ij}]$ with $a_{ij} = 0$ for $i \neq j$, (25.24g)
- **idempotent matrix** if $\underline{A}^2 = \underline{A}$, (25.24h)
- **nilpotent matrix** if $\underline{A}^k = \underline{0}$ for some integer k. (25.24i)

26 Vector Spaces

A n-vector $\mathbf{x}$ is said to live in an n-dimensional **vector space**. Vectors in the vector space have the following operations:

- Addition of vectors commutative and associative:

$$\mathbf{x}+\mathbf{y}=\mathbf{y}+\mathbf{x} \qquad \text{and} \qquad (\mathbf{x}+\mathbf{y})+\mathbf{z}=\mathbf{x}+(\mathbf{y}+\mathbf{z})\,. \tag{26.1}$$

- Multiplication by a scalar is distributive and associative:

$$a(\mathbf{x}+\mathbf{y})=a\mathbf{x}+b\mathbf{y} \qquad \text{and} \qquad a(b\mathbf{x})=(ab)\mathbf{x}\,. \tag{26.2}$$

Multiplication by 1 leaves a vector unchanged: $1\mathbf{x}=\mathbf{x}$.
Multiplication by 0 results in a null vector $0\mathbf{x}=\mathbf{0}$ for which $\mathbf{x}+\mathbf{0}=\mathbf{x}$.
Multiplication by -1 results in a vector $-\mathbf{x}$ for which $\mathbf{x}+(-\mathbf{x})=\mathbf{0}$.

A set of vectors $\mathbf{x}, \mathbf{y}, \ldots, \mathbf{z}$, are **linearly independent** if there are no values of $a, b, \ldots, c$ for which

$$a\mathbf{x}+b\mathbf{y}+\cdots+c\mathbf{z}=\mathbf{0} \tag{26.3}$$

except for $a=b=\cdots=c=0$.

In an n-dimensional vector space, there exists sets of n linearly independent vectors, but there does not exist $n+1$ linearly independent vectors.

Let $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$ be n linearly independent vectors in a n-dimensional vector space. These are known as **basis vectors**. Then, for any vector $\mathbf{x}$, we can find values $x_1, x_2, \ldots, x_n$ for which

$$x_1\mathbf{e}_1+x_2\mathbf{e}_2+\cdots+x_n\mathbf{e}_n-\mathbf{x}=\mathbf{0}\,. \tag{26.4}$$

Thus the basis vectors are complete and define a **coordinate system**. The values $x_1, x_2, \ldots, x_n$ that satisfy the above equation are the **components** of $\mathbf{x}$. That is, the vector $\mathbf{x}$ can be written in terms of its components x_i, $i=1\ldots n$, as

$$\mathbf{x}=\sum_{i=1}^{n} x_i\mathbf{e}_i\,. \tag{26.5}$$

We will find it convenient to express the components of the vector $\mathbf{x}$ as a column vector $\underline{x}=[x_i]$.

Linear Operators

A **linear operator** $\mathcal{A}$ is a map from one vector in a vector space to another

$$\mathbf{y} = \mathcal{A}\,\mathbf{x} \tag{26.6}$$

having the property

$$\mathcal{A}(a\mathbf{x} + b\mathbf{y}) = a\mathcal{A}\,\mathbf{x} + b\mathcal{A}\,\mathbf{y} \tag{26.7}$$

Linear operators do not generally commute, $\mathcal{A}\mathcal{B} \neq \mathcal{B}\mathcal{A}$. If an inverse operator $\mathcal{A}^{-1}$ exists then

$$\mathcal{A}\mathcal{A}^{-1} = \mathcal{A}^{-1}\mathcal{A} = 1\,. \tag{26.8}$$

Consider the application of a linear operator $\mathcal{A}$ to a set of basis vectors:

$$\mathbf{a}_j = \mathcal{A}\,\mathbf{e}_j\,, \quad j = 1\ldots n\,. \tag{26.9}$$

We can write these vectors in terms of their components:

$$\mathbf{a}_j = \sum_{i=1}^{n} a_{ij}\mathbf{e}_i\,, \quad j = 1\ldots n \tag{26.10}$$

where a_{ij} is the ith component of the vector $\mathbf{a}_j$ in a particular basis.

These n^2 components are sufficient to define the operator $\mathcal{A}$: for any vector $\mathbf{x}$,

$$\mathbf{y} = \mathcal{A}\,\mathbf{x} = \mathcal{A}\sum_{j=1}^{n} x_j\mathbf{e}_j = \sum_{j=1}^{n} x_j\mathcal{A}\,\mathbf{e}_j = \sum_{j=1}^{n} x_j \sum_{i=1}^{n} a_{ij}\mathbf{e}_i \tag{26.11a}$$

$$= \sum_{i=1}^{n}\left(\sum_{j=1}^{n} a_{ij}x_j\right)\mathbf{e}_i \tag{26.11b}$$

but

$$\mathbf{y} = \sum_{i=1}^{n} y_i\mathbf{e}_i \tag{26.11c}$$

thus

$$y_i = \sum_{j=1}^{n} a_{ij}x_j\,, \quad i = 1\ldots n\,. \tag{26.11d}$$

Therefore if, in some basis, we have the components $\underline{\mathrm{A}} = [a_{ij}]$ of a linear operator $\mathcal{A}$, then the components $\underline{y} = [y_i]$ of the vector $\mathbf{y} = \mathcal{A}\,\mathbf{x}$ are related to the components $\underline{x} = [x_i]$ of the vector $\mathbf{x}$ by the matrix equation

$$\underline{y} = \underline{\mathrm{A}}\,\underline{x}\,. \tag{26.12}$$

Coordinate Transformations

Suppose that we change from one set of basis vectors to another set of basis vectors by an invertable linear transformation $\mathcal{P}$

$$\mathbf{e}'_j = \mathcal{P}\,\mathbf{e}_j \qquad \text{or} \qquad \mathbf{e}'_j = \sum_{i=1}^{n} p_{ij}\mathbf{e}_i\,, \quad j = 1\ldots n\,. \tag{26.13}$$

Here $\underline{\mathrm{P}} = [p_{ij}]$ is called the **transformation matrix**.
In the new bases, a vector $\mathbf{x}$ is

$$\mathbf{x} = \sum_{i=1}^{n} x_j\mathbf{e}_j = \sum_{j=1}^{n} x'_j\mathbf{e}'_j = \sum_{j=1}^{n} x'_j \sum_{i=1}^{n} p_{ij}\mathbf{e}_i = \sum_{i=1}^{n} \underbrace{\left(\sum_{j=1}^{n} p_{ij}x'_j\right)}_{x_i}\mathbf{e}_i \tag{26.14}$$

so

$$x_i = \sum_{j=1}^{n} p_{ij}x'_j\,, \quad i = 1\ldots n \qquad \text{or} \qquad \underline{\mathrm{x}} = \underline{\mathrm{P}}\,\underline{\mathrm{x}}' \tag{26.15}$$

where we express the components as column vectors $\underline{\mathrm{x}} = [x_i]$ and $\underline{\mathrm{x}}' = [x'_i]$.

We can now determine the effect of the change of basis on the components of other linear operators. Suppose

$$\mathbf{y} = \mathcal{A}\,\mathbf{x} \tag{26.16}$$

then

$$\underline{\mathrm{y}} = \underline{\mathrm{A}}\,\underline{\mathrm{x}} \qquad \text{and} \qquad \underline{\mathrm{y}}' = \underline{\mathrm{A}}'\underline{\mathrm{x}}'\,. \tag{26.17}$$

Therefore

$$\underline{\mathrm{P}}\,\underline{\mathrm{y}}' = \underline{\mathrm{A}}(\underline{\mathrm{P}}\,\underline{\mathrm{x}}') \quad \text{or} \quad \underline{\mathrm{y}}' = \underline{\mathrm{P}}^{-1}\underline{\mathrm{A}}\,\underline{\mathrm{P}}\,\underline{\mathrm{x}}'\,. \tag{26.18}$$

We thus identify

$$\underline{\mathrm{A}}' = \underline{\mathrm{P}}^{-1}\underline{\mathrm{A}}\,\underline{\mathrm{P}}\,. \tag{26.19}$$

This is known as a **similarity transformation**.

We can apply similarity transforms to any matrix equation:

$$\underline{\mathrm{A}}\,\underline{\mathrm{B}} = \underline{\mathrm{C}} \quad \Longrightarrow \quad \underline{\mathrm{P}}^{-1}\underline{\mathrm{A}}(\underline{\mathrm{P}}\,\underline{\mathrm{P}}^{-1})\underline{\mathrm{B}}\,\underline{\mathrm{P}} = \underline{\mathrm{P}}^{-1}\underline{\mathrm{C}}\,\underline{\mathrm{P}} \quad \Longrightarrow \quad \underline{\mathrm{A}}'\underline{\mathrm{B}}' = \underline{\mathrm{C}}'\,. \tag{26.20}$$

Inner Product

A **scalar product** or **inner product** or **dot product** between two vectors

$$\mathbf{x}\cdot\mathbf{y} \tag{26.21}$$

is a scalar-valued function of the two vectors with the properties:

- Conjugate symmetry $\quad \mathbf{x}\cdot\mathbf{y}=(\mathbf{y}\cdot\mathbf{x})^*$ (26.22a)
- Linearity $\quad (a\mathbf{x}+b\mathbf{y})\cdot\mathbf{z}=a(\mathbf{x}\cdot\mathbf{z})+b(\mathbf{y}\cdot\mathbf{z})$ (26.22b)
- Positive definite $\quad \mathbf{x}\cdot\mathbf{x}>0$ for $\mathbf{x}\neq\mathbf{0}$ (26.22c)

The **length** of a vector $\mathbf{x}$ is $\|\mathbf{x}\|=(\mathbf{x}\cdot\mathbf{x})^{1/2}$.
If $\mathbf{x}\cdot\mathbf{y}=0$ then the two vectors are **orthogonal**.
The dot product of two vectors is related to their lengths and the angle θ between them by $\mathbf{x}\cdot\mathbf{y}=\|\mathbf{x}\|\,\|\mathbf{y}\|\cos\theta$.

Suppose we define the inner product in some basis as

$$\mathbf{x}\cdot\mathbf{y}=\sum_{i=1}^{n}x_i y_i^*=\underline{y}^\dagger\underline{x} \tag{26.23}$$

where x_i and y_i are the components of the vectors $\mathbf{x}$ and $\mathbf{y}$ respectively in that basis. It then follows that the basis vectors are **orthonormal** with respect to our inner product:

$$\mathbf{e}_i\cdot\mathbf{e}_j=\delta_{ij}\,. \tag{26.24}$$

If we wish to find a new orthonormal basis $\mathbf{e}'_i=\mathcal{P}\,\mathbf{e}_i$, $i=1\ldots n$, with respect to the same inner product, then

$$\delta_{ij}=\mathbf{e}'_i\cdot\mathbf{e}'_j=\left(\sum_{k=1}^{n}p_{ki}\mathbf{e}_k\right)\cdot\left(\sum_{\ell=1}^{n}p_{\ell j}\mathbf{e}_\ell\right)=\sum_{k=1}^{n}\sum_{\ell=1}^{n}p_{ki}p^*_{\ell j}\underbrace{\mathbf{e}_k\cdot\mathbf{e}_\ell}_{\delta_{k\ell}} \tag{26.25a}$$

$$=\sum_{k=1}^{n}p_{ki}p^*_{kj} \tag{26.25b}$$

or

$$\underline{1}=\underline{P}^\dagger\underline{P} \tag{26.25c}$$

so the transformation matrix must be unitary. If the vector space is real then the transformation matrix must be orthogonal.

Note that

$$\mathbf{e}'_j\cdot\mathbf{e}_i=\left(\sum_{k=1}^{n}p_{kj}\mathbf{e}_k\right)\cdot\mathbf{e}_i=\sum_{k=1}^{n}p_{kj}\underbrace{\mathbf{e}_k\cdot\mathbf{e}_i}_{\delta_{ki}}=p_{ij} \tag{26.26}$$

and since $\mathbf{e}_i$ and $\mathbf{e}'_j$ are both unit vectors, p_{ij} is the **direction cosine** between the two different basis vectors, and $\underline{P}$ is the matrix of direction cosines.

Ex. 26.1. Passive and active rotations.

Consider a vector $\mathbf{x}$ in a 2-dimensional vector space. First suppose we rotate the basis vectors as in the left panel of Fig. 26.1 so that the direction cosines are

$$\begin{aligned} p_{11} &= \mathbf{e}'_1 \cdot \mathbf{e}_1 = \cos\theta & p_{12} &= \mathbf{e}'_2 \cdot \mathbf{e}_1 = \cos(\pi/2+\theta) \\ p_{21} &= \mathbf{e}'_1 \cdot \mathbf{e}_2 = \cos(\pi/2-\theta) & p_{22} &= \mathbf{e}'_2 \cdot \mathbf{e}_2 = \cos\theta \end{aligned} \tag{26.27a}$$

or

$$\underline{\mathsf{P}} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}. \tag{26.27b}$$

Then, from Eq. (26.15), $\underline{x}' = \underline{\mathsf{P}}^{-1}\underline{x}$ and since $\underline{\mathsf{P}}^{-1} = \underline{\mathsf{P}}^{\mathsf{T}}$ (it is orthogonal)

$$\begin{bmatrix} x'_1 \\ x'_2 \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}. \tag{26.28}$$

This is known as a **passive** or **alias rotation**.

Alternatively, one could apply the linear operation $\mathcal{P}$ to the vector $\mathbf{x}$ to obtain an new vector $\mathbf{x}' = \mathcal{P}\mathbf{x}$ as shown in the right panel of Fig. 26.1. The components of $\mathbf{x}'$ in the (unchanged) basis, according to Eq. (26.12), is $\underline{x}' = \underline{\mathsf{P}}\,\underline{x}$ or

$$\begin{bmatrix} x'_1 \\ x'_2 \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}. \tag{26.29}$$

This is known as a **active** or **alabi rotation**.

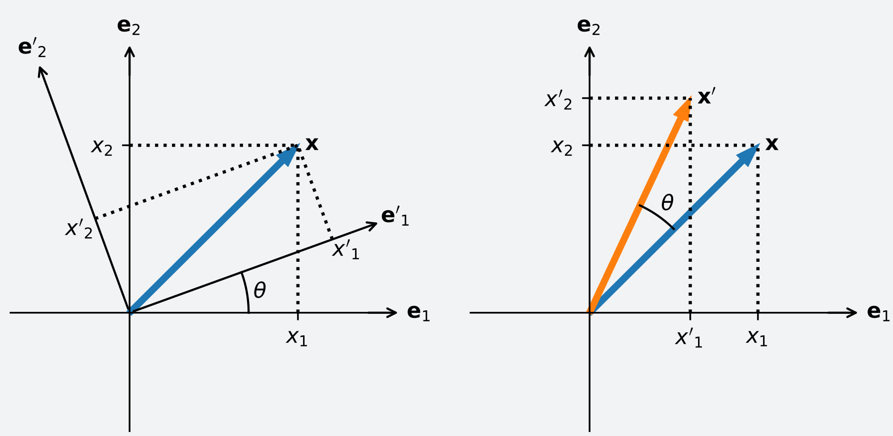


Figure 26.1: Passive or alias (left) and active or alibi (right) rotations.

Vector or Cross Product

In a 3-dimensional real vector space, a **vector product** or **cross product**

$$\mathbf{x} \times \mathbf{y} \tag{26.30}$$

is a vector-valued function of the two vectors with the properties:

- Linearity and distributivity $\quad (a\mathbf{x} + b\mathbf{y}) \times \mathbf{z} = a(\mathbf{x} \times \mathbf{z}) + b(\mathbf{y} \times \mathbf{z}) \quad$ (26.31a)
- Anticommutativity $\quad \mathbf{x} \times \mathbf{y} = -\mathbf{y} \times \mathbf{x} \quad$ (26.31b)
- **Jacobi identity** $\quad \mathbf{x} \times (\mathbf{y} \times \mathbf{z}) + \mathbf{z} \times (\mathbf{x} \times \mathbf{y}) + \mathbf{y} \times (\mathbf{z} \times \mathbf{x}) = \mathbf{0} \quad$ (26.31c)

In a particular basis it is conventional to define the cross product as

$$\mathbf{z} = \mathbf{x} \times \mathbf{y} \quad \Longleftrightarrow \quad z_i = \sum_{j=1}^{3} \sum_{k=1}^{3} \epsilon_{ijk} x_j y_k \tag{26.32a}$$

where ϵ_{ijk} is the Levi-Civita symbol, or

$$z_1 = x_2 y_3 - x_3 y_2 \,, \quad z_2 = x_3 y_1 - x_1 y_3 \,, \quad \text{and} \quad z_3 = x_1 y_2 - x_2 y_1 \,. \tag{26.32b}$$

We see that

$$\mathbf{e}_1 \times \mathbf{e}_2 = \mathbf{e}_3 \,, \quad \mathbf{e}_2 \times \mathbf{e}_3 = \mathbf{e}_1 \,, \quad \text{and} \quad \mathbf{e}_3 \times \mathbf{e}_1 = \mathbf{e}_2 \,. \tag{26.33}$$

The cross product of two vectors is orthogonal to both of those vectors: $\mathbf{x} \cdot (\mathbf{x} \times \mathbf{y}) = \mathbf{y} \cdot (\mathbf{x} \times \mathbf{y}) = 0$.

The magnitude of the cross product is related to the lengths of the two vectors and the angle θ between them by $\|\mathbf{x} \times \mathbf{y}\| = \|\mathbf{x}\| \, \|\mathbf{y}\| \sin\theta$.

The cross product of two vectors $\mathbf{x}$ and $\mathbf{y}$ gives the (directed) area of the parallelogram with sides defined by $\mathbf{x}$ and $\mathbf{y}$.

The **scalar triple product** is

$$\mathbf{x} \cdot (\mathbf{y} \times \mathbf{z}) = \mathbf{y} \cdot (\mathbf{z} \times \mathbf{x}) = \mathbf{z} \cdot (\mathbf{x} \times \mathbf{y}) = \det \begin{bmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{bmatrix} . \tag{26.34}$$

This is the volume of a parallelepiped with sides defined by $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$.

The **vector triple product** is

$$\mathbf{x} \times (\mathbf{y} \times \mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})\mathbf{y} - (\mathbf{x} \cdot \mathbf{y})\mathbf{z} \,. \tag{26.35}$$

Eigenvalue Problems

If a linear operator $\mathcal{A}$ acts on a vector $\mathbf{x}$ in such a manner that the result is proportional to $\mathbf{x}$,

$$\mathcal{A}\,\mathbf{x} = \lambda \mathbf{x}\,, \tag{26.36}$$

then λ is known as an **eigenvalue** of the operator $\mathcal{A}$ and $\mathbf{x}$ is the **eigenvector** belonging to λ.

The matrix version of the eigenvalue problem is

$$\underline{\mathrm{A}}\,\underline{\mathrm{x}} = \lambda \underline{\mathrm{x}}\,. \tag{26.37}$$

This equation can be rearranged as follows:

$$(\underline{\mathrm{A}} - \lambda \underline{1})\underline{\mathrm{x}} = \underline{0}\,. \tag{26.38}$$

Note that if $(\underline{\mathrm{A}} - \lambda \underline{1})$ is invertible then the solution is the trivial solution $\underline{\mathrm{x}} = \underline{0}$. Therefore, in order for there to be non-trivial solutions to the eigenvalue equation, $(\underline{\mathrm{A}} - \lambda \underline{1})$ must be non-invertible and so its determinant must vanish:

$$\det(\underline{\mathrm{A}} - \lambda \underline{1}) = 0\,. \tag{26.39}$$

This is called the **secular** or **characteristic equation**. The determinant will produce a polynomial in λ which is called the **characteristic polynomial** which will have n roots (not necessarily all real though). These roots are the eigenvalues. Then, for a particular eigenvalue, λ_p, the eigenvector $\underline{\mathrm{x}}_p$ that belongs to it can be determined up to an overall constant by solving

$$(\underline{\mathrm{A}} - \lambda_p \underline{1})\underline{\mathrm{x}}_p = \underline{0} \tag{26.40}$$

for the components of $\underline{\mathrm{x}}_p$. This is an underdetermined system of equations so there will be one (or more if the eigenvalue is degenerate) degrees of freedom. Normally we supplement the system of equations with one additional equation requiring the eigenvector to be normalized

$$\underline{\mathrm{x}}_p^\dagger \underline{\mathrm{x}}_p = 1\,. \tag{26.41}$$

Ex. 26.2. Consider the (active) rotation of a vector **x** through angle θ about the z-axis $\mathcal{R}_z$ described by the rotation matrix

$$\underline{\mathrm{R}}_z = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{26.42}$$

We want to solve the eigenvalue problem

$$\mathcal{R}_z\,\mathbf{x} = \lambda\mathbf{x} \qquad \text{or} \qquad \underline{\mathrm{R}}_z\underline{\mathrm{x}} = \lambda\underline{\mathrm{x}} \tag{26.43}$$

that is, we seek a vector that is left unchanged, apart from a possible scale, when rotated by θ about the z-axis. (It should be obvious what this vector is.)

The secular equation is

$$\det[\underline{\mathrm{R}}_z - \lambda\underline{1}] = (1-\lambda)[(\cos\theta-\lambda)^2 + \sin^2\theta] \tag{26.44a}$$

$$= (1-\lambda)(\lambda^2 - 2\lambda\cos\theta + 1) \tag{26.44b}$$

$$= (1-\lambda)(\lambda - e^{i\theta})(\lambda - e^{-i\theta})\,. \tag{26.44c}$$

This has one real eigenvalue, $\lambda = 1$, unless $\theta = 0$ or $\theta = \pi$. We'll come back to those at the end of the example.

To find the eigenvector for the $\lambda = 1$ eigenvalue we solve

$$\begin{bmatrix} \cos\theta - 1 & -\sin\theta & 0 \\ \sin\theta & \cos\theta - 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{26.45}$$

for which the solution is $x = y = 0$ and z is undetermined. Requiring the eigenvector to be normalized we find $z = 1$ and thus the eigenvector is $\mathbf{e}_z$.

Now for the case $\theta = 0$, $\lambda = 1$ is a triply-degenerate eigenvector. We have $\underline{\mathrm{R}}_z\big|_{\theta=0} = \underline{1}$ and it is obvious that any vector $\underline{\mathrm{x}}$ will solve the equation $\underline{1}\,\underline{\mathrm{x}} = \underline{\mathrm{x}}$. A orthonormal set of eigenvectors is $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$.

Finally for the case $\theta = \pi$, we have the usual eigenvalue $\lambda = 1$ and the eigenvector $\mathbf{e}_z$ that belongs to it but now we also have a doubly-degenerate eigenvalue $\lambda = -1$. The eigenvalue equation is

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} = - \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad \Longrightarrow \quad \begin{aligned} -x &= -x \\ -y &= -y \\ z &= -z \end{aligned} \tag{26.46}$$

for which the solution is $z = 0$ and x and y are unspecified. An orthonormal set of eigenvectors is $\mathbf{e}_x$ and $\mathbf{e}_y$. We see that any vector on the x-y plane simply changes its sign when rotated by an angle π about the z axis.

If $\underline{H} = [h_{ij}]$ is a Hermitian matrix, $\underline{H}^\dagger = \underline{H}$, with two eigenvectors $\underline{x}_p$ and $\underline{x}_q$ belonging to eigenvalues λ_p and λ_q respectively then

$$\underline{H}\,\underline{x}_p = \lambda_p \underline{x}_p \qquad \text{and} \qquad \underline{H}\,\underline{x}_q = \lambda_q \underline{x}_q\,. \tag{26.47}$$

Then we have

$$\begin{aligned}
\underline{x}_q^\dagger(\lambda_p \underline{x}_p) &= \underline{x}_q^\dagger \underline{H}\,\underline{x}_p & (26.48a)\\
&= \sum_{i=1}^{n} x_{qi}^* \sum_{j=1}^{n} h_{ij} x_{pj} & (26.48b)\\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} (x_{qi} h_{ij}^* x_{pj}^*)^* & (26.48c)\\
&= \left[\sum_{j=1}^{n} x_{pj}^* \sum_{i=1}^{n} h_{ij}^* x_{qi}\right]^* & (26.48d)\\
&= \left[\underline{x}_p^\dagger(\underline{H}^\dagger\,\underline{x}_q)\right]^* & (26.48e)\\
&= \left[\underline{x}_p^\dagger(\underline{H}\,\underline{x}_q)\right]^* & (26.48f)\\
&= \left[\underline{x}_p^\dagger(\lambda_q \underline{x}_q)\right]^*. & (26.48g)
\end{aligned}$$

Since $\underline{x}_q^\dagger \underline{x}_p = (\underline{x}_p^\dagger \underline{x}_q)^*$ we find

$$(\lambda_p - \lambda_q^*)\underline{x}_q^\dagger \underline{x}_p = 0\,. \tag{26.49}$$

- If $p = q$ and $\underline{x}_p \neq \underline{0}$ so that $\underline{x}_p^\dagger \underline{x}_p > 0$ then we have $\lambda_p = \lambda_p^*$. *The eigenvalues of a Hermitian matrix are real.*
- If $\lambda_p \neq \lambda_q$ then $\underline{x}_p^\dagger \underline{x}_q = 0$ or $\mathbf{x}_p \cdot \mathbf{x}_q = 0$. *The eigenvectors belonging to different eigenvalues of a Hermitian matrix are orthogonal.*
- If $\lambda_p = \lambda_q$ are degenerate eigenvalues then the eigenvectors belonging to them need not be orthogonal. However, a linear combination of them can be made orthogonal. Let

  $$\mathbf{u} = \mathbf{x}_p \qquad \text{and} \qquad \mathbf{v} = \mathbf{u} + \alpha \mathbf{x}_q \tag{26.50}$$

  where α is some constant. Then

  $$\mathbf{v}\cdot\mathbf{u} = 0 \quad \Longrightarrow \quad \alpha = -\frac{\mathbf{x}_q\cdot\mathbf{x}_p}{\mathbf{x}_p\cdot\mathbf{x}_p}\,. \tag{26.51}$$

  This procedure can be generalized to multiply degenerate eigenvalues and it is just the Gram-Schmidt orthogonalization described in §23.

We see that all n eigenvalues of a Hermitian operator are real, and that we can construct an orthogonal set of n eigenvectors belonging to these eigenvalues. This set of eigenvectors is also complete.

The eigenvectors $\mathbf{x}$ of a linear operator $\mathcal{A}$ do not depend on the choice of basis vectors. Suppose that in one basis we have

$$\underline{A}\,\underline{x} = \lambda\underline{x} \tag{26.52}$$

and we use a transformation matrix $\underline{P}$ to go to a different basis:

$$\underline{P}^{-1}\underline{A}\,\underline{P}\,\underline{P}^{-1}\underline{x} = \lambda\underline{P}^{-1}\underline{x} \qquad \text{or} \qquad \underline{A}'\underline{x}' = \lambda\underline{x}' \tag{26.53}$$

where $\underline{A}' = \underline{P}^{-1}\underline{A}\,\underline{P}$ and $\underline{x}' = \underline{P}^{-1}\underline{x}$. We see that the transformed column vector $\underline{x}'$ is an eigenvector of the transformed matrix $\underline{A}'$ belonging to the same eigenvalue λ.

Two other important invariants of a similarity transformation are the trace and determinant of the matrix:

$$\operatorname{Tr}\underline{A}' = \operatorname{Tr}(\underline{P}^{-1}\underline{A}\,\underline{P}) = \operatorname{Tr}(\underline{P}\,\underline{P}^{-1}\underline{A}) = \operatorname{Tr}\underline{A} \tag{26.54}$$

$$\det\underline{A}' = \det(\underline{P}^{-1}\underline{A}\,\underline{P}) = \det(\underline{P}\,\underline{P}^{-1}\underline{A}) = \det\underline{A}\,. \tag{26.55}$$

Suppose our linear operator has a complete set of orthonormal eigenvectors and suppose that we make a coordinate transformation so that the new basis vectors are these eigenvectors so that

$$\mathcal{A}\,\mathbf{e}_i' = \lambda_i\mathbf{e}_i' \quad \Longrightarrow \quad (\mathcal{A}\,\mathbf{e}_i')\cdot\mathbf{e}_j' = \lambda_i\mathbf{e}_i'\cdot\mathbf{e}_j' = \lambda_i\delta_{ij}\,. \tag{26.56}$$

However, $(\mathcal{A}\,\mathbf{e}_i')\cdot\mathbf{e}_j' = a_{ij}'$ where $\underline{A}' = [a_{ij}']$, so

$$a_{ij}' = \lambda_i\delta_{ij}\,. \tag{26.57}$$

Therefore, the coordinate transformation to the basis set by the orthonormal set of eigenvectors has diagonalized the matrix and the diagonal elements of $\underline{A}'$ are the eigenvalues.

Recall that the transformation matrix $\underline{P} = [p_{ij}]$ has elements $p_{ij} = \mathbf{e}_j'\cdot\mathbf{e}_i$ in our original (unprimed) basis, i.e., the jth column contains the components of $\mathbf{e}_j'$ (the eigenvectors) in the original basis:

$$\underline{P} = \left[\, \underline{e}_1' \,\middle|\, \underline{e}_2' \,\middle|\, \cdots \,\middle|\, \underline{e}_n' \,\right]. \tag{26.58}$$

Therefore, once a complete set of orthonormal eigenvectors of a matrix $\underline{A}$ are found, we can use them to diagonalize the matrix.

Ex. 26.3. Vibrational modes of the linear triatomic carbon dioxide molecule.

We consider only the vibrational modes along the axis of the linear triatomic molecule. Let s_1, s_2, and s_3 be the displacements away from the equilibrium positions of the leftmost oxygen atom, the carbon atom, and the rightmost oxygen atom respectively (see Fig. 26.2). The two double bonds are represented by springs with spring constant k. Newton's equations of motion are

$$m_O \frac{d^2 s_1}{dt^2} = -k(s_1 - s_2) \tag{26.59a}$$

$$m_C \frac{d^2 s_2}{dt^2} = -k(s_2 - s_3) + k(s_1 - s_2) \tag{26.59b}$$

$$m_O \frac{d^2 s_3}{dt^2} = k(s_2 - s_3)\,. \tag{26.59c}$$

Assume the motion is oscillatory with angular frequency ω and let $s_1(t) = x_1 e^{i\omega t}$, $s_2(t) = x_2 e^{i\omega t}$, and $s_3(t) = x_3 e^{i\omega t}$. Then

$$-m_O \omega^2 x_1 = -k(x_1 - x_2) \tag{26.60a}$$

$$-m_C \omega^2 x_2 = -k(-x_3 + 2x_2 - x_1) \tag{26.60b}$$

$$-m_O \omega^2 x_3 = -k(x_3 - x_2)\,. \tag{26.60c}$$

These equations can be expressed in matrix form as

$$\begin{bmatrix} 1 & -1 & 0 \\ -q & 2q & -q \\ 0 & -1 & 1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad \text{with} \quad q = \frac{m_O}{m_C} \quad \text{and} \quad \lambda = \frac{\omega^2}{k/m_O}\,. \tag{26.61}$$

This is now in the form of an eigenvalue problem where the eigenvalues λ will determine the eigenfrequencies $\omega = \sqrt{\lambda}\sqrt{k/m_O}$ and the eigenvectors will be the normal modes.

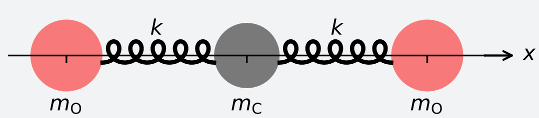


Figure 26.2: CO_2 Molecule

First we compute the eigenvalues from the secular equation

$$0 = \det\begin{bmatrix} 1-\lambda & -1 & 0 \\ -q & 2q-\lambda & -q \\ 0 & -1 & 1-\lambda \end{bmatrix} \tag{26.62a}$$

$$= (1-\lambda)[(1-\lambda)(2q-\lambda)-q]-(-1)[-q(1-\lambda)] \tag{26.62b}$$

$$= \lambda(1-\lambda)(\lambda-2q-1)\,. \tag{26.62c}$$

We see that the eigenvalues are $\lambda = 0$, $\lambda = 1$, and $\lambda = 2q+1$.

Next we find the eigenvectors belonging to these eigenfunctions.

- Case $\lambda = 0$: Solve

$$\begin{bmatrix} 1 & -1 & 0 \\ -q & 2q & -q \\ 0 & -1 & 1 \end{bmatrix}\cdot\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad\Longrightarrow\quad \begin{aligned} x_1 - x_2 &= 0 \\ -qx_1 + 2qx_2 - qx_3 &= 0 \\ -x_2 + x_3 &= 0 \end{aligned} \tag{26.63}$$

  and so we have $x_1 = x_2 = x_3$. With suitable normalization the eigenvector is $\frac{1}{\sqrt{3}}\left[\begin{smallmatrix}1\\1\\1\end{smallmatrix}\right]$.

  This is a zero-frequency mode that corresponds to rigid translation of the whole molecule along its axis as seen in the top panel of Fig. 26.3.

- Case $\lambda = 1$: Solve

$$\begin{bmatrix} 1 & -1 & 0 \\ -q & 2q & -q \\ 0 & -1 & 1 \end{bmatrix}\cdot\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad\Longrightarrow\quad \begin{aligned} \cancel{x_1} - x_2 &= \cancel{x_1} \\ -qx_1 + 2qx_2 - qx_3 &= x_2 \\ -x_2 + \cancel{x_3} &= \cancel{x_3} \end{aligned} \tag{26.64}$$

  and so we have $x_2 = 0$ and $x_1 = -x_3$. The normalized eigenvector is $\frac{1}{\sqrt{2}}\left[\begin{smallmatrix}1\\0\\-1\end{smallmatrix}\right]$.

  This is a symmetric mode of oscillation with frequency $\omega_s = \sqrt{k/m_O}$ in which the carbon atom remains stationary and the two oxygen atoms vibrate out-of-phase with each other along the axis as seen in the middle panel of Fig. 26.3.

- Case $\lambda = 2q+1$: Solve

$$\begin{bmatrix} 1 & -1 & 0 \\ -q & 2q & -q \\ 0 & -1 & 1 \end{bmatrix}\cdot\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = (2q+1)\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad\Longrightarrow\quad \begin{aligned} \cancel{x_1} - x_2 &= (2q+\cancel{1})x_1 \\ -qx_1 + \cancel{2qx_2} - qx_3 &= (\cancel{2q}+1)x_2 \\ -x_2 + \cancel{x_3} &= (2q+\cancel{1})x_3 \end{aligned} \tag{26.65}$$

  and so we have $x_1 = x_3$ and $x_2 = -2qx_1$. The eigenvector is $\frac{1}{\sqrt{4q^2+2}}\left[\begin{smallmatrix}1\\-2q\\1\end{smallmatrix}\right]$.

  This is a asymmetric mode of oscillation with frequency $\omega_a = \sqrt{2k/m_C + k/m_O}$ in which the two oxygen atoms move in phase while the carbon atom moves out of phase along the axis in such a way to preserve the center of mass as seen in the bottom panel of Fig. 26.3.

The general solution to the longitudinal motion is

$$\begin{bmatrix} s_1 \\ s_2 \\ s_3 \end{bmatrix} = (s_0 + vt)\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + a\cos(\omega_s t + \phi_s)\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} + b\cos(\omega_a t + \phi_a)\begin{bmatrix} 1 \\ -2m_O/m_C \\ 1 \end{bmatrix} \quad (26.66)$$

where a, b, s_0, v, ϕ_s, and ϕ_a are constants determined by the initial conditions. (Note: the solution to $d^2s/dt^2 = -\omega^2 s$ for $\omega = 0$ is $s = s_0 + vt$.)

For the CO_2 molecule, $m_O \approx 16$ amu and $m_C \approx 12$ amu and we find $\omega_a \approx \sqrt{3}\omega_s$.

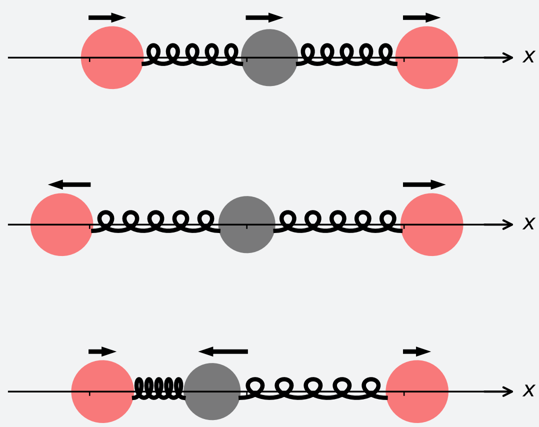


Figure 26.3: Vibration modes of the CO_2 molecule along its axis. Top: a zero-frequency rigid translation along the axis. Middle: symmetric stretching in which the oxygen atoms move out of phase and the carbon atom remains at rest. Bottom: antisymmetric stretching in which the oxygen atoms move in phase while the carbon atom moves out of phase preserving the center of mass.

27 Vector Calculus

Derivatives

Consider a scalar function of multiple variables, $\varphi(x,y,z)$. The **partial derivative** of this function with respect to x at $(x,y,z)=(a,b,c)$ is the derivative of the related univariate function $f(x)$ constructed by holding the other variables at fixed values, $y=b$ and $z=c$, $f(x)=\varphi(x,b,c)$:

$$\left.\frac{\partial\varphi(x,y,z)}{\partial x}\right|_{x=a,y=b,z=c} = \left.\frac{df(x)}{dx}\right|_{x=a} = \lim_{h\to 0}\frac{\varphi(x+h,b,c)-\varphi(x,b,c)}{h}\,. \tag{27.1}$$

The antiderivative of a partial derivative results in a "constant" of integration that is in fact a function of the remaining variables: if

$$\psi(x,y,z) = \frac{\partial\varphi(x,y,z)}{\partial x} \tag{27.2a}$$

then

$$\varphi(x,y,z) = \int \psi(x,y,z)\,dx + \chi(y,z)\,. \tag{27.2b}$$

Differentiating a function with respect to one variable and then with respect to another results in a mixed partial derivative. If all mixed partial derivatives are continuous at a point then the order with which the procedure is done does not matter:

$$\frac{\partial^2\varphi}{\partial x\partial y} = \frac{\partial^2\varphi}{\partial y\partial x}\,. \tag{27.3}$$

The **gradient** of a function $\varphi(x,y,z)$ is a **vector field** whose components are the partial derivatives of the function:

$$\boldsymbol{\nabla}\varphi(x,y,z) = \frac{\partial\varphi(x,y,z)}{\partial x}\,\mathbf{e}_x + \frac{\partial\varphi(x,y,z)}{\partial y}\,\mathbf{e}_y + \frac{\partial\varphi(x,y,z)}{\partial z}\,\mathbf{e}_z. \tag{27.4}$$

Ex. 27.1. Compute the gradient of the function of two variables

$$\varphi(x, y) = xe^{-(x^2+y^2)/2}. \tag{27.5}$$

The partial derivatives are

$$\frac{\partial\varphi(x, y)}{\partial x} = e^{-(x^2+y^2)/2} - x^2 e^{-(x^2+y^2)/2} \tag{27.6a}$$

and

$$\frac{\partial\varphi(x, y)}{\partial y} = -xye^{-(x^2+y^2)/2} \tag{27.6b}$$

so we have

$$\nabla\varphi(x, y) = (1 - x^2)e^{-(x^2+y^2)/2}\mathbf{e}_x - xye^{-(x^2+y^2)/2}\mathbf{e}_y. \tag{27.7}$$

Figure 27.1 shows a contour plot of $\varphi(x, y)$ along with the vector field $\nabla\varphi(x, y)$. Notice that the vectors are normal to the contours.

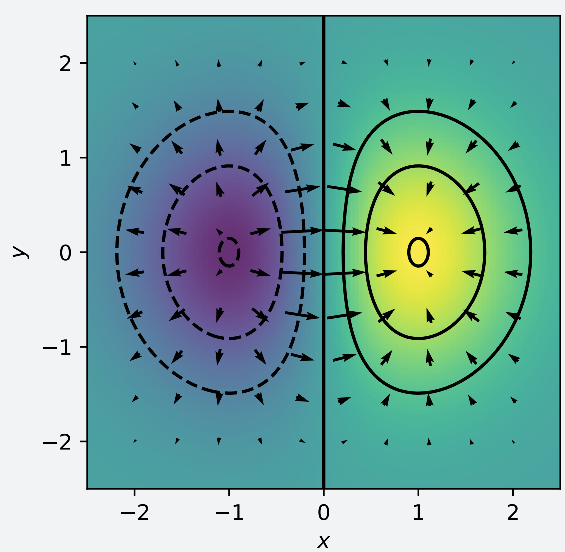


Figure 27.1: The function $\varphi(x, y) = xe^{-(x^2+y^2)/2}$ and its gradient $\nabla\varphi(x, y)$. The color density plot and with contours shows $\varphi(x, y)$ while the arrows (length and direction) represent the vector field $\nabla\varphi(x, y)$.

The gradient of a scalar function is an example of a vector field. More generally, a vector field is a vector-valued function over space of the form

$$\mathbf{A}(x,y,z) = A_x(x,y,z)\mathbf{e}_x + A_y(x,y,z)\mathbf{e}_y + A_z(x,y,z)\mathbf{e}_z \tag{27.8}$$

where $A_x(x,y,z)$, $A_y(x,y,z)$, and $A_z(x,y,z)$ are scalar functions that give the x-, y-, and z-components of a vector at each point in space.

The **divergence** of a vector field is given by

$$\begin{aligned}\nabla\cdot\mathbf{A} &= \sum_{i=1}^{3}\frac{\partial}{\partial x_i}A_i = \begin{bmatrix}\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z}\end{bmatrix}\cdot\begin{bmatrix}A_x\\A_y\\A_z\end{bmatrix}\\ &= \frac{\partial A_x}{\partial x}+\frac{\partial A_y}{\partial y}+\frac{\partial A_z}{\partial z}\,.\end{aligned} \tag{27.9}$$

The **curl** of a vector field is given by

$$\begin{aligned}\nabla\times\mathbf{A} &= \sum_{i=1}^{3}\sum_{j=1}^{3}\sum_{k=1}^{3}\epsilon_{ijk}\mathbf{e}_i\frac{\partial}{\partial x_j}A_k = \det\begin{bmatrix}\mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z\\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z}\\ A_x & A_y & A_z\end{bmatrix}\\ &= \left(\frac{\partial A_z}{\partial y}-\frac{\partial A_y}{\partial z}\right)\mathbf{e}_x+\left(\frac{\partial A_x}{\partial z}-\frac{\partial A_z}{\partial x}\right)\mathbf{e}_y+\left(\frac{\partial A_y}{\partial x}-\frac{\partial A_x}{\partial y}\right)\mathbf{e}_z\end{aligned} \tag{27.10}$$

where ϵ_{ijk} is the Levi-Civita symbol.

Figure 27.2 shows vector fields with non-zero divergence (left) and non-zero curl (right).

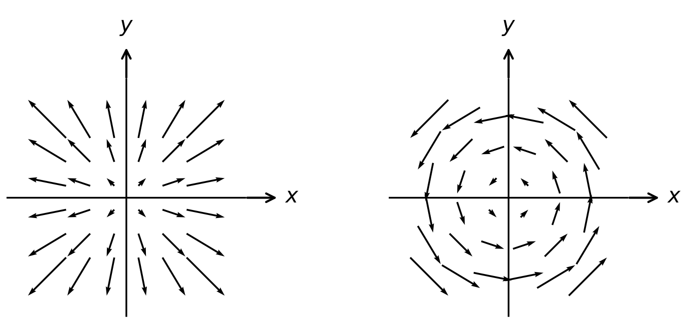


Figure 27.2: Vector fields $\mathbf{A} = x\mathbf{e}_x + y\mathbf{e}_y$ (left) and $\mathbf{A} = -y\mathbf{e}_x + x\mathbf{e}_y$ (right). The former has vanishing curl but non-vanishing divergence while the latter has vanishing divergence but non-vanishing curl.

Some useful identities involving the gradient, divergence, and curl:

- Gradient.

$$\nabla(\psi+\varphi) = \nabla\psi + \nabla\varphi \tag{27.11a}$$
$$\nabla(\psi\varphi) = \varphi\nabla\psi + \psi\nabla\varphi \tag{27.11b}$$
$$\nabla(\mathbf{A}\cdot\mathbf{B}) = (\mathbf{A}\cdot\nabla)\mathbf{B} + (\mathbf{B}\cdot\nabla)\mathbf{A} + \mathbf{A}\times(\nabla\times\mathbf{B}) + \mathbf{B}\times(\nabla\times\mathbf{A})\,. \tag{27.11c}$$

- Divergence.

$$\nabla\cdot(\mathbf{A}+\mathbf{B}) = \nabla\cdot\mathbf{A} + \nabla\cdot\mathbf{B} \tag{27.12a}$$
$$\nabla\cdot(\psi\mathbf{A}) = \psi\nabla\cdot\mathbf{A} + (\nabla\psi)\cdot\mathbf{A} \tag{27.12b}$$
$$\nabla\cdot(\mathbf{A}\times\mathbf{B}) = (\nabla\times\mathbf{A})\cdot\mathbf{B} - (\nabla\times\mathbf{B})\cdot\mathbf{A}\,. \tag{27.12c}$$

- Curl.

$$\nabla\times(\mathbf{A}+\mathbf{B}) = \nabla\times\mathbf{A} + \nabla\times\mathbf{B} \tag{27.13a}$$
$$\nabla\times(\psi\mathbf{A}) = \psi\nabla\times\mathbf{A} + (\nabla\psi)\times\mathbf{A} \tag{27.13b}$$
$$\nabla\times(\mathbf{A}\times\mathbf{B}) = \mathbf{A}(\nabla\cdot\mathbf{B}) - \mathbf{B}(\nabla\cdot\mathbf{A}) + (\mathbf{B}\cdot\nabla)\mathbf{A} - (\mathbf{A}\cdot\nabla)\mathbf{B} \tag{27.13c}$$

- Second derivatives.

$$\nabla\cdot(\nabla\times\mathbf{A}) = 0 \tag{27.14a}$$
$$\nabla\times(\nabla\psi) = \mathbf{0} \tag{27.14b}$$
$$\nabla\cdot(\nabla\psi) = \nabla^2\psi \tag{27.14c}$$
$$\nabla\times(\nabla\times\mathbf{A}) = \nabla(\nabla\cdot\mathbf{A}) - \nabla^2\mathbf{A} \tag{27.14d}$$

  where we define the scalar and vector **Laplacian** ∇^2 by

$$\nabla^2\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} \tag{27.15a}$$

  and

$$\nabla^2\mathbf{A} = (\nabla^2 A_x)\mathbf{e}_x + (\nabla^2 A_y)\mathbf{e}_y + (\nabla^2 A_z)\mathbf{e}_x\,. \tag{27.15b}$$

- Other miscellaneous results.

$$\nabla\|\mathbf{x}\| = \mathbf{x}/\|\mathbf{x}\| \tag{27.16a}$$
$$\nabla\cdot\mathbf{x} = 3 \tag{27.16b}$$
$$\nabla\times\mathbf{x} = \mathbf{0} \tag{27.16c}$$
$$(\mathbf{A}\cdot\nabla)\mathbf{x} = \mathbf{A} \tag{27.16d}$$

Integrals

A curve C is a set of points

$$C = \left\{ \mathbf{x}(t) : a \le t \le b \right\} \tag{27.17}$$

(see Fig. 27.3).

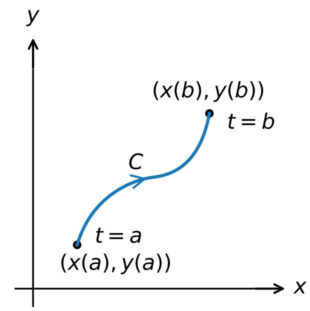


Figure 27.3: Curve in 2-Dimensions.

The directed length element along this curve is

$$d\mathbf{s} = \mathbf{x}'(t)\, dt\,. \tag{27.18}$$

A **line integral** of a scalar field $\varphi(\mathbf{x})$ is

$$\int_C \varphi(\mathbf{x})\, ds = \int_a^b \varphi(\mathbf{x}(t)) \|\mathbf{x}'(t)\|\, dt \tag{27.19}$$

which is invariant under re-parameterization of the curve.

A scalar line integral of a vector field $\mathbf{A}(\mathbf{x})$ is

$$\int_C \mathbf{A}(\mathbf{x}) \cdot d\mathbf{s} = \int_a^b \mathbf{A}(\mathbf{x}(t)) \cdot \mathbf{x}'(t)\, dt \tag{27.20}$$

and the vector line integral of the vector field is

$$\int_C \mathbf{A}(\mathbf{x}) \times d\mathbf{s} = \int_a^b \mathbf{A}(\mathbf{x}(t)) \times \mathbf{x}'(t)\, dt \tag{27.21}$$

A **double integral** of a scalar field $\varphi(x, y)$ over a domain D bounded by two functions $y = \alpha(x)$ and $y = \beta(x)$ with $a \le x \le b$ as shown in Fig. 27.4 is given by

$$\iint_D \varphi(\mathbf{x})\, d\mathcal{A} = \int_{x=a}^{x=b} \int_{y=\alpha(x)}^{y=\beta(x)} \varphi(x, y)\, dy\, dx\,. \tag{27.22}$$

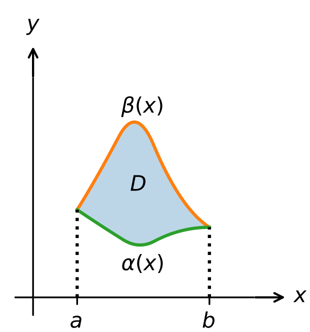


Figure 27.4: Double Integral

This generalizes to **volume integrals** with $\alpha(x, y) \le z \le \beta(x, y)$ and (x, y) in D:

$$\iiint_V \varphi(\mathbf{x})\, dV = \iint_D \int_{z=\alpha(x,y)}^{\beta(x,y)} \varphi(x, y, z)\, dz\, dx\, dy \tag{27.23}$$

and so on for higher dimensional integrals.

A change of variables from $\mathbf{x}$ to $\mathbf{q}$ specified by $\mathbf{x}(\mathbf{q})$ can be performed. In doing so, the volume element $dx\,dy\,dz$ must also be transformed:

$$\iiint_V \varphi(\mathbf{x})\,dV = \iiint_V \varphi(\mathbf{x}(\mathbf{q}))\rho(\mathbf{q})\,dq_1\,dq_2\,dq_3 \tag{27.24}$$

where $\rho(\mathbf{q})$ is a density that we now determine. Consider a volume element that is a parallelepiped formed by three vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, with displacements dq_1, dq_2, and dq_3 along the q_1-, q_2-, and q_3-axes respectively:

$$\mathbf{a} = dq_1\left(\frac{\partial x}{\partial q_1}\mathbf{e}_x + \frac{\partial y}{\partial q_1}\mathbf{e}_y + \frac{\partial z}{\partial q_1}\mathbf{e}_z\right) \tag{27.25a}$$

$$\mathbf{b} = dq_2\left(\frac{\partial x}{\partial q_2}\mathbf{e}_x + \frac{\partial y}{\partial q_2}\mathbf{e}_y + \frac{\partial z}{\partial q_2}\mathbf{e}_z\right) \tag{27.25b}$$

and

$$\mathbf{c} = dq_3\left(\frac{\partial x}{\partial q_3}\mathbf{e}_x + \frac{\partial y}{\partial q_3}\mathbf{e}_y + \frac{\partial z}{\partial q_3}\mathbf{e}_z\right). \tag{27.25c}$$

The volume of this parallelepiped is $\det\begin{bmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{bmatrix}$:

$$dV = \det\begin{bmatrix} \frac{\partial x}{\partial q_1}dq_1 & \frac{\partial y}{\partial q_1}dq_1 & \frac{\partial z}{\partial q_1}dq_1 \\ \frac{\partial x}{\partial q_2}dq_2 & \frac{\partial y}{\partial q_2}dq_2 & \frac{\partial z}{\partial q_2}dq_2 \\ \frac{\partial x}{\partial q_3}dq_3 & \frac{\partial y}{\partial q_3}dq_3 & \frac{\partial z}{\partial q_3}dq_3 \end{bmatrix} = \det(\underline{\mathsf{J}})\,dq_1\,dq_2\,dq_3\,. \tag{27.26}$$

where we define the **Jacobian matrix**

$$\underline{\mathsf{J}} = \begin{bmatrix} \frac{\partial x}{\partial q_1} & \frac{\partial y}{\partial q_1} & \frac{\partial z}{\partial q_1} \\ \frac{\partial x}{\partial q_2} & \frac{\partial y}{\partial q_2} & \frac{\partial z}{\partial q_2} \\ \frac{\partial x}{\partial q_3} & \frac{\partial y}{\partial q_3} & \frac{\partial z}{\partial q_3} \end{bmatrix} \tag{27.27}$$

and then we have $\rho(\mathbf{q}) = \det(\underline{\mathsf{J}})$ and so

$$\iiint_V \varphi(\mathbf{x})\,dV = \iiint_V \varphi(\mathbf{x}(\mathbf{q}))\det(\underline{\mathsf{J}})\,dq_1\,dq_2\,dq_3\,. \tag{27.28}$$

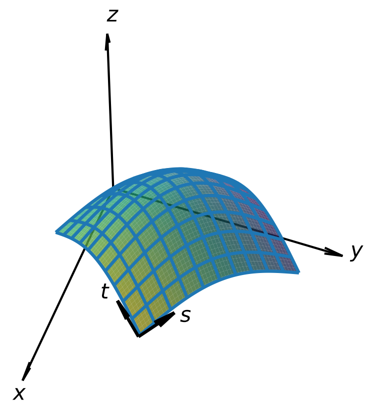


Figure 27.5: Surface

A surface S is a set of points

$$S = \left\{ \mathbf{x}(s,t) : (s,t) \in D \right\} \tag{27.29}$$

for some domain D (see Fig. 27.5).

A directed surface area element of a parallelogram with sides given by vectors **a** and **b** with displacements ds and dt along the s- and t-directions is given by

$$d\mathbf{S} = \mathbf{a} \times \mathbf{b} = \frac{\partial \mathbf{x}}{\partial s} \times \frac{\partial \mathbf{x}}{\partial t}\, ds\, dt. \tag{27.30}$$

The **surface integral** of a scalar field $\varphi(\mathbf{x})$ is

$$\iint_S \varphi(\mathbf{x})\, dS = \iint_S \varphi(\mathbf{x}(s,t)) \left\| \frac{\partial \mathbf{x}}{\partial s} \times \frac{\partial \mathbf{x}}{\partial t} \right\| ds\, dt. \tag{27.31}$$

A scalar surface integral of a vector field $\mathbf{A}(\mathbf{x})$ is

$$\iint_S \mathbf{A}(\mathbf{x}) \cdot d\mathbf{S} = \iint_S \mathbf{A}(\mathbf{x}(s,t)) \cdot \left(\frac{\partial \mathbf{x}}{\partial s} \times \frac{\partial \mathbf{x}}{\partial t} \right) ds\, dt. \tag{27.32}$$

A vector surface integral of a vector field $\mathbf{A}(\mathbf{x})$ is

$$\iint_S \mathbf{A}(\mathbf{x}) \times d\mathbf{S} = \iint_S \mathbf{A}(\mathbf{x}(s,t)) \times \left(\frac{\partial \mathbf{x}}{\partial s} \times \frac{\partial \mathbf{x}}{\partial t} \right) ds\, dt. \tag{27.33}$$

If we parameterize our surface as $z = z(x,y)$ where (x,y) is in a domain D on the x-y plane then we have

$$\frac{\partial \mathbf{x}}{\partial x} \times \frac{\partial \mathbf{x}}{\partial y} = \left(\mathbf{e}_x + \frac{\partial z}{\partial x} \mathbf{e}_z \right) \times \left(\mathbf{e}_y + \frac{\partial z}{\partial y} \mathbf{e}_z \right) = -\frac{\partial z}{\partial x} \mathbf{e}_x - \frac{\partial z}{\partial y} \mathbf{e}_y + \mathbf{e}_z \tag{27.34}$$

and then we find

$$\iint_S \mathbf{A} \cdot d\mathbf{S} = \iint_D \left(-A_x \frac{\partial z}{\partial x} - A_y \frac{\partial z}{\partial y} + A_z \right) dx\, dy. \tag{27.35}$$

Ex. 27.2. Area of a unit sphere.

A unit sphere is parameterized by a polar angle θ and an azimuthal angle ϕ as

$$\mathrm{x}(\theta,\phi) = \sin\theta\cos\phi\,\mathbf{e}_x + \sin\theta\sin\phi\,\mathbf{e}_y + \cos\theta\,\mathbf{e}_z\,, \quad 0 \le \theta \le \pi\,,\, 0 \le \phi \le 2\pi\,. \tag{27.36}$$

We have

$$\frac{\partial \mathrm{x}}{\partial\theta} = \cos\theta\cos\phi\,\mathbf{e}_x + \cos\theta\sin\phi\,\mathbf{e}_y - \sin\theta\,\mathbf{e}_z \tag{27.37a}$$

and

$$\frac{\partial \mathrm{x}}{\partial\phi} = -\sin\theta\sin\phi\,\mathbf{e}_x + \sin\theta\cos\phi\,\mathbf{e}_y \tag{27.37b}$$

so

$$\frac{\partial \mathrm{x}}{\partial\theta} \times \frac{\partial \mathrm{x}}{\partial\phi} = \sin^2\theta\cos\phi\,\mathbf{e}_x + \sin^2\theta\sin\phi\,\mathbf{e}_y + \sin\theta\cos\theta\,\mathbf{e}_z \tag{27.37c}$$

and

$$\left\|\frac{\partial \mathrm{x}}{\partial\theta} \times \frac{\partial \mathrm{x}}{\partial\phi}\right\| = \sqrt{\sin^4\theta\cos^2\phi + \sin^4\theta\sin^2\phi + \sin^2\theta\cos^2\theta} = \sin\theta\,. \tag{27.37d}$$

The area of the sphere is thus

$$A = \int_S dS = \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} \sin\theta\,d\theta\,d\phi = 4\pi\,. \tag{27.38}$$

Green's theorem

Consider two scalar fields in two dimensions, $\varphi(x, y)$ and $\psi(x, y)$ defined over a domain D with boundary given by the closed curve C. We write the boundary as $C = \partial D$. Then

$$\oint_{\partial D} (\varphi\, dx + \psi\, dy) = \iint_D \left(\frac{\partial \psi}{\partial x} - \frac{\partial \varphi}{\partial y} \right) dx\, dy \tag{27.39}$$

where the line integral over the boundary is taken in a counter-clockwise sense.

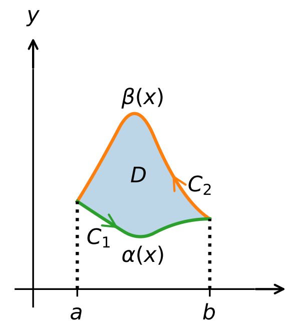


Figure 27.6: Green's Theorem

Proof. The domain D is given by

$$D = \Big\{ (x, y) : a \le x \le b\,,\; \alpha(x) \le y \le \beta(x) \Big\} \tag{27.40}$$

and let the boundary of this domain be divided into two curves, $\partial D = C = C_1 + C_2$ where C_1 is given by $\alpha(x)$ and C_2 is given by $\beta(x)$ and note that the second curve is traversed from $x = b$ to $x = a$ as shown in Fig. 27.6. We have

$$\oint_C \varphi\, dx = \int_{C_1} \varphi(x, y)\, dx + \int_{C_2} \varphi(x, y)\, dx \tag{27.41a}$$

$$= \int_a^b \varphi(x, \alpha(x))\, dx + \int_b^a \varphi(x, \beta(x))\, dx \tag{27.41b}$$

$$= \int_a^b \varphi(x, \alpha(x))\, dx - \int_a^b \varphi(x, \beta(x))\, dx\,. \tag{27.41c}$$

Also,

$$\iint_D \frac{\partial \varphi}{\partial y}\, dx\, dy = \int_{x=a}^{b} \int_{y=\alpha(x)}^{\beta(x)} \frac{\partial \varphi(x, y)}{\partial y}\, dx\, dy \tag{27.42a}$$

$$= \int_a^b \left[\varphi(x, \beta(x)) - \varphi(x, \alpha(x)) \right] dx\,. \tag{27.42b}$$

We thus see that

$$\oint_C \varphi\, dx = -\iint_D \frac{\partial \varphi}{\partial y}\, dx\, dy\,. \tag{27.43}$$

Similarly, if D is taken to be bounded by two functions of y and roles of x and y are interchanged in the above argument, we have

$$\oint_C \psi\, dy = \iint_D \frac{\partial \psi}{\partial x}\, dx\, dy\,. \tag{27.44}$$

Combining this with the previous result proves Green's theorem. □

Stokes's theorem

Green's theorem is a special case of the more general **Stokes's theorem:** if $\mathbf{F}(\mathbf{x})$ is a vector field and S is a surface with boundary ∂S then

$$\oint_{\partial S} \mathbf{F}\cdot d\mathbf{s} = \iint_S (\nabla\times\mathbf{F})\cdot d\mathbf{S}\,. \qquad (27.45)$$

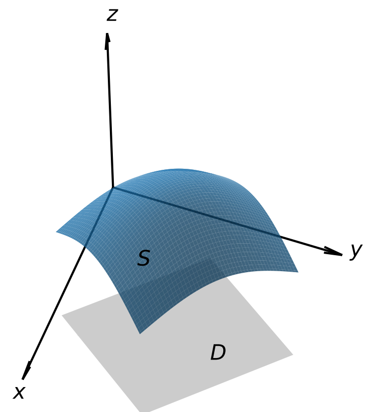


Figure 27.7: Stokes's Theorem

Proof. Suppose the surface S is given by $z = z(x,y)$ with (x,y) in the domain D as shown in Fig. 27.7. Then we have

$$\oint_{\partial S} \mathbf{F}\cdot d\mathbf{s} = \int_a^b \left(F_x\frac{dx}{dt} + F_y\frac{dy}{dt} + F_z\frac{dz}{dt}\right) dt \qquad (27.46)$$

but

$$\frac{dz}{dt} = \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt} \qquad (27.47)$$

so

$$\oint_{\partial S} \mathbf{F}\cdot d\mathbf{s} = \int_a^b \left[\left(F_x + F_z\frac{\partial z}{\partial x}\right)\frac{dx}{dt} + \left(F_y + F_z\frac{\partial z}{\partial y}\right)\frac{dy}{dt}\right] \qquad (27.48a)$$

$$= \int_D \Bigg[\underbrace{\left(F_x + F_z\frac{\partial z}{\partial x}\right)}_{\varphi(x,y)} dx + \underbrace{\left(F_y + F_z\frac{\partial z}{\partial y}\right)}_{\psi(x,y)} dy\Bigg] \qquad (27.48b)$$

where we define

$$\varphi(x,y) = F_x(x,y,z(x,y)) + F_z(x,y,z(x,y))\frac{\partial z(x,y)}{\partial x} \qquad (27.49a)$$

and

$$\psi(x,y) = F_y(x,y,z(x,y)) + F_z(x,y,z(x,y))\frac{\partial z(x,y)}{\partial y} \qquad (27.49b)$$

and now employ Green's theorem

$$\oint_{\partial S} \mathbf{F}\cdot d\mathbf{s} = \iint_D \left(\frac{\partial\psi}{\partial x} - \frac{\partial\varphi}{\partial y}\right) dx\,dy\,. \qquad (27.50)$$

Now

$$\frac{\partial\psi}{\partial x}-\frac{\partial\varphi}{\partial y}=\left(\frac{\partial F_y}{\partial x}+\frac{\partial F_y}{\partial z}\frac{\partial z}{\partial x}+\frac{\partial F_z}{\partial x}\frac{\partial z}{\partial y}+\frac{\partial F_z}{\cancel{\partial z}}\frac{\partial z}{\partial x}\cancel{\frac{\partial z}{\partial y}}+F_z\cancel{\frac{\partial^2 z}{\partial x\partial y}}\right)$$
$$-\left(\frac{\partial F_x}{\partial y}+\frac{\partial F_x}{\partial z}\frac{\partial z}{\partial y}+\frac{\partial F_z}{\partial y}\frac{\partial z}{\partial x}+\frac{\partial F_z}{\cancel{\partial z}}\frac{\partial z}{\partial y}\cancel{\frac{\partial z}{\partial x}}+F_z\cancel{\frac{\partial^2 z}{\partial y\partial x}}\right) \quad (27.51)$$

so we have

$$\oint_{\partial S}\mathbf{F}\cdot d\mathbf{s} = \iint_D\left[-\underbrace{\left(\frac{\partial F_z}{\partial y}-\frac{\partial F_y}{\partial z}\right)}_{A_x}\frac{\partial z}{\partial x}-\underbrace{\left(\frac{\partial F_x}{\partial z}-\frac{\partial F_z}{\partial y}\right)}_{A_y}\frac{\partial z}{\partial y}+\underbrace{\left(\frac{\partial F_y}{\partial x}-\frac{\partial F_x}{\partial y}\right)}_{A_z}\right]dx\,dy\,. \quad (27.52)$$

Here we have identified the components of the vector $\mathbf{A}=\nabla\times\mathbf{F}$.

Comparing this with Eq. (27.35) we arrive at

$$\oint_{\partial S}\mathbf{F}\cdot d\mathbf{s}=\iint_S(\nabla\times\mathbf{F})\cdot d\mathbf{S}\,. \quad (27.53)$$

□

Ex. 27.3. Conservative fields.

Suppose $\mathbf{F}$ is a curl-free vector field, $\nabla\times\mathbf{F}=\mathbf{0}$. Suppose C is any closed curve and let S be a surface whose boundary is C. Then, by Stokes's theorem

$$\oint_C\mathbf{F}\cdot d\mathbf{s}=0\,. \quad (27.54)$$

From this result it is easy to show that line integral of $\mathbf{F}$ depends only on the endpoints. We say that such a field $\mathbf{F}$ is a **conservative vector field**.

It can also be shown that if $\mathbf{F}$ is a conservative field then it is the gradient of some function. Suppose C is a curve from $(0,0,0)$ to (x,y,z) and define

$$-\varphi(x,y,z)=\int_C\mathbf{F}\cdot d\mathbf{s}\,. \quad (27.55)$$

Let C be three straight lines connecting the points $(0,0,0)$, $(x,0,0)$, $(x,y,0)$, and (x,y,z):

$$-\varphi(x,y,z)=\int_0^x F_x(t,0,0)\,dt+\int_0^y F_y(x,t,0)\,dt+\int_0^z F_z(x,y,t)\,dt\,. \quad (27.56)$$

Clearly $-\partial\varphi/\partial z=F_z$. Permuting x, y, and z we see $\mathbf{F}=-\nabla\varphi$.

Since $\nabla\times\nabla\varphi=\mathbf{0}$ it follows that $\nabla\times\mathbf{F}=\mathbf{0} \iff \mathbf{F}=-\nabla\varphi$.

Gauss's theorem

Consider a vector field $\mathbf{F}(\mathbf{x})$ defined in a volume V which has a boundary that is a closed surface $S = \partial V$. Then

$$\oiint_{\partial V} \mathbf{F} \cdot d\mathbf{S} = \iiint_V \boldsymbol{\nabla} \cdot \mathbf{F}\, dV\,. \qquad (27.57)$$

Here we assume that directed surface elements are directed outwards from the volume. This is known as **Gauss's theorem** or the **divergence theorem**.

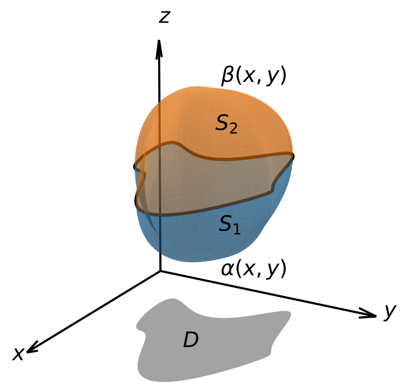


Figure 27.8: Gauss's Theorem

Proof. Let $\mathbf{F} = \varphi\,\mathbf{e}_x + \chi\,\mathbf{e}_y + \psi\,\mathbf{e}_z$. Then Gauss's theorem becomes

$$\oiint_{\partial V} \varphi\,\mathbf{e}_x \cdot d\mathbf{S} + \oiint_{\partial V} \chi\,\mathbf{e}_y \cdot d\mathbf{S} + \oiint_{\partial V} \psi\,\mathbf{e}_z \cdot d\mathbf{S} = \iiint_V \frac{\partial \varphi}{\partial x}\, dV + \iiint_V \frac{\partial \chi}{\partial y}\, dV + \iiint_V \frac{\partial \psi}{\partial z}\, dV\,. \qquad (27.58)$$

Let the volume be (see Fig. 27.8)

$$V = \Big\{(x, y, z) : (x, y) \in D\,,\ \alpha(x, y) \le z \le \beta(x, y)\Big\} \qquad (27.59)$$

which is bounded by a lower surface S_1 with $z = \alpha(x, y)$ for (x, y) in D and an upper surface S_2 with $z = \beta(x, y)$ for (x, y) in D so that $S_1 + S_2 = \partial V$.

Consider

$$\oiint_{\partial V} \psi\,\mathbf{e}_z \cdot d\mathbf{S} = \iint_{S_1} \psi\,\mathbf{e}_z \cdot d\mathbf{S} + \iint_{S_2} \psi\,\mathbf{e}_z \cdot d\mathbf{S} \qquad (27.60a)$$

$$= -\iint_D \psi(x, y, \alpha(x, y))\, dx\, dy + \iint_D \psi(x, y, \beta(x, y))\, dx\, dy \qquad (27.60b)$$

where the minus sign arises because $\mathbf{e}_z \cdot d\mathbf{S}$ is negative on the lower surface.

Now consider

$$\iiint_V \frac{\partial \psi}{\partial z}\, dV = \iint_R \int_{z=\alpha(x,y)}^{\beta(x,y)} \frac{\partial \psi}{\partial z}\, dz\, dx\, dy \qquad (27.61a)$$

$$= \iint_D \Big[\psi(x, y, \beta(x, y)) - \psi(x, y, \alpha(x, y))\Big]\, dx\, dy\,. \qquad (27.61b)$$

Thus we have

$$\oiint_{\partial V} \psi\,\mathbf{e}_z \cdot d\mathbf{S} = \iiint_V \frac{\partial \psi}{\partial z}\, dV\,. \qquad (27.62)$$

A similar argument for the x- and y-components completes the proof. □

Ex. 27.4. Gauss's law can be expressed as follows: if V is some volume and x_0 is some vector then

$$\oiint_{\partial V} \frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3} \cdot d\mathbf{S} = \begin{cases} 4\pi & \text{if } \mathrm{x}_0 \in V \\ 0 & \text{otherwise.} \end{cases} \tag{27.63}$$

To show this, use Gauss's theorem

$$\oiint_{\partial V} \frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3} \cdot d\mathbf{S} = \iiint_V \boldsymbol{\nabla}\cdot\left(\frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3}\right) dV\,. \tag{27.64}$$

It is straightforward to show that

$$\boldsymbol{\nabla}\cdot\left(\frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3}\right) = 0 \quad \text{for } \mathrm{x} \neq \mathrm{x}_0 \tag{27.65}$$

which proves the case for $\mathrm{x}_0 \notin V$.

Now consider a spherical ball V_ϵ, $\|\mathrm{x}-\mathrm{x}_0\| < \epsilon$, which is a ball of radius ϵ centered on x_0:

$$\iiint_{V_\epsilon} \boldsymbol{\nabla}\cdot\left(\frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3}\right) dV = \oiint_{\partial V_\epsilon} \frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3} \cdot d\mathbf{S} = \oiint_{\partial V_\epsilon} \frac{\epsilon^2}{\epsilon^4}\, dS = 4\pi \tag{27.66}$$

since the normal to the ∂V_ϵ is $(\mathrm{x}-\mathrm{x}_0)/\epsilon$ and the area of the surface is $4\pi\epsilon^2$.
Taking the limit $\epsilon \to 0$ we obtain the identity

$$\boldsymbol{\nabla}\cdot\left(\frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3}\right) = 4\pi\delta^3(\mathrm{x}-\mathrm{x}_0) \tag{27.67}$$

where the three-dimensional Dirac delta function is

$$\delta^3(\mathrm{x}) = \delta(x)\delta(y)\delta(z)\,. \tag{27.68}$$

Also, since

$$\frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3} = -\boldsymbol{\nabla}\frac{1}{\|\mathrm{x}-\mathrm{x}_0\|} \tag{27.69}$$

we have the identity

$$\nabla^2 \frac{1}{\|\mathrm{x}-\mathrm{x}_0\|} = -4\pi\delta^3(\mathrm{x}-\mathrm{x}_0)\,. \tag{27.70}$$

Therefore, for the case $\mathrm{x}_0 \in V$, let $V' = V - V_\epsilon$ be the volume with an infinitesimal ball about x_0 removed and we have

$$\oiint_{\partial V} \frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3} \cdot d\mathbf{S} = \underbrace{\iiint_{V'} \boldsymbol{\nabla}\cdot\left(\frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3}\right) dV}_{0 \text{ since } \mathrm{x}_0 \notin V'} + \underbrace{\iiint_{V_\epsilon} \boldsymbol{\nabla}\cdot\left(\frac{\mathrm{x}-\mathrm{x}_0}{\|\mathrm{x}-\mathrm{x}_0\|^3}\right) dV}_{4\pi} \tag{27.71a}$$

$$= 4\pi\,. \tag{27.71b}$$

In electrostatics, Coulomb's law states that the force on a charge q at position $\mathbf{x}$ produced by another charge q_0 at position $\mathbf{x}_0$ is

$$\mathbf{F} = \frac{q q_0}{4\pi\epsilon_0} \frac{\mathbf{x}-\mathbf{x}_0}{\|\mathbf{x}-\mathbf{x}_0\|^3} \tag{27.72}$$

where ϵ_0 is the permittivity of free space. Define the electric field $\mathbf{E} = \mathbf{F}/q$ so

$$\mathbf{E}(\mathbf{x}) = \frac{q_0}{4\pi\epsilon_0} \frac{\mathbf{x}-\mathbf{x}_0}{\|\mathbf{x}-\mathbf{x}_0\|^3}\,. \tag{27.73}$$

Then Gauss's law has the more familiar form

$$\oiint_{\partial V} \mathbf{E}(\mathbf{x}) \cdot d\mathbf{S} = \begin{cases} q_0/\epsilon_0 & \text{if } q_0 \text{ is contained in } V \\ 0 & \text{otherwise.} \end{cases} \tag{27.74}$$

In addition we have

$$\nabla \cdot \mathbf{E}(\mathbf{x}) = \frac{q_0}{\epsilon_0} \delta^3(\mathbf{x}-\mathbf{x}_0)\,. \tag{27.75}$$

A continuous charge distribution $\rho(\mathbf{x})$ can be thought of as a sum over point charges in the neighborhood of $\mathbf{x}$. Since the Coulomb forces combine as a linear vector sum, we can write

$$\mathbf{E}(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \sum_{n=1}^{N} q_i \frac{\mathbf{x}-\mathbf{x}_i}{\|\mathbf{x}-\mathbf{x}_i\|^3} = \frac{1}{4\pi\epsilon_0} \iiint \rho(\mathbf{x}') \frac{\mathbf{x}-\mathbf{x}'}{\|\mathbf{x}-\mathbf{x}'\|^3}\, dV' \tag{27.76}$$

and

$$\begin{aligned} \nabla \cdot \mathbf{E}(\mathbf{x}) &= \frac{1}{4\pi\epsilon_0} \iiint \rho(\mathbf{x}') \nabla \cdot \left(\frac{\mathbf{x}-\mathbf{x}'}{\|\mathbf{x}-\mathbf{x}'\|^3} \right) dV' && (27.77\text{a}) \\ &= \frac{1}{4\pi\epsilon_0} \iiint \rho(\mathbf{x}') 4\pi \delta^3(\mathbf{x}-\mathbf{x}')\, dV' && (27.77\text{b}) \\ &= \frac{\rho(\mathbf{x})}{\epsilon_0} && (27.77\text{c}) \end{aligned}$$

which is also known as Gauss's law.

Now Gauss's theorem results in the following form of Gauss's law:

$$\oiint_{\partial V} \mathbf{E}(\mathbf{x}) \cdot d\mathbf{S} = \iiint_V \nabla \cdot \mathbf{E}(\mathbf{x})\, dV = \iiint_V \rho(\mathbf{x})\, dV = Q \tag{27.78}$$

where Q is the total charge contained in V.

Green's identities and other useful identities

From the divergence theorem with $\mathbf{F} = \psi \boldsymbol{\nabla} \varphi$ we obtain **Green's first identity**

$$\oiint_{\partial V} \psi \boldsymbol{\nabla} \varphi \cdot d\mathbf{S} = \iiint_V (\psi \nabla^2 \varphi + \boldsymbol{\nabla} \varphi \cdot \boldsymbol{\nabla} \psi)\, dV \tag{27.79a}$$

and from this we obtain **Green's second identity**

$$\oiint_{\partial V} (\psi \boldsymbol{\nabla} \varphi - \varphi \boldsymbol{\nabla} \psi) \cdot d\mathbf{S} = \iiint_V (\psi \nabla^2 \varphi - \varphi \nabla^2 \psi)\, dV\,. \tag{27.79b}$$

Other useful identities are

$$\oiint_{\partial V} \varphi\, d\mathbf{S} = \iiint_V \boldsymbol{\nabla} \varphi\, dV \tag{27.80a}$$

$$\oiint_{\partial V} \mathbf{A} \times d\mathbf{S} = -\iiint_V \boldsymbol{\nabla} \times \mathbf{A}\, dV \tag{27.80b}$$

$$\oint_{\partial S} \varphi\, d\mathbf{s} = -\iint_S \boldsymbol{\nabla} \varphi \times d\mathbf{S}\,. \tag{27.80c}$$

Integration by parts for volume gives the rule

$$\iiint_V \mathbf{A} \cdot \boldsymbol{\nabla} \varphi\, dV = \oiint_{\partial V} \varphi \mathbf{A} \cdot d\mathbf{S} - \iiint_V \varphi \boldsymbol{\nabla} \cdot \mathbf{A}\, dV \tag{27.81a}$$

or, written the other way,

$$\iiint_V \varphi \boldsymbol{\nabla} \cdot \mathbf{A}\, dV = \oiint_{\partial V} \varphi \mathbf{A} \cdot d\mathbf{S} - \iiint_V \mathbf{A} \cdot \boldsymbol{\nabla} \varphi\, dV\,. \tag{27.81b}$$

Helmholtz's theorem

Any vector $\mathbf{F}(\mathbf{x})$ defined in a volume V can be decomposed as

$$\mathbf{F}(\mathbf{x}) = -\boldsymbol{\nabla}\varphi(\mathbf{x}) + \boldsymbol{\nabla}\times\mathbf{A}(\mathbf{x}) \tag{27.82a}$$

where

$$\varphi(\mathbf{x}) = \frac{1}{4\pi}\iiint_V \frac{\boldsymbol{\nabla}'\cdot\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV' - \frac{1}{4\pi}\oiint_{\partial V}\frac{\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\cdot d\mathbf{S}' \tag{27.82b}$$

$$\mathbf{A}(\mathbf{x}) = \frac{1}{4\pi}\iiint_V \frac{\boldsymbol{\nabla}'\times\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV' + \frac{1}{4\pi}\oiint_{\partial V}\frac{\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\times d\mathbf{S}' \tag{27.82c}$$

and $\boldsymbol{\nabla}'$ is the gradient operator acting on $\mathbf{x}'$. If V is all space and $\mathbf{F}$ vanishes faster than $1/\|\mathbf{x}\|$ as $\|\mathbf{x}\|\to\infty$ then the surface terms vanish.

Since $\boldsymbol{\nabla}\times\boldsymbol{\nabla}\varphi = \mathbf{0}$ and $\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\mathbf{A}) = 0$, Helmholtz's theorem implies any vector field can be decomposed into a **longitudinal** field $\mathbf{F}_L$ and a **transverse** field $\mathbf{F}_T$

$$\mathbf{F}(\mathbf{x}) = \mathbf{F}_L(\mathbf{x}) + \mathbf{F}_T(\mathbf{x}) \quad \text{where} \quad \boldsymbol{\nabla}\times\mathbf{F}_L(\mathbf{x}) = \mathbf{0} \quad \text{and} \quad \boldsymbol{\nabla}\cdot\mathbf{F}_T(\mathbf{x}) = 0\,. \tag{27.83}$$

Proof. We now prove Helmholtz's theorem:

$$\mathbf{F}(\mathbf{x}) = \iiint_V \mathbf{F}(\mathbf{x}')\delta^3(\mathbf{x}-\mathbf{x}')\,dV' \tag{27.84a}$$

$$= \iiint_V \mathbf{F}(\mathbf{x}')\left(-\frac{1}{4\pi}\nabla^2\frac{1}{\|\mathbf{x}-\mathbf{x}'\|}\right)dV' \tag{27.84b}$$

$$= \nabla^2\frac{1}{4\pi}\iiint_V \frac{\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV' \tag{27.84c}$$

$$= \boldsymbol{\nabla}\underbrace{\left(\boldsymbol{\nabla}\cdot\frac{1}{4\pi}\iiint_V\frac{\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV'\right)}_{\varphi(\mathbf{x})} - \boldsymbol{\nabla}\times\underbrace{\left(\boldsymbol{\nabla}\times\frac{1}{4\pi}\iiint_V\frac{\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV'\right)}_{-\mathbf{A}(\mathbf{x})} \tag{27.84d}$$

Now

$$\varphi(\mathbf{x}) = \boldsymbol{\nabla}\cdot\frac{1}{4\pi}\iiint_V\frac{\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV' \tag{27.85a}$$

$$= \frac{1}{4\pi}\iiint_V \mathbf{F}(\mathbf{x}')\cdot\boldsymbol{\nabla}\frac{1}{\|\mathbf{x}-\mathbf{x}'\|}\,dV' \tag{27.85b}$$

$$= -\frac{1}{4\pi}\iiint_V \mathbf{F}(\mathbf{x}')\cdot\boldsymbol{\nabla}'\frac{1}{\|\mathbf{x}-\mathbf{x}'\|}\,dV' \tag{27.85c}$$

since $\boldsymbol{\nabla}\dfrac{1}{\|\mathbf{x}-\mathbf{x}'\|} = -\boldsymbol{\nabla}'\dfrac{1}{\|\mathbf{x}-\mathbf{x}'\|}$ and now use the integration by parts rule

$$= -\oiint_{\partial V}\frac{\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\cdot d\mathbf{S} + \iiint_V\frac{\boldsymbol{\nabla}'\cdot\mathbf{F}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV' \tag{27.85d}$$

A similar manipulation for $\mathbf{A}(\mathbf{x})$ completes the proof. □

Uniqueness.

If both $\nabla\cdot\mathbf{F}$ and $\nabla\times\mathbf{F}$ are specified in V as well as the normal component of $\mathbf{F}$ on ∂V, then $\mathbf{F}$ is uniquely determined. This is shown as follows: suppose $\mathbf{G}$ is a different vector having the same divergence and curl in V and normal component on ∂V. Then

$$\nabla\cdot(\mathbf{F}-\mathbf{G})=0 \qquad \text{and} \qquad \nabla\times(\mathbf{F}-\mathbf{G})=\mathbf{0}\,. \tag{27.86}$$

The second implies we can write $\mathbf{F}-\mathbf{G}=-\nabla\varphi$ and then the first implies $\nabla^2\varphi=0$. Now use Green's first identity, Eq. (27.79a), with $\psi=\varphi$:

$$\oiint_{\partial V}\varphi\nabla\varphi\cdot d\mathbf{S}=\iiint_V(\varphi\cancelto{0}{\nabla^2\varphi}+\nabla\varphi\cdot\nabla\varphi)\,dV\,. \tag{27.87}$$

But $\nabla\varphi\cdot d\mathbf{S}=0$ on the surface ∂V since the normal component of $\mathbf{F}$ and $\mathbf{G}$ are the same on the surface so surface integral vanishes. Thus

$$\iiint_V\|\nabla\varphi\|^2\,dV=0\,. \tag{27.88}$$

The integrand is non-negative, so this implies $\nabla\phi=0$ and hence $\mathbf{F}=\mathbf{G}$. We thus see that the Helmholtz decomposition is unique.

Ex. 27.5. Electrostatics and magnetostatics.

In electrostatics the electric field $\mathbf{E}(\mathbf{x})$ satisfies

$$\nabla\cdot\mathbf{E}(\mathbf{x})=\frac{\rho(\mathbf{x})}{\epsilon_0} \qquad \text{and} \qquad \nabla\times\mathbf{E}(\mathbf{x})=\mathbf{0} \tag{27.89}$$

and in magnetostatics the magnetic field $\mathbf{B}(\mathbf{x})$ satisfies

$$\nabla\cdot\mathbf{B}(\mathbf{x})=0 \qquad \text{and} \qquad \nabla\times\mathbf{B}(\mathbf{x})=\mu_0\mathbf{j}(\mathbf{x}) \tag{27.90}$$

where $\rho(\mathbf{x})$ is a static electric charge density, $\mathbf{j}(\mathbf{x})$ is a steady electric current density, and μ_0 is the permeability of free space.

By Helmholtz's theorem, the unique solutions to these equations are

$$\mathbf{E}(\mathbf{x})=-\nabla\frac{1}{4\pi\epsilon_0}\iiint\frac{\rho(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV'=\frac{1}{4\pi\epsilon_0}\iiint\rho(\mathbf{x}')\frac{\mathbf{x}-\mathbf{x}'}{\|\mathbf{x}-\mathbf{x}'\|^3}\,dV' \tag{27.91}$$

and

$$\mathbf{B}(\mathbf{x})=\nabla\times\frac{\mu_0}{4\pi}\iiint\frac{\mathbf{j}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV'=\frac{\mu_0}{4\pi}\iiint\mathbf{j}(\mathbf{x}')\times\frac{\mathbf{x}-\mathbf{x}'}{\|\mathbf{x}-\mathbf{x}'\|^3}\,dV'\,. \tag{27.92}$$

These are the Coulomb law and the Biot-Savart law respectively.

28 Curvilinear Coordinates

General curvilinear coordinates $\mathbf{q}$ are specified by three functions $\mathsf{x}(\mathbf{q})$ or by their inverse $\mathbf{q}(\mathsf{x})$.

Basis vectors $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ are normal to surfaces of constant q_1, q_2, and q_3 respectively. In this basis the components of a vector A are A_1, A_2, and A_3 where

$$\mathsf{A} = A_1\,\mathbf{e}_1 + A_2\,\mathbf{e}_2 + A_3\,\mathbf{e}_3\,. \tag{28.1}$$

Infinitesimal displacements are

$$dx = \frac{\partial x}{\partial q_1}\,dq_1 + \frac{\partial x}{\partial q_2}\,dq_2 + \frac{\partial x}{\partial q_3}\,dq_3 \tag{28.2a}$$

$$dy = \frac{\partial y}{\partial q_1}\,dq_1 + \frac{\partial y}{\partial q_2}\,dq_2 + \frac{\partial y}{\partial q_3}\,dq_3 \tag{28.2b}$$

$$dz = \frac{\partial z}{\partial q_1}\,dq_1 + \frac{\partial z}{\partial q_2}\,dq_2 + \frac{\partial z}{\partial q_3}\,dq_3\,. \tag{28.2c}$$

Pythagoras's law requires that

$$(ds)^2 = \|d\mathsf{x}\|^2 = (dx)^2 + (dy)^2 + (dz)^2 \tag{28.3}$$

is invariant. We thus have

$$\begin{aligned}(ds)^2 &= \left(\frac{\partial x}{\partial q_1}\,dq_1 + \frac{\partial x}{\partial q_2}\,dq_2 + \frac{\partial x}{\partial q_3}\,dq_3\right)^2 \\ &\quad + \left(\frac{\partial y}{\partial q_1}\,dq_1 + \frac{\partial y}{\partial q_2}\,dq_2 + \frac{\partial y}{\partial q_3}\,dq_3\right)^2 \\ &\quad + \left(\frac{\partial z}{\partial q_1}\,dq_1 + \frac{\partial z}{\partial q_2}\,dq_2 + \frac{\partial z}{\partial q_3}\,dq_3\right)^2 \qquad (28.4a) \\ &= \sum_{i=1}^{3}\sum_{j=1}^{3} g_{ij}\,dq_i\,dq_j \qquad (28.4b)\end{aligned}$$

where

$$g_{ij} = \frac{\partial x}{\partial q_i}\frac{\partial x}{\partial q_j} + \frac{\partial y}{\partial q_i}\frac{\partial y}{\partial q_j} + \frac{\partial z}{\partial q_i}\frac{\partial z}{\partial q_j} \tag{28.4c}$$

are the components of the **metric**.

We restrict attention to orthogonal coordinate systems for which

$$g_{ij} = 0 \quad \text{for} \quad i \neq j\,. \tag{28.5}$$

Then it is conventional to define the scale factors $h_i = \sqrt{g_{ii}}$ and then

$$(ds)^2 = (h_1\, dq_1)^2 + (h_2\, dq_2)^2 + (h_3\, dq_3)^2\,. \tag{28.6}$$

We see that $h_1\, dq_1$, $h_2\, dq_2$, and $h_3\, dq_3$ take the place of orthogonal rectilinear elements dx_1, dx_2, and dx_3 which can be oriented so that $dx_1 = h_1\, dq_1$ is a displacement in the $\mathbf{e}_1$ direction, $dx_2 = h_2\, dq_2$ is a displacement in the $\mathbf{e}_2$ direction, and $dx_3 = h_3\, dq_3$ is a displacement in the $\mathbf{e}_3$ direction. For these rectilinear coordinates aligned with the curvilinear coordinate surfaces

$$h_1 = \left|\frac{\partial x_1}{\partial q_1}\right|, \quad h_2 = \left|\frac{\partial x_2}{\partial q_2}\right|, \quad \text{and} \quad h_3 = \left|\frac{\partial x_3}{\partial q_3}\right|. \tag{28.7}$$

Note that the orientation of the basis vectors of the curvilinear coordinates $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ relative to a fixed rectilinear basis $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$ will change from point to point.

Integrals

The line element is

$$d\mathbf{s} = h_1\, dq_1\, \mathbf{e}_1 + h_2\, dq_2\, \mathbf{e}_2 + h_3\, dq_3\, \mathbf{e}_3 \tag{28.8}$$

and the line integral is therefore

$$\int_C \mathbf{A} \cdot d\mathbf{s} = \int_C (A_1 h_1\, dq_1 + A_2 h_2\, dq_2 + A_3 h_3\, dq_3)\,. \tag{28.9}$$

Similarly the area and volume elements are

$$d\boldsymbol{\mathcal{A}} = h_2 h_3\, dq_2\, dq_3\, \mathbf{e}_1 + h_3 h_1\, dq_3\, dq_1\, \mathbf{e}_2 + h_1 h_2\, dq_1\, dq_2\, \mathbf{e}_3 \tag{28.10}$$

and

$$dV = h_1 h_2 h_3\, dq_1\, dq_2\, dq_3 \tag{28.11}$$

and so, for example, a double integral on a surface of constant q_3 and $(q_1, q_2) \in D$ would be

$$\iint_D \varphi\, d\mathcal{A} = \iint_D \varphi\, h_1 h_2\, dq_1\, dq_2 \tag{28.12}$$

while a volume integral would be

$$\iiint_V \varphi\, dV = \iiint_V \varphi\, h_1 h_2 h_3\, dq_1\, dq_2\, dq_3\,. \tag{28.13}$$

Derivatives

The gradient of a scalar field is

$$\begin{aligned}\nabla\varphi &= \frac{\partial\varphi}{\partial x_1}\mathbf{e}_1 + \frac{\partial\varphi}{\partial x_2}\mathbf{e}_2 + \frac{\partial\varphi}{\partial x_3}\mathbf{e}_3 \\ &= \frac{\partial q_1}{\partial x_1}\frac{\partial\varphi}{\partial q_1}\mathbf{e}_1 + \frac{\partial q_2}{\partial x_2}\frac{\partial\varphi}{\partial q_2}\mathbf{e}_2 + \frac{\partial q_3}{\partial x_3}\frac{\partial\varphi}{\partial q_3}\mathbf{e}_3 \end{aligned} \tag{28.14}$$

and so

$$\boxed{\nabla\varphi = \frac{1}{h_1}\frac{\partial\varphi}{\partial q_1}\mathbf{e}_1 + \frac{1}{h_2}\frac{\partial\varphi}{\partial q_2}\mathbf{e}_2 + \frac{1}{h_3}\frac{\partial\varphi}{\partial q_3}\mathbf{e}_3} \tag{28.15}$$

To obtain a formula for the divergence of a vector field, consider an infinitesimal volume of sides $dx_1 = h_1\, dq_1$, $dx_2 = h_2\, dq_2$, $dx_3 = h_3\, dq_3$ at point (q_1, q_2, q_3) and use Gauss's theorem $\iiint \nabla\cdot \mathsf{A}\, dV = \oint\!\!\!\oint \mathsf{A}\cdot d\mathbf{S}$

$$\nabla\cdot \mathsf{A}\, h_1 h_2 h_3\, dq_1\, dq_2\, dq_3 \tag{28.16a}$$

$$\begin{aligned} &= \left[(A_1 h_2 h_3)\Big|_{(q_1+h_1\,dq_1, q_2, q_3)} - (A_1 h_2 h_3)\Big|_{(q_1,q_2,q_3)} \right] dq_2\, dq_3 \\ &\quad + \left[(A_2 h_3 h_1)\Big|_{(q_1, q_2+h_2\,dq_2, q_3)} - (A_2 h_3 h_1)\Big|_{(q_1,q_2,q_3)} \right] dq_3\, dq_1 \\ &\quad + \left[(A_3 h_1 h_2)\Big|_{(q_1, q_2, q_3+h_3\,dq_3)} - (A_3 h_1 h_2)\Big|_{(q_1,q_2,q_3)} \right] dq_1\, dq_2\,. \end{aligned} \tag{28.16b}$$

$$\begin{aligned} &\approx \frac{\partial(A_1 h_2 h_3)}{h_1\,\partial q_1} h_1\, dq_1\, dq_2\, dq_3 \\ &\quad + \frac{\partial(A_2 h_3 h_1)}{h_2\,\partial q_2} h_2\, dq_2\, dq_3\, dq_1 \\ &\quad + \frac{\partial(A_3 h_1 h_2)}{h_3\,\partial q_3} h_3\, dq_3\, dq_1\, dq_2 \end{aligned} \tag{28.16c}$$

The right hand side is the surface integral over all six faces.
Divide both sides by the volume element $dV = h_1 h_2 h_3\, dq_1\, dq_2\, dq_3$:

$$\boxed{\nabla\cdot \mathsf{A} = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}(A_1 h_2 h_3) + \frac{\partial}{\partial q_2}(A_2 h_3 h_1) + \frac{\partial}{\partial q_3}(A_3 h_1 h_2) \right].} \tag{28.17}$$

The Laplacian $\nabla^2\varphi$ is obtained by setting $\mathsf{A} = \nabla\varphi$ and computing $\nabla\cdot \mathsf{A}$:

$$\boxed{\nabla^2\varphi = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}\left(\frac{h_2 h_3}{h_1}\frac{\partial\varphi}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_3 h_1}{h_2}\frac{\partial\varphi}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(\frac{h_1 h_2}{h_3}\frac{\partial\varphi}{\partial q_3}\right) \right].} \tag{28.18}$$

We derive the formula for the curl on a component-by-component basis. Consider a square of sides $dx_1 = h_1\, dq_1$ and $dx_2 = h_2\, dq_2$ on the q_3 = const surface at point (q_1, q_2, q_3). By Stokes's theorem, $\iint (\boldsymbol{\nabla}\times \mathsf{A})\cdot d\mathbf{S} = \oint \mathsf{A}\cdot d\mathbf{s}$,

$$
\begin{aligned}
&(\boldsymbol{\nabla}\times \mathsf{A})\cdot \mathbf{e}_3\, h_1 h_2\, dq_1\, dq_2 \\
&\quad = \left[(A_1 h_1)\Big|_{(q_1,q_2,q_3)} - (A_1 h_1)\Big|_{(q_1,q_2+h_2\, dq_2,q_2,q_3)} \right] dq_1 \\
&\qquad + \left[(A_2 h_2)\Big|_{(q_1+h_1\, dq_1,q_2,q_3)} - (A_2 h_2)\Big|_{(q_1,q_2,q_2,q_3)} \right] dq_2 && \text{(28.19a)} \\
&\quad \approx -\frac{\partial (A_1 h_1)}{h_2\, \partial q_2} h_2\, dq_2\, dq_1 + \frac{\partial (A_2 h_2)}{h_1\, \partial q_1} h_1\, dq_1\, dq_2 && \text{(28.19b)}
\end{aligned}
$$

and so

$$
(\boldsymbol{\nabla}\times \mathsf{A})\cdot \mathbf{e}_3 = \frac{1}{h_1 h_2}\left[\frac{\partial (A_2 h_2)}{\partial q_1} - \frac{\partial (A_1 h_1)}{\partial q_2} \right]. \qquad \text{(28.19c)}
$$

A similar treatment for the other components of $\boldsymbol{\nabla}\times \mathsf{A}$ results in

$$
\begin{aligned}
\boldsymbol{\nabla}\times \mathsf{A} &= \sum_{i=1}^{3}\sum_{j=1}^{3}\sum_{k=1}^{3} \epsilon_{ijk}\mathbf{e}_i \frac{1}{h_j h_k}\frac{\partial}{\partial x_j}(A_k h_k) && \text{(28.20a)} \\
&= \frac{1}{h_1 h_2 h_3} \det \begin{bmatrix} \mathbf{e}_1 h_1 & \mathbf{e}_2 h_2 & \mathbf{e}_3 h_3 \\ \dfrac{\partial}{\partial q_1} & \dfrac{\partial}{\partial q_2} & \dfrac{\partial}{\partial q_3} \\ A_1 h_1 & A_2 h_2 & A_3 h_3 \end{bmatrix} && \text{(28.20b)} \\
&= \frac{1}{h_2 h_3}\left[\frac{\partial (A_3 h_3)}{\partial q_2} - \frac{\partial (A_2 h_2)}{\partial q_3} \right] \mathbf{e}_1 \\
&\quad + \frac{1}{h_3 h_1}\left[\frac{\partial (A_1 h_1)}{\partial q_3} - \frac{\partial (A_3 h_3)}{\partial q_1} \right] \mathbf{e}_2 \\
&\quad + \frac{1}{h_1 h_2}\left[\frac{\partial (A_2 h_2)}{\partial q_1} - \frac{\partial (A_1 h_1)}{\partial q_2} \right] \mathbf{e}_3 && \text{(28.20c)}
\end{aligned}
$$

where ϵ_{ijk} is the Levi-Civita symbol.

The vector Laplacian in general curvilinear coordinates is obtained from the above rules for the gradient, divergence, and curl via the formula

$$
\nabla^2 \mathsf{A} = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot \mathsf{A}) - \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times \mathsf{A}). \qquad \text{(28.21)}
$$

In curvilinear coordinates it is *not* $\nabla^2 A_1\, \mathbf{e}_1 + \nabla^2 A_2\, \mathbf{e}_2 + \nabla^2 A_3\, \mathbf{e}_3$, which is true only in rectilinear coordinates.

Cylindrical Coordinates

The **cylindrical coordinates** (ρ, ϕ, z) are defined by

$$x = \rho\cos\phi\,, \quad y = \rho\sin\phi\,, \quad \text{and} \quad z = z \tag{28.22}$$

or

$$\rho = \sqrt{x^2+y^2}\,, \quad \phi = \arctan\frac{y}{x}\,, \quad \text{and} \quad z = z \tag{28.23}$$

where $0 \le \rho < \infty$, $0 \le \phi \le 2\pi$, and $-\infty < z < \infty$.

The scale factors are

$$h_\rho = 1\,, \quad h_\phi = \rho\,, \quad \text{and} \quad h_z = 1 \tag{28.24}$$

and the basis vectors are related to the Cartesian basis by

$$\mathbf{e}_\rho = \cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y \quad \text{and} \quad \mathbf{e}_\phi = -\sin\phi\,\mathbf{e}_x + \cos\phi\,\mathbf{e}_y \tag{28.25}$$

or

$$\mathbf{e}_x = \cos\phi\,\mathbf{e}_\rho - \sin\phi\,\mathbf{e}_\phi \quad \text{and} \quad \mathbf{e}_y = \sin\phi\,\mathbf{e}_\rho + \cos\phi\,\mathbf{e}_\phi\,. \tag{28.26}$$

The line, area, and volume elements are

$$d\mathbf{s} = d\rho\,\mathbf{e}_\rho + \rho\,d\phi\,\mathbf{e}_\phi + dz\,\mathbf{e}_z \tag{28.27}$$

$$d\boldsymbol{\mathcal{A}} = \rho\,d\phi\,dz\,\mathbf{e}_\rho + dz\,d\rho\,\mathbf{e}_\phi + \rho\,d\rho\,d\phi\,\mathbf{e}_z \tag{28.28}$$

$$dV = \rho\,d\rho\,d\phi\,dz\,. \tag{28.29}$$

The differential operators are

$$\boldsymbol{\nabla}\psi = \frac{\partial\psi}{\partial\rho}\mathbf{e}_\rho + \frac{1}{\rho}\frac{\partial\psi}{\partial\phi}\mathbf{e}_\phi + \frac{\partial\psi}{\partial z}\mathbf{e}_z \tag{28.30}$$

$$\boldsymbol{\nabla}\cdot\mathbf{A} = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho A_\rho) + \frac{1}{\rho}\frac{\partial A_\phi}{\partial\phi} + \frac{\partial A_z}{\partial z} \tag{28.31}$$

$$\boldsymbol{\nabla}\times\mathbf{A} = \left(\frac{1}{\rho}\frac{\partial A_z}{\partial\phi} - \frac{\partial A_\phi}{\partial z}\right)\mathbf{e}_\rho + \left(\frac{\partial A_\rho}{\partial z} - \frac{\partial A_z}{\partial\rho}\right)\mathbf{e}_\phi + \frac{1}{\rho}\left(\frac{\partial}{\partial\rho}(\rho A_\phi) - \frac{\partial A_\rho}{\partial\phi}\right)\mathbf{e}_z \tag{28.32}$$

$$\nabla^2\psi = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2} \tag{28.33}$$

$$\begin{aligned}\nabla^2\mathbf{A} = &\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial A_\rho}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 A_\rho}{\partial\phi^2} + \frac{\partial^2 A_\rho}{\partial z^2} - \frac{1}{\rho^2}A_\rho - \frac{2}{\rho^2}\frac{\partial A_\phi}{\partial\phi}\right]\mathbf{e}_\rho \\ &+ \left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial A_\phi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 A_\phi}{\partial\phi^2} + \frac{\partial^2 A_\phi}{\partial z^2} - \frac{1}{\rho^2}A_\phi - \frac{2}{\rho^2}\frac{\partial A_\rho}{\partial\phi}\right]\mathbf{e}_\phi \\ &+ \left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial A_z}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 A_z}{\partial\phi^2} + \frac{\partial^2 A_z}{\partial z^2}\right]\mathbf{e}_z\,.\end{aligned} \tag{28.34}$$

Spherical Polar Coordinates

The **spherical polar coordinates** (r, θ, ϕ) are defined by

$$x = r \sin\theta \cos\phi\,, \quad y = r \sin\theta \sin\phi\,, \quad \text{and} \quad z = r\cos\theta \tag{28.35}$$

or

$$r = \sqrt{x^2 + y^2 + z^2}\,, \quad \phi = \arctan\frac{y}{x}\,, \quad \text{and} \quad z = \arccos\frac{z}{\sqrt{x^2+y^2+z^2}} \tag{28.36}$$

where $0 \le r < \infty$, $0 \le \theta \le \pi$, and $0 \le \phi \le 2\pi$.

The scale factors are

$$h_r = 1\,, \quad h_\theta = r\,, \quad \text{and} \quad h_\phi = r\sin\theta \tag{28.37}$$

and the basis vectors are related to the Cartesian basis by

$$\mathbf{e}_r = \sin\theta\cos\phi\,\mathbf{e}_x + \sin\theta\sin\phi\,\mathbf{e}_y + \cos\theta\,\mathbf{e}_z \tag{28.38a}$$
$$\mathbf{e}_\theta = \cos\theta\cos\phi\,\mathbf{e}_x + \cos\theta\sin\phi\,\mathbf{e}_y - \sin\theta\,\mathbf{e}_z \tag{28.38b}$$
$$\mathbf{e}_\phi = -\sin\phi\,\mathbf{e}_x + \cos\phi\,\mathbf{e}_y \tag{28.38c}$$

or

$$\mathbf{e}_x = \sin\theta\cos\phi\,\mathbf{e}_r + \cos\theta\cos\phi\,\mathbf{e}_\theta - \sin\phi\,\mathbf{e}_\phi \tag{28.39a}$$
$$\mathbf{e}_y = \sin\theta\sin\phi\,\mathbf{e}_r + \cos\theta\sin\phi\,\mathbf{e}_\theta + \cos\phi\,\mathbf{e}_\phi \tag{28.39b}$$
$$\mathbf{e}_z = \cos\theta\,\mathbf{e}_r - \cos\theta\,\mathbf{e}_\theta\,. \tag{28.39c}$$

The line, area, and volume elements are

$$d\mathbf{s} = dr\,\mathbf{e}_r + r\,d\theta\,\mathbf{e}_\theta + r\sin\theta\,d\phi\,\mathbf{e}_\phi \tag{28.40}$$
$$d\mathcal{A} = r^2\sin\theta\,d\theta\,d\phi\,\mathbf{e}_r + r\sin\theta\,d\phi\,dr\,\mathbf{e}_\theta + r\,dr\,d\theta\,\mathbf{e}_\phi \tag{28.41}$$
$$dV = r^2\sin\theta\,dr\,d\theta\,d\phi\,. \tag{28.42}$$

The differential operators are

$$\boldsymbol{\nabla}\psi = \frac{\partial\psi}{\partial r}\,\mathbf{e}_r + \frac{1}{r}\frac{\partial\psi}{\partial\theta}\,\mathbf{e}_\theta + \frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}\,\mathbf{e}_\phi \tag{28.43}$$

$$\boldsymbol{\nabla}\cdot\mathbf{A} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 A_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_\theta) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial\phi} \tag{28.44}$$

$$\begin{aligned}\boldsymbol{\nabla}\times\mathbf{A} = {}& \frac{1}{r\sin\theta}\left(\frac{\partial}{\partial\theta}(\sin\theta A_\phi) - \frac{\partial A_\theta}{\partial\phi}\right)\mathbf{e}_r \\ & + \frac{1}{r}\left(\frac{1}{\sin\theta}\frac{\partial A_r}{\partial\phi} - \frac{\partial}{\partial r}(rA_\phi)\right)\mathbf{e}_\theta \\ & + \frac{1}{r}\left(\frac{\partial}{\partial r}(rA_\theta) - \frac{\partial A_r}{\partial\theta}\right)\mathbf{e}_\phi\end{aligned} \tag{28.45}$$

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} \tag{28.46}$$

$$\begin{aligned}\nabla^2\mathbf{A} = {}& \left[\nabla^2 A_r - \frac{2}{r^2}A_r - \frac{2}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_\theta) - \frac{2}{r^2\sin\theta}\frac{\partial A_\phi}{\partial\phi}\right]\mathbf{e}_r \\ & + \left[\nabla^2 A_\theta - \frac{1}{r^2\sin^2\theta}A_\theta + \frac{2}{r^2}\frac{\partial A_r}{\partial\theta} - \frac{2\cos\theta}{r^2\sin^2\theta}\frac{\partial A_\phi}{\partial\phi}\right]\mathbf{e}_\theta \\ & + \left[\nabla^2 A_\phi - \frac{1}{r^2\sin^2\theta}A_\phi + \frac{2}{r^2\sin^2\theta}\frac{\partial A_r}{\partial\phi} + \frac{2\cos\theta}{r^2\sin^2\theta}\frac{\partial A_\theta}{\partial\phi}\right]\mathbf{e}_\phi\,.\end{aligned} \tag{28.47}$$

Problems

Problem 34.

Find the eigenvalues and normalized eigenvectors of the matrix $\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$.
Keep 3 significant figures in your numerical answer.

Problem 35.

a) Let $\mathbf{a}$ and $\mathbf{b}$ be any two vectors in a linear vector space and let $\mathbf{c} = \mathbf{a} + \lambda\mathbf{b}$ where λ is a scalar. By requiring $\mathbf{c} \cdot \mathbf{c} \geq 0$ for all λ, derive the **Cauchy-Schwarz inequality**

$$(\mathbf{a} \cdot \mathbf{a})(\mathbf{b} \cdot \mathbf{b}) \geq |\mathbf{a} \cdot \mathbf{b}|^2 .$$

b) In an infinite-dimensional vector space with a set of n orthonormal vectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$ satisfying $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$, $i, j = 1 \ldots n$, use the results of part (a) to obtain **Bessel's inequality**

$$\sum_{i=1}^{n} |x_i|^2 \leq \mathbf{x} \cdot \mathbf{x} \qquad \text{where} \qquad x_i = \mathbf{x} \cdot \mathbf{e}_i \,, \quad i = 1 \ldots n \,.$$

Problem 36.

In 2-dimensions, show that if λ is the charge at the origin, then Gauss's law is

$$\varphi = -\frac{\lambda}{2\pi\epsilon_0} \ln \rho \qquad \text{and} \qquad \mathbf{E} = -\boldsymbol{\nabla}\varphi = \frac{\lambda}{2\pi\epsilon_0} \frac{1}{\rho} \mathbf{e}_\rho$$

where ρ is the radial distance from the charge.

Module VIII

Partial Differential Equations

Motivation

Fundamental physical laws, from electrodynamics to quantum mechanics, are formulated as partial differential equations. Here we examine methods to solve these equations.

In this module we will solve several types of partial differential equations in a series of examples. We will focus on second-order partial differential equations involving the Laplacian operator ∇^2 as these types of equations are the ones most commonly encountered in basic physics problems.

29 Classification

Some commonly encountered partial differential equations:

- Vibrating string / 1-dimensional **wave equation**

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} \quad \text{with} \quad c^2 = \frac{\text{tension of string}}{\text{linear density of string}}\,. \tag{29.1}$$

  This is a **hyperbolic equation**.

- **Laplace's equation**

$$\nabla^2 \psi = \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}\right) = 0\,. \tag{29.2}$$

  This is an **elliptic equation**.

- 3-dimensional wave equation

$$\nabla^2 \psi - \frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} = 0\,. \tag{29.3}$$

  This is another hyperbolic equation.

- **Diffusion equation**

$$\nabla^2 \psi - \frac{1}{\alpha}\frac{\partial \psi}{\partial t} = 0 \tag{29.4}$$

  where α is the diffusion constant, e.g., if ψ is temperature then

$$\alpha = \frac{\text{thermal conductivity}}{(\text{specific heat capacity}) \cdot (\text{density})}\,. \tag{29.5}$$

  This is a **parabolic equation**.

- **Schrödinger equation**

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{x})\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{29.6}$$

  where $\psi(\mathbf{x})$ is the wavefunction of a particle, m is the mass of the particle, $V(\mathbf{x})$ is the potential the particle moves in, and $\hbar$ is the reduced Planck constant. This is again a parabolic equation.

  If $\psi \propto e^{-iEt/\hbar}$ where E is the energy, the time-independent Schrödinger equation is

$$\nabla^2\psi + \frac{2m}{\hbar^2}[E - V(\mathbf{x})]\psi = 0\,. \tag{29.7}$$

  This is an elliptic equation.

All of these are **linear**, **second order**, and **homogeneous**. The last implies that if ψ is a solution, any multiple of ψ is also a solution.

If a "force" or "source" is present, the equation is **inhomogeneous**, e.g.,

$$\frac{\partial^2\psi}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = -\frac{1}{\text{tension}}f(x,t) \tag{29.8}$$

where $f(x,t)$ is the force per unit length acting on the string.

An equation may be inhomogeneous due to a boundary condition, e.g., a vibrating string in which the end $x = 0$ is prescribed to move in a particular way:

$$\psi(0,t) = g(t)\,. \tag{29.9}$$

The general solution is made up of any particular solution plus the general solution of the corresponding homogeneous problem.

Boundary Conditions

There are three commonly used types of boundary conditions:

- **Dirichlet boundary conditions** are ones in which ψ is specified at each point on the boundary.
- **Neumann boundary conditions** are ones in which the normal derivative $\mathbf{n} \cdot \nabla \psi$ is specified at each point on the boundary where $\mathbf{n}$ is the unit normal vector to the boundary surface.
- **Cauchy boundary conditions** are ones in which both ψ and $\mathbf{n} \cdot \nabla \psi$ are specified at each point on the boundary.

The goal is to choose appropriate boundary conditions so that a unique solution is obtained.

Generally we use Dirichlet or Neumann boundary conditions for elliptic or parabolic systems, and Cauchy boundary conditions for hyperbolic systems.

Ex. 29.1. Simplest hyperbolic equation.

$$\frac{\partial^2\psi}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = 0\,. \tag{29.10}$$

Change variables to

$$u = x - ct \qquad \text{and} \qquad v = x + ct\,. \tag{29.11}$$

Lines of $u = \text{const}$ and $v = \text{const}$ are known as **characteristics**.
We have

$$\frac{\partial}{\partial x} = \frac{\partial u}{\partial x}\frac{\partial}{\partial u} + \frac{\partial v}{\partial x}\frac{\partial}{\partial v} = \frac{\partial}{\partial u} + \frac{\partial}{\partial v} \tag{29.12a}$$

$$\frac{\partial}{\partial t} = \frac{\partial u}{\partial t}\frac{\partial}{\partial u} + \frac{\partial v}{\partial t}\frac{\partial}{\partial v} = -c\frac{\partial}{\partial u} + c\frac{\partial}{\partial v} \tag{29.12b}$$

and so

$$\left(\frac{\partial}{\partial u} + \frac{\partial}{\partial v}\right)^2 \psi - \left(-\frac{\partial}{\partial u} + \frac{\partial}{\partial v}\right)^2 \psi = 0 \tag{29.12c}$$

or

$$\frac{\partial^2\psi}{\partial u \partial v} = 0\,. \tag{29.12d}$$

This is the hyperbolic equation in its **normal form**.

The solution is immediate:

$$\psi(u,v) = f(u) + g(v) \qquad \text{or} \qquad \psi(x,y) = f(x-ct) + g(x+ct) \tag{29.13}$$

where f and g are arbitrary functions, i.e., a superposition of a left-going wave and a right-going wave.

Suppose we specify the Cauchy boundary conditions $\psi(t=0,x)$ and $\dfrac{\partial\psi}{\partial t}(t=0,x)$. Then

$$f(x) + g(x) = \psi(t=0,x) \tag{29.14a}$$

$$-f'(x) + g'(x) = \frac{1}{c}\frac{\partial\psi}{\partial t}(t=0,x) \quad \Longrightarrow \quad -f(x) + g(x) = \frac{1}{c}\int \frac{\partial\psi}{\partial t}(t=0,x)\,dx\,. \tag{29.14b}$$

Therefore

$$f(x) = \frac{1}{2}\psi(t=0,x) - \frac{1}{2c}\int \frac{\partial\psi}{\partial t}(t=0,x)\,dx \tag{29.15a}$$

$$g(x) = \frac{1}{2}\psi(t=0,x) + \frac{1}{2c}\int \frac{\partial\psi}{\partial t}(t=0,x)\,dx\,. \tag{29.15b}$$

Note: the arbitrary constant of integration is irrelevant as it cancels in the sum $\psi = f + g$.

30 Separation of Variables

Ex. 30.1. Wave equation in spherical-polar coordinates.

The 3-dimensional wave equation is

$$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = 0\,. \tag{30.1}$$

Look for a solution where t and $\mathbf{x}$ dependence factors:

$$\psi(t,\mathbf{x}) = T(t)X(\mathbf{x}) \tag{30.2a}$$

$$\implies \quad T\nabla^2 X - \frac{X}{c^2}\frac{\partial^2 T}{\partial t^2} = 0 \tag{30.2b}$$

$$\implies \quad \underbrace{\frac{\nabla^2 X}{X}}_{\substack{\text{function of}\\ \mathbf{x}\text{ only}}} = \underbrace{\frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2}}_{\substack{\text{function of}\\ t\text{ only}}}\,. \tag{30.2c}$$

In order for this to hold for all t and all $\mathbf{x}$, each side must be constant.

Let $-k^2$ be the separation constant. Then

$$\frac{\nabla^2 X}{X} = -k^2 \qquad \text{and} \qquad \frac{1}{c^2}\frac{1}{T}\frac{d^2T}{dt^2} = -k^2\,. \tag{30.3}$$

Note that the second is an *ordinary* differential equation which we now solve:

$$\implies \quad \frac{d^2T}{dt^2} + \omega^2 T = 0 \qquad \text{with} \qquad \omega = ck \tag{30.4a}$$

$$\implies \quad T(t) = e^{\pm i\omega t} \quad \text{or} \quad T(t) = \begin{cases}\sin\omega t\\ \cos\omega t\end{cases} \tag{30.4b}$$

(the choice depends on the initial conditions).

The other equation, involving $X(\mathbf{x})$, is

$$\boxed{\nabla^2 X + k^2 X = 0\,.} \tag{30.5}$$

This is the **Helmholtz equation**. We want to solve this in spherical-polar coordinates.

Express the Laplacian in spherical polar coordinates:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial X}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial X}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2 X}{\partial\phi^2}+k^2X=0\,. \tag{30.6}$$

Let $X(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$ and divide by X:

$$\frac{1}{R}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{\Theta}\frac{1}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\underbrace{\frac{1}{\Phi}\frac{1}{r^2\sin^2\theta}\frac{d^2\Phi}{d\phi^2}}_{\substack{\text{only term that}\\ \text{depends on }\phi}}+k^2=0\,. \tag{30.7}$$

Multiply by $r^2\sin^2\theta$:

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\underbrace{\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}}_{\substack{\text{depends only on }\phi\\ \Longrightarrow\ \text{separates!}}}+k^2r^2\sin^2\theta=0\,. \tag{30.8}$$

Let the separation constant be $-m^2$. Then

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=-m^2 \qquad\Longrightarrow\qquad \Phi(\phi)=e^{\pm im\phi} \tag{30.9}$$

and

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-m^2+k^2r^2\sin^2\theta=0\,. \tag{30.10}$$

Divide by $\sin^2\theta$:

$$\underbrace{\left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+k^2r^2\right]}_{\text{depends only on }r}+\underbrace{\left[\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\frac{m^2}{\sin^2\theta}\right]}_{\text{depends only on }\theta}=0. \tag{30.11}$$

This equation again separates. Let the separation constant be $\ell(\ell+1)$. We then arrive at an angular equation

$$\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\frac{m^2}{\sin^2\theta}=-\ell(\ell+1) \tag{30.12}$$

and a radial equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left[k^2-\frac{\ell(\ell+1)}{r^2}\right]R=0\,. \tag{30.13}$$

Solve the angular equation first. Let $x = \cos\theta$:

$$\frac{d}{d\theta} = \frac{dx}{d\theta}\frac{d}{dx} = -\sin\theta\frac{d}{dx} \tag{30.14}$$

and so

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = \frac{d}{dx}\left[\sin^2\theta\frac{d\Theta}{dx}\right] \tag{30.15a}$$

$$= \frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right] \tag{30.15b}$$

$$= (1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx}\,. \tag{30.15c}$$

The angular equation is thus

$$(1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx}\,. + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right]\Theta = 0\,. \tag{30.16}$$

This is the associated Legendre equation so the solutions are

$$\Theta(x) = \begin{cases} P_\ell^m(x) \\ Q_\ell^m(x)\,. \end{cases} \tag{30.17}$$

Note that when we choose the associated Legendre functions of the first kind, $P_\ell^m(x)$, which are the ones that are defined in $-1 \le x \le 1$ or $0 \le \theta \le \pi$, we have

$$\Theta(\theta)\Phi(\phi) = P_\ell^m(\cos\theta)e^{im\phi} \propto Y_\ell^m(\theta,\phi) \tag{30.18}$$

so the ℓ and m separation constants separates the solution into terms in which the angular part are spherical harmonics.

Now solve the radial equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[k^2 - \frac{\ell(\ell+1)}{r^2}\right] = 0 \tag{30.19a}$$

$$\implies \quad r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + [k^2r^2 - \ell(\ell+1)]R = 0\,. \tag{30.19b}$$

Solutions to this equation are the spherical Bessel functions

$$R(r) = \begin{cases} j_\ell(kr) \\ y_\ell(kr)\,. \end{cases} \tag{30.20}$$

However, if $k = 0$ (corresponding to $\partial\psi/\partial t = 0$ so solving Laplace's equation rather than the wave equation), we have instead

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{\ell(\ell+1)}{r^2}R = 0 \tag{30.21}$$

and the solutions to this equation are

$$R(r) = \begin{cases} r^{\ell} \\ r^{-(\ell+1)} \end{cases}. \tag{30.22}$$

Therefore the solutions have the form

$$\nabla^2\psi + \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = 0 \ :$$
$$\psi(t,r,\theta,\phi) = \left\{ \begin{array}{c} e^{ikct} \\ e^{-ikct} \end{array} \right\} \cdot \left\{ \begin{array}{c} e^{im\phi} \\ e^{-im\phi} \end{array} \right\} \cdot \left\{ \begin{array}{c} P_\ell^m(\cos\theta) \\ Q_\ell^m(\cos\theta) \end{array} \right\} \cdot \left\{ \begin{array}{c} j_\ell(kr) \\ y_\ell(kr) \end{array} \right\} \tag{30.23}$$

$$\nabla^2\psi = 0 \ :$$
$$\psi(r,\theta,\phi) = \left\{ \begin{array}{c} e^{im\phi} \\ e^{-im\phi} \end{array} \right\} \cdot \left\{ \begin{array}{c} P_\ell^m(\cos\theta) \\ Q_\ell^m(\cos\theta) \end{array} \right\} \cdot \left\{ \begin{array}{c} r^{\ell} \\ r^{-(\ell+1)} \end{array} \right\}. \tag{30.24}$$

Any linear combination is a solution, but boundary conditions limit allowed types of solutions.

Ex. 30.2. Vibrations of a round drum head.

We now solve the 2-dimensional wave equation

$$\nabla^2 u = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \tag{30.25}$$

in polar coordinates.

The **normal modes** are periodic solutions $u(t, \mathrm{x}) = u(\mathrm{x})e^{i\omega t}$

$$\implies \quad \nabla^2 u + k^2 u = 0 \tag{30.26}$$

where $k = \dfrac{\omega}{c}$ is the wave number.

In 2-dimensional polar coordinates, this is

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \phi^2} + k^2 u = 0\,. \tag{30.27}$$

Let $u = R(r)\Phi(\phi)$ and separate:

$$\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0 \qquad \implies \qquad \Phi(\phi) = e^{\pm im\phi} \tag{30.28a}$$

$$\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} + \left(k^2 - \frac{m^2}{r^2}\right)R = 0 \qquad \implies \qquad R(r) = \begin{cases} J_m(kr) \\ Y_m(kr) \end{cases} \tag{30.28b}$$

(the second is Bessel's equation) and so our solutions are of the form

$$u(r, \phi) = \left\{ \begin{array}{c} e^{im\phi} \\ e^{-im\phi} \end{array} \right\} \cdot \left\{ \begin{array}{c} J_m(kr) \\ Y_m(kr) \end{array} \right\}. \tag{30.29}$$

Boundary conditions:

- Require solutions to be periodic in ϕ so that $u(r, \phi = 0) = u(r, \phi = 2\pi)$
  $\implies \quad m$ is an integer.
- Dirichlet boundary conditions on edge or drum requires $u(r = a, \phi) = 0$
  $\implies \quad J_m(ka) = 0\,.$
  Note: $Y_m(kr)$ solutions are unacceptable because they are not regular at $r = 0$.
  Thus, only certain values of k are allowed:

$$k_{mn} = \frac{x_{mn}}{a} \tag{30.30}$$

  where x_{mn} is the nth zero of $J_m(x)$:

$$J_0(x) = 0 \quad \text{for} \quad x_{01} \approx 2.40,\ x_{02} \approx 5.52,\ x_{03} \approx 8.65, \ldots \tag{30.31a}$$

$$J_1(x) = 0 \quad \text{for} \quad x_{11} \approx 3.83,\ x_{12} \approx 7.02,\ x_{13} \approx 10.17, \ldots \tag{30.31b}$$

$$J_2(x) = 0 \quad \text{for} \quad x_{21} \approx 5.14,\ x_{22} \approx 8.42,\ x_{23} \approx 11.62, \ldots \tag{30.31c}$$

The lowest-frequency modes have

- $k_{01} = \dfrac{2.40}{a}, \quad \omega_{01} = 2.40\dfrac{c}{a}, \quad u \propto J_0\left(2.40\dfrac{r}{a}\right)$

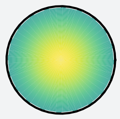


Figure 30.1: Drum 01 Mode

There are no nodes inside the rim.

- $k_{11} = \dfrac{3.83}{a}, \quad \omega_{11} = 3.83\dfrac{c}{a}, \quad u \propto J_1\left(3.83\dfrac{r}{a}\right)\begin{cases}\cos\phi \\ \sin\phi\end{cases}$

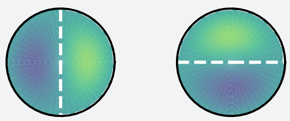


Figure 30.2: Drum 11 Modes

The white dashed lines are the nodes.
Note: there are two degenerate modes belonging to the same eigenfrequency.

- $k_{21} = \dfrac{5.14}{a}, \quad \omega_{21} = 5.14\dfrac{c}{a}, \quad u \propto J_2\left(5.14\dfrac{r}{a}\right)\begin{cases}\cos 2\phi \\ \sin 2\phi\end{cases}$

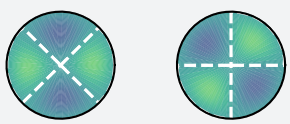


Figure 30.3: Drum 21 Modes

The white dashed lines are the nodes.
Note: there are two degenerate modes belonging to the same eigenfrequency.

- $k_{02} = \dfrac{5.52}{a}, \quad \omega_{02} = 5.52\dfrac{c}{a}, \quad u \propto J_0\left(5.52\dfrac{r}{a}\right)$

Figure 30.4: Drum 02 Mode

The white dashed line is the node.

The generalization to a cylinder is straightforward: first separate out the z-dependence (with separation constant α) then proceed as in the 2-dimensional example.

The Laplacian in cylindrical coordinates (ρ, ϕ, z) is

$$\nabla^2 = \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}\,. \tag{30.32}$$

- Laplace's equation

$$\nabla^2 \psi = 0\ :$$
$$\psi(\rho,\phi,z) = \left\{ \begin{array}{c} J_m(\alpha\rho) \\ Y_m(\alpha\rho) \end{array} \right\} \cdot \left\{ \begin{array}{c} e^{\alpha z} \\ e^{-\alpha z} \end{array} \right\} \cdot \left\{ \begin{array}{c} e^{im\phi} \\ e^{-im\phi} \end{array} \right\}. \tag{30.33}$$

- Helmholtz equation

$$\nabla^2 \psi + k^2 \psi = 0\ :$$
$$\psi(\rho,\phi,z) = \left\{ \begin{array}{c} J_m\left(\sqrt{k^2-\alpha^2}\rho\right) \\ Y_m\left(\sqrt{k^2-\alpha^2}\rho\right) \end{array} \right\} \cdot \left\{ \begin{array}{c} e^{i\alpha z} \\ e^{-i\alpha z} \end{array} \right\} \cdot \left\{ \begin{array}{c} e^{im\phi} \\ e^{-im\phi} \end{array} \right\}. \tag{30.34}$$

Ex. 30.3. Cube in a hot bath.

A cube with sides L is immersed in a heat bath at temperature $T = T_0$. The initial temperature of the cube is $T = 0$. The warming of the cube is described by the **heat equation**

$$\nabla^2 T = \frac{1}{\alpha}\frac{\partial T}{\partial t} \qquad \text{with} \qquad \alpha = \frac{k}{c\rho} \tag{30.35}$$

where k is the thermal conductivity, c is the specific heat capacity, and ρ is the density of the cube.

Let $T \propto e^{-\lambda t}$. Then

$$\nabla^2 T + \frac{\lambda}{\alpha} T = 0 \tag{30.36a}$$

$$\implies \quad \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} = -\frac{\lambda}{\alpha} T\,. \tag{30.36b}$$

Now separate the spatial variables: $T \propto e^{iax} e^{iby} e^{icz}$

$$\implies \quad a^2 + b^2 + c^2 = \frac{\lambda}{\alpha}\,. \tag{30.37}$$

Boundary conditions: all six faces must be at $T = T_0$.

This is an inhomogeneous boundary condition. A particular solution is $T_p = T_0$.

Now we need to find the complementary function T_c which must satisfy the homogeneous boundary conditions:

$$T = 0 \quad \text{for} \quad x = 0, L \quad y = 0, L \quad z = 0, L\,. \tag{30.38}$$

We find

$$T_c \propto \sin\left(\frac{\ell \pi x}{L}\right) \sin\left(\frac{m \pi y}{L}\right) \sin\left(\frac{n \pi z}{L}\right) \tag{30.39a}$$

with

$$\left(\frac{\ell\pi}{L}\right)^2 + \left(\frac{m\pi}{L}\right)^2 + \left(\frac{n\pi}{L}\right)^2 = \frac{\lambda}{\alpha}\,. \tag{30.39b}$$

Therefore, $T = T_p + T_c$:

$$T = T_0 + \sum_{\ell=1}^{\infty} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_{\ell mn} \sin\left(\frac{\ell \pi x}{L}\right) \sin\left(\frac{m \pi y}{L}\right) \sin\left(\frac{n \pi z}{L}\right) e^{-\lambda_{\ell mn} t} \tag{30.40a}$$

where

$$\lambda_{\ell mn} = \alpha \frac{\pi^2}{L^2}(\ell^2 + m^2 + n^2)\,. \tag{30.40b}$$

To determine the coefficients $c_{\ell mn}$ use the condition $T = 0$ at $t = 0$:

$$\sum_{\ell=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} c_{\ell mn}\sin\left(\frac{\ell\pi x}{L}\right)\sin\left(\frac{m\pi y}{L}\right)\sin\left(\frac{n\pi z}{L}\right) = -T_0\,. \tag{30.41}$$

Multiply by $\sin\left(\frac{\ell'\pi x}{L}\right)\sin\left(\frac{m'\pi y}{L}\right)\sin\left(\frac{n'\pi z}{L}\right)$ and integrate $\int_{x=0}^{L} dx$, $\int_{y=0}^{L} dy$, $\int_{z=0}^{L} dz$ (i.e., over the whole cube). Then we obtain

$$c_{\ell mn} = \begin{cases} -\dfrac{64}{\pi^3 \ell mn} & \ell,\, m,\, n \text{ all odd} \\ 0 & \text{otherwise.} \end{cases} \tag{30.42}$$

We have finally

$$T(t,x,y,z) = T_0 - \frac{64}{\pi^3}T_0 \sum_{\substack{\ell=1 \\ \ell,\, m,\, n \text{ all odd}}}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{1}{\ell mn}\sin\left(\frac{\ell\pi x}{L}\right)\sin\left(\frac{m\pi y}{L}\right)\sin\left(\frac{n\pi z}{L}\right) \times \exp\left[-\frac{(\ell^2+m^2+n^2)\pi^2}{L^2}\alpha t\right]. \tag{30.43}$$

This series solution works well at late times when the exponential kills all but the lowest modes, but at early times we will need to keep a large number of terms in the sums to get an accurate result.

Ex. 30.4. Heating of a slab.

Consider a slab of thickness d in the x-direction that is infinite in y- and z-directions as shown in Fig. 30.5.

The face at $x = d$ is insulated while the face at $x = 0$ is heated at a constant rate q.

Initially the slab is at $T = 0$.

We must solve the 1-dimensional diffusion equation

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\alpha}\frac{\partial T}{\partial t} = 0\,, \quad \alpha = \frac{k}{c\rho} \tag{30.44}$$

with inhomogeneous boundary conditions.

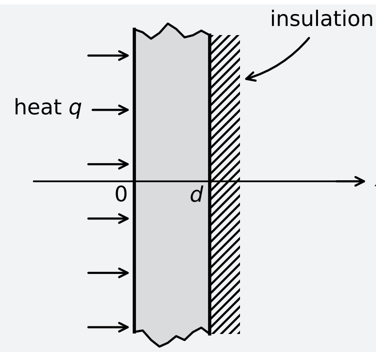


Figure 30.5: Slab Heating

As before, we seek a particular solution T_p to which we will add a complementary function T_c,

$$T = T_p + T_c \tag{30.45}$$

where T_c is a solution to the problem with homogeneous boundary conditions.

- *Particular solution.*

  Eventually we expect the temperature to rise linearly with time as heat is added. Try

$$T_p(t,x) = u(x) + \kappa t\,. \tag{30.46}$$

This results in a separation of variables:

$$\frac{d^2 u}{dx^2} = \frac{\kappa}{\alpha} \tag{30.47a}$$

$$\Longrightarrow \quad u(x) = \frac{1}{2}\frac{\kappa}{\alpha}x^2 + ax + b\,. \tag{30.47b}$$

To determine a and b, we employ the boundary conditions.
From **Fourier's law of conduction**, $\mathbf{q} = -k\boldsymbol{\nabla} T$ where $\mathbf{q}$ is the heat flux density, the temperature gradient is

$$u'(0) = -\frac{q}{\alpha} \qquad \text{and} \qquad u'(d) = 0 \quad \text{(insulated)} \tag{30.48}$$

so we find

$$u(x) = \frac{1}{2}\frac{q}{kd}(x-d)^2 \qquad \text{and} \qquad \kappa = \frac{q\alpha}{kd} = \frac{q}{c\rho d}\,. \tag{30.49}$$

Therefore

$$T_p(t,x) = \frac{1}{2}\frac{q}{kd}(x-d)^2 + \frac{q}{kd}\alpha t\,. \tag{30.50}$$

To this we need to add a complementary function (that satisfies the homogeneous boundary conditions) in order to satisfy the initial condition

$$T(t=0,x) = T_p(t=0,x) + T_c(t=0,x) = 0\,. \tag{30.51}$$

- *Characteristic function.*
  Write $T_c(t,x) \propto e^{-\lambda t} e^{iax} \quad \Longrightarrow \quad a^2 = \dfrac{\lambda}{\alpha}$.
  The homogeneous boundary conditions (Neumann) are:

$$\left.\frac{\partial T_c}{\partial x}\right|_{x=0} = \left.\frac{\partial T_c}{\partial x}\right|_{x=d} = 0 \tag{30.52}$$

  and so e^{iax} becomes $\cos(ax)$ with $a = n\pi/d$ so

$$T_c(t,x) = \frac{A_0}{2} + \sum_{n=1}^{\infty} A_n \cos\left(\frac{n\pi x}{d}\right) e^{-\lambda_n t}\,, \qquad \lambda_n = \alpha\frac{\pi^2 n^2}{d^2}\,. \tag{30.53}$$

  At $t=0$, $T_c = -T_p$ so

$$\frac{A_0}{2} + \sum_{n=1}^{\infty} A_n \cos\left(\frac{n\pi x}{d}\right) = -\frac{1}{2}\frac{q}{kd}(x-d)^2 \tag{30.54a}$$

  and we solve for A_0 and A_n, $n = 1, 2, \ldots$:

$$A_0 = \left(\frac{2}{d}\right)\left[-\frac{1}{2}\frac{q}{kd}\int_0^d (x-d)^2\,dx\right] = -\frac{1}{3}\frac{qd}{k} \tag{30.54b}$$

$$A_n = \left(\frac{2}{d}\right)\left[-\frac{1}{2}\frac{q}{kd}\int_0^d (x-d)^2 \cos\left(\frac{n\pi x}{d}\right)dx\right] = -2\frac{qd}{k}\frac{1}{(n\pi)^2}\,. \tag{30.54c}$$

The complete solution is

$$T(t,x) = \frac{1}{2}\frac{q}{kd}(x-d)^2 + \frac{q}{kd}\alpha t - \frac{qd}{k}\left\{\frac{1}{3} + \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\cos\left(\frac{n\pi x}{d}\right)e^{-\alpha n^2\pi^2 t/d^2}\right\}. \tag{30.55}$$

31 Integral Transform Method

Ex. 31.1. Find the temperature distribution $T(t,x)$ of an infinite solid if we are given an initial distribution $T(t=0,x)=f(x)$.

Note: there is no y- or z-dependence so this is a 1-dimensional problem:

$$\frac{\partial^2 T}{\partial x^2}=\frac{1}{\alpha}\frac{\partial T}{\partial t}\,. \tag{31.1}$$

Let

$$T(t,x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}F(t,k)e^{ikx}\,dk \qquad \Longleftrightarrow \qquad F(t,k)=\int_{-\infty}^{\infty}T(t,x)e^{-ikx}\,dx\,. \tag{31.2}$$

Then

$$-k^2F(t,k)=\frac{1}{\alpha}\frac{\partial F(t,k)}{\partial t} \qquad \Longrightarrow \qquad F(t,k)=g(k)e^{-k^2\alpha t} \tag{31.3}$$

where we must determine $g(k)$ from the initial conditions.

At $t=0$,

$$F(t=0,k)=\int_{-\infty}^{\infty}T(0,x)e^{-ikx}\,dx=\int_{-\infty}^{\infty}f(x)e^{-ikx}\,dx \tag{31.4}$$

but $F(t=0,k)=g(k)$ so

$$g(k)=\int_{-\infty}^{\infty}f(x)e^{-ikx}\,dx\,. \tag{31.5}$$

Thus

$$F(t,k)=\int_{-\infty}^{\infty}e^{-k^2\alpha t}f(x)e^{-ikx}\,dx\,. \tag{31.6}$$

Therefore

$$T(t,x) = \frac{1}{2\pi}\int_{k=-\infty}^{\infty}\int_{x'=-\infty}^{\infty} e^{-k^2\alpha t} f(x') e^{-ikx'} e^{ikx}\, dx'\, dk \tag{31.7a}$$

$$= \int_{x'=-\infty}^{\infty} f(x') \underbrace{\frac{1}{2\pi}\int_{k=-\infty}^{\infty} e^{ik(x-x')} e^{-k^2\alpha t}\, dk}_{\sqrt{\frac{1}{4\pi\alpha t}}\, e^{-(x-x')^2/4\alpha t}}\, dx' \tag{31.7b}$$

and so we have

$$T(t,x) = \int_{-\infty}^{\infty} f(x')\sqrt{\frac{1}{4\pi\alpha t}}\, e^{-(x-x')^2/4\alpha t}\, dx'\,. \tag{31.8}$$

Note:

$$G(t,x;x') = \sqrt{\frac{1}{4\pi\alpha t}}\, e^{-(x-x')^2/4\alpha t} \tag{31.9}$$

is a **Green function** for this problem.

Suppose the initial source is the plane source $f(x) = \delta(x)$. Then

$$T(t,x) = \sqrt{\frac{1}{4\pi\alpha t}}\, e^{-x^2/4\alpha t} = G(t,x;0)\,, \quad t > 0\,. \tag{31.10}$$

This is a Gaussian of width $\sqrt{2\alpha t}$. We see that an initial delta-like distribution spatially diffuses with time as shown in Fig. 31.1.

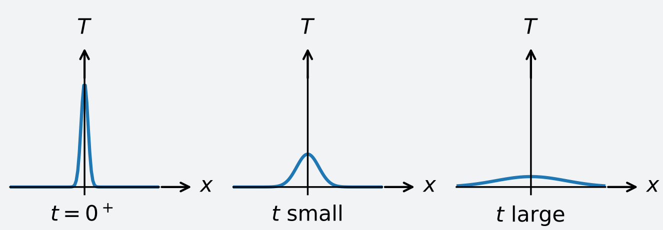


Figure 31.1: Heat Diffusion

We can use this solution to find the distribution from a point source $\delta^3(\mathrm{x})$.

Let $G(t,x;0)$ be the response to the plane source $\delta(x)$ at $t=0$.
Let $g(t,r)$ be the response to the point source $\delta^3(\mathrm{x})$ at $t=0$.
Then we must have (see Fig. 31.2)

$$G(t,x;0) = 2\pi \int_0^\infty g(t,r)\rho\, d\rho \tag{31.11}$$

(a superposition of points lying on the $x=0$ plane)
and $r^2 = \rho^2 + x^2 \implies r\,dr = \rho\, d\rho$ so

$$G(t,x;0) = 2\pi \int_x^\infty g(t,r)\, r\, dr\,. \tag{31.12}$$

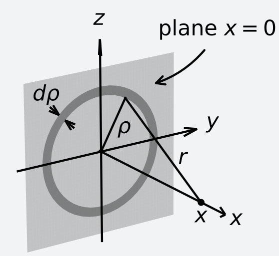


Figure 31.2: Point Source Integral

$$\implies \quad \frac{\partial G(t,x;0)}{\partial x} = -2\pi x g(t,x) \tag{31.13a}$$

$$\implies \quad g(t,r) = -\frac{1}{2\pi r}\left.\frac{\partial G(t,x;0)}{\partial x}\right|_{x=r} \tag{31.13b}$$

We find

$$g(t,r) = \left(\frac{1}{4\pi\alpha t}\right)^{3/2} e^{-r^2/4\alpha t}\,, \quad t>0\,. \tag{31.14}$$

Thus the Green function for an infinite solid is

$$G(t,\mathrm{x};\mathrm{x}') = \left(\frac{1}{4\pi\alpha t}\right)^{3/2} e^{-\|\mathrm{x}-\mathrm{x}'\|^2/4\alpha t}\,, \quad t>0\,. \tag{31.15}$$

Ex. 31.2. Consider the response of a semi-infinite solid $x > 0$ to a point initial temperature distribution at $x = a$, $y = z = 0$, $\delta(x-a)\delta(y)\delta(z)$, if the entire solid is initially at $T = 0$ (except at the point) and the boundary $x = 0$ is maintained at $T = 0$, as shown in Fig. 31.3.

We will solve this using the **method of images**.

In the previous example we saw that the Green function for a point source in an *infinite* solid is

$$G(t, \mathbf{x}; \mathbf{x}') = \left(\frac{1}{4\pi\alpha t}\right)^{3/2} e^{-\|\mathbf{x}-\mathbf{x}'\|^2/4\alpha t}, \quad t > 0\,. \tag{31.16}$$

To enforce the boundary condition $T = 0$ at $x = 0$ for the *semi*-infinite solid, superimpose a source function at $x = a$, $y = z = 0$, with a negative source function at $x = -a$, $y = z = 0$:

$$T(t, x, y, z) = \left(\frac{1}{4\pi\alpha t}\right)^{3/2} \left\{ \exp\left[-\frac{(x-a)^2 + y^2 + z^2}{4\alpha t}\right] \right. \\ \left. - \underbrace{\exp\left[-\frac{(x+a)^2 + y^2 + z^2}{4\alpha t}\right]}_{\substack{\text{fictitious image source} \\ \text{required to maintain} \\ T = 0 \text{ at } x = 0}} \right\}, \quad t > 0\,,\ x > 0\,. \tag{31.17}$$

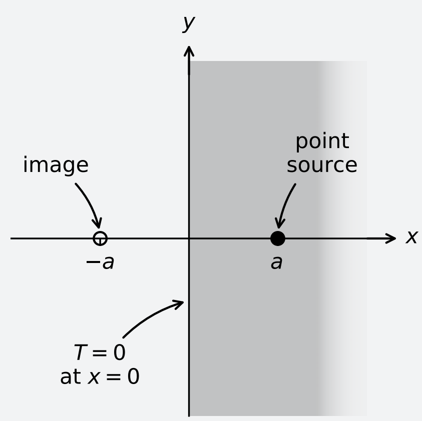


Figure 31.3: Image Source

32 Green Functions

We have the following methods for finding Green functions:

- Sum over eigenfunctions (discussed previously).
- Use solutions to the homogeneous equation and boundary conditions on either side of a surface containing the source point that are matched on that surface with the required jump.
- Take the sum of a singular fundamental solution and a smooth solution of the homogeneous problem which fixes the boundary conditions.

Explore the latter two methods in the following example.

Ex. 32.1. Circular drum.

$$\nabla^2 u + k^2 u = 0 \tag{32.1}$$

with $u = 0$ when $r = a$.
Clearly $G(\mathrm{x}, \mathrm{x}')$ depends only on r, r', and θ. We have

$$\nabla^2 G + k^2 G = \delta^2(\mathrm{x} - \mathrm{x}')\,. \tag{32.2}$$

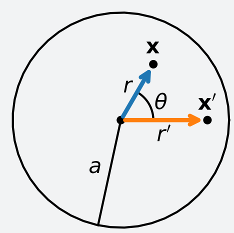


Figure 32.1: Circular Drum

For $\mathrm{x} \neq \mathrm{x}'$, $\nabla^2 G + k^2 G = 0$ so the solution that satisfies the boundary conditions is

$$G = \begin{cases} \sum_{m=0}^{\infty} A_m J_m(kr) \cos m\theta & r < r' \\ \sum_{m=0}^{\infty} B_m [J_m(kr) Y_m(ka) - Y_m(kr) J_m(ka)] \cos m\theta & r > r'\,. \end{cases} \tag{32.3}$$

Note that the factor in square brackets vanishes automatically when $r = a$.
Note also that G is an even function of θ periodic in 2π.

To determine A_m and B_m we must match the solutions along the circle $r = r'$.
G is continuous but its gradient is discontinuous at $r = r'$.

We need to determine what the jump in the gradient across this surface.

Recall Gauss's theorem, $\iiint \nabla \cdot \mathbf{F}\, dV = \oiint \mathbf{F} \cdot d\mathbf{S}$. In 2-dimensions, with $\mathbf{F} = \nabla G$, we have

$$\iint \nabla^2 G\, d\mathcal{A} = \oint \mathbf{n} \cdot \nabla G\, ds\,. \tag{32.4}$$

Integrate the inhomogeneous equation over the area element shown in Fig. 32.2:

$$\underbrace{\iint \nabla^2 G\, d\mathcal{A}}_{\oint \mathbf{n}\cdot\nabla G\, ds} + k^2 \underbrace{\iint G\, d\mathcal{A}}_{0 \text{ as } \epsilon\to 0} = \underbrace{\iint \delta^2(\mathbf{x}-\mathbf{x}')\, d\mathcal{A}}_{1} \tag{32.5a}$$

so, as $\epsilon \to 0$, only the arcs above and below $r = r'$ contribute to the line integral

$$\int_{r'+\epsilon} \frac{\partial G}{\partial r}\, ds - \int_{r'-\epsilon} \frac{\partial G}{\partial r}\, ds = 1 \tag{32.5b}$$

and, since $ds = r'\, d\theta$ for the arcs

$$\int \left(\frac{\partial G}{\partial r}\bigg|_{r'+\epsilon} - \frac{\partial G}{\partial r}\bigg|_{r'-\epsilon} \right) d\theta = \frac{1}{r'} \tag{32.5c}$$

provided $\theta = 0$ is in the domain of integration

$$\Longrightarrow \quad \frac{\partial G}{\partial r}\bigg|_{r'+\epsilon} - \frac{\partial G}{\partial r}\bigg|_{r'-\epsilon} = \frac{1}{r'}\delta(\theta)\,. \tag{32.5d}$$

Let

$$\frac{\partial G}{\partial r}\bigg|_{r'+\epsilon} - \frac{\partial G}{\partial r}\bigg|_{r'-\epsilon} = \sum_{m=0}^{\infty} c_m \cos m\theta \tag{32.5e}$$

$$\Longrightarrow \quad \sum_{m=0}^{\infty} c_m \cos m\theta = \frac{1}{r'}\delta(\theta)\,. \tag{32.5f}$$

Multiply both sides by $\cos m'\theta$ and integrate $\int_{-\pi}^{\pi} d\theta$ to get

$$2\pi c_0 = \frac{1}{r'} \qquad \text{and} \qquad \pi c_m = \frac{1}{r'}\,, \quad m = 1, 2, \ldots\,. \tag{32.5g}$$

Therefore

$$\frac{\partial G}{\partial r}\bigg|_{r'+\epsilon} - \frac{\partial G}{\partial r}\bigg|_{r'-\epsilon} = \frac{1}{2\pi r'} + \frac{1}{\pi r'} \sum_{m=1}^{\infty} \cos m\theta\,. \tag{32.5h}$$

This is the requirement for the discontinuity of the gradient of G at $r = r'$.

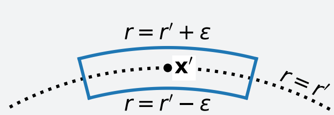


Figure 32.2: Green Function Integral

Thus, at $r' = r$, we require

$$A_m J_m(kr') = B_m[J_m(kr')Y_m(ka) - Y_m(kr')J_m(ka)], \quad m = 0, 1, 2, \ldots \tag{32.6a}$$

$$B_0[J_0'(kr')Y_0(ka) - Y_0'(kr')J_0(ka)] - A_0 J_0'(kr') = \frac{1}{2\pi kr'} \tag{32.6b}$$

$$B_m[J_m'(kr')Y_m(ka) - Y_m'(kr')J_m(ka)] - A_m J_m'(kr') = \frac{1}{\pi kr'}, \quad m = 1, 2, \ldots. \tag{32.6c}$$

The solution is

$$A_0 = \frac{J_0(ka)Y_0(kr') - J_0(kr')Y_0(ka)}{4J_0(ka)} \tag{32.7a}$$

$$B_0 = -\frac{J_0(kr')}{4J_0(ka)} \tag{32.7b}$$

$$A_m = \frac{J_m(ka)Y_m(kr') - J_m(kr')Y_m(ka)}{2J_m(ka)} \qquad m = 1, 2, \ldots \tag{32.7c}$$

$$B_m = -\frac{J_m(kr')}{2J_m(ka)} \qquad m = 1, 2, \ldots \tag{32.7d}$$

where we have used $J_m(x)Y_m'(x) - J_m'(x)Y_m(x) = \dfrac{2}{\pi x}$.

Thus the Green function is

$$G(\mathbf{x}, \mathbf{x}') = \frac{J_0(kr_<)[J_0(ka)Y_0(kr_>) - J_0(kr_>)Y_0(ka)]}{4J_0(ka)} + \sum_{m=1}^{\infty} \frac{J_m(kr_<)[J_m(ka)Y_m(kr_>) - J_m(kr_>)Y_m(ka)]}{2J_m(ka)} \cos m\theta \tag{32.8}$$

with

$$r_< = \begin{cases} r & r < r' \\ r' & r > r' \end{cases} \quad \text{and} \quad r_> = \begin{cases} r' & r < r' \\ r & r > r' \end{cases} \tag{32.9}$$

where $r = \|\mathbf{x}\|$, $r' = \|\mathbf{x}'\|$, and $\cos\theta = \mathbf{x} \cdot \mathbf{x}'/rr'$.

Ex. 32.1 (continued)**.** *Alternative approach for the circular drum.*

Note that we want to solve $\nabla^2 G + k^2 G = \delta^2(\mathbf{x}-\mathbf{x}')$ so G must
(i) have the proper singular behavior at $\mathbf{x}=\mathbf{x}'$, and
(ii) satisfy the boundary conditions.

Therefore we seek a solution of the form

$$G(\mathbf{x},\mathbf{x}') = u(\mathbf{x},\mathbf{x}') + v(\mathbf{x},\mathbf{x}') \tag{32.10}$$

where $u(\mathbf{x},\mathbf{x}')$, known as the **fundamental solution**, is singular at $\mathbf{x}=\mathbf{x}'$ but does not satisfy the boundary conditions, and $v(\mathbf{x},\mathbf{x}')$ is a smooth solution of the *homogeneous* problem that fixes the boundary conditions.

To find $u(\mathbf{x},\mathbf{x}')$, let $\rho = \|\mathbf{x}-\mathbf{x}'\|$ and write $u = u(\rho)$. Integrate over a small circular disk about $\rho = 0$:

$$\underbrace{2\pi\int_0^\rho \nabla^2 u\, d\rho}_{2\pi\rho\frac{du}{d\rho}} + \underbrace{2\pi\int_0^\rho k^2 u\, d\rho}_{\text{vanishes as } \rho\to 0} = \underbrace{\iint \delta^2(\mathbf{x}-\mathbf{x}')\, d\mathcal{A}}_{1}\,. \tag{32.11}$$

As $\rho \to 0$, have $2\pi\rho\frac{du}{d\rho} = 1$ so

$$u(\rho) \sim \frac{1}{2\pi}\ln\rho + \text{const} \quad \text{as } \rho \to 0. \tag{32.12}$$

Recall the singular solution to $\nabla^2 u + k^2 u = 0$ is

$$Y_0(k\rho) \sim \frac{2}{\pi}\ln\rho + \text{const} \quad \text{as } \rho\to 0 \tag{32.13}$$

so take $u(\rho) = \frac{1}{4}Y_0(k\rho)$ and so

$$G = \frac{1}{4}Y_0(k\rho) + v(\mathbf{x},\mathbf{x}')\,. \tag{32.14}$$

We now find $v(\mathbf{x},\mathbf{x}')$ by fixing the boundary conditions.

Since v is a solution to the homogeneous equation, it can be written as

$$v = \sum_{n=0}^{\infty} A_n J_n(kr) \cos n\theta\,. \tag{32.15}$$

Thus, at $r = a$, we have

$$G(r=a) = 0 = \frac{1}{4} Y_0\Big(k \underbrace{\sqrt{a^2 + r'^2 - 2ar'\cos\theta}}_{\text{this is } \rho(r=a)}\Big) + \sum_{n=0}^{\infty} A_n J_n(kr) \cos n\theta\,. \tag{32.16a}$$

so

$$A_0 = -\frac{1}{8\pi J_0(ka)} \int_0^{2\pi} Y_0\Big(k\sqrt{a^2 + r'^2 - 2ar'\cos\theta}\Big)\, d\theta \tag{32.16b}$$

and

$$A_n = -\frac{1}{4\pi J_n(ka)} \int_0^{2\pi} Y_0\Big(k\sqrt{a^2 + r'^2 - 2ar'\cos\theta}\Big) \cos n\theta\, d\theta \tag{32.16c}$$

for $n = 1, 2, \ldots$.

Therefore, another form of the Green function is

$$\begin{aligned} G(\mathrm{x}, \mathrm{x}') = {} & \frac{1}{4} Y_0\left(k\|\mathrm{x} - \mathrm{x}'\|\right) \\ & - \frac{J_0(kr)}{4\pi J_0(ka)} \int_0^{\pi} Y_0\Big(k\sqrt{a^2 + r'^2 - 2ar'\cos\theta'}\Big)\, d\theta' \\ & - \sum_{n=1}^{\infty} \frac{J_n(kr)\cos n\theta}{2\pi J_n(ka)} \int_0^{\pi} Y_0\Big(k\sqrt{a^2 + r'^2 - 2ar'\cos\theta'}\Big) \cos n\theta'\, d\theta'\,. \end{aligned} \tag{32.17}$$

Ex. 32.2. Heating of a slab (redux).

We've seen that problems that are inhomogeneous due to the boundary conditions rather than the differential equation may still be written in terms of a Green function.

Alternatively, a homogeneous equation with inhomogeneous boundary conditions can be transformed into an inhomogeneous equation with homogeneous boundary conditions (and vice versa).

Recall from Ex. 30.4 our infinite slab of thickness d, initially at zero temperature, heated at constant rate q at $x = 0$ and insulated at $x = d$ as shown in Fig. 32.3:

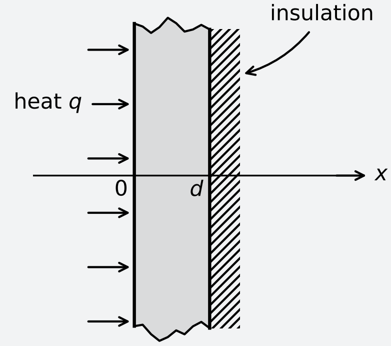


Figure 32.3: Slab Heating Redux

$$\frac{\partial^2 u(t,x)}{\partial x^2} - \frac{1}{\alpha}\frac{\partial u(t,x)}{\partial t} = 0\,, \quad \alpha = \frac{k}{c\rho} \tag{32.18a}$$

with inhomogeneous boundary conditions

$$u(t=0,x) = 0\,, \quad \left.\frac{\partial u}{\partial x}\right|_{x=d} = 0\,, \quad \text{and} \quad \left.\frac{\partial u}{\partial x}\right|_{x=0} = -\frac{q}{k}\,. \tag{32.18b}$$

Transform to a problem with homogeneous boundary conditions with a change of variables:

$$v(t,x) = u(t,x) - w(x) \tag{32.19}$$

where $w(x)$ satisfies

$$\left.\frac{dw}{dx}\right|_{x=d} = 0 \qquad \text{and} \qquad \left.\frac{dw}{dx}\right|_{x=0} = -\frac{q}{k} \tag{32.20}$$

and also choose it so that d^2w/dx^2 gives a simple result. The simplest choice is

$$w(x) = \frac{1}{2}\frac{q}{kd}(x-d)^2 \tag{32.21}$$

which satisfies the boundary conditions and now

$$\frac{\partial^2 v}{\partial x^2} - \frac{1}{\alpha}\frac{\partial v}{\partial t} = -\frac{d^2 w}{dx^2} = -\frac{q}{kd}\,. \tag{32.22a}$$

where v must now satisfy the boundary conditions

$$\left.\frac{\partial v}{\partial x}\right|_{x=d} = \left.\frac{\partial v}{\partial x}\right|_{x=0} = 0\,. \tag{32.22b}$$

We have achieved our goal of transforming to an inhomogeneous equation for v with homogeneous boundary conditions.

An almost trivial particular solution is

$$v_p = \frac{q\alpha}{kd}t \tag{32.23a}$$

and so

$$u_p(t,x) = \frac{q}{kd}\alpha t + \frac{1}{2}\frac{q}{kd}(x-d)^2\,. \tag{32.23b}$$

This is the same particular solution we saw in Ex. 30.4.

We proceed as we did before in Ex. 30.4 to find the characteristic function u_c to satisfy the initial conditions.

Ex. 32.3. Laplace's equation

$$\nabla^2\varphi = 0 \tag{32.24}$$

in an infinite region with $\varphi \to 0$ as $r \to \infty$.

The Green function is a solution to

$$\nabla^2\varphi(\mathbf{x}) = \delta^3(\mathbf{x}-\mathbf{x}')\,. \tag{32.25}$$

Note: φ can only depend on $r = \|\mathbf{x}-\mathbf{x}'\|$ so we take the origin of spherical coordinates to be the point $\mathbf{x}'$.

For $\mathbf{x} \neq \mathbf{x}'$, $\nabla^2\varphi(\mathbf{x}) = 0$ so solutions have the form

$$\varphi(r,\theta,\phi) = \left\{ \begin{matrix} r^{\ell} \\ r^{-(\ell+1)} \end{matrix} \right\} P_\ell^m(\cos\theta)e^{\pm im\phi}\,. \tag{32.26}$$

Spherical symmetry implies $\ell = m = 0$.

The boundary condition $\varphi \to 0$ as $r \to \infty$ then implies

$$\varphi(r) = \frac{A}{r} \tag{32.27}$$

where we now must determine A.

Integrate the inhomogeneous equation over a spherical ball of radius a about the origin:

$$\iiint_{r<a} \nabla^2\varphi\,dV = \iiint_{r<a} \delta^3(\mathbf{x}-\mathbf{x}')\,dV = 1 \tag{32.28a}$$

but, using Gauss's theorem,

$$\iiint_{r<a} \nabla^2\varphi\,dV = \oiint_{r=a} \left(\frac{\partial\varphi}{\partial r}\right) dS = 4\pi a^2 \left[-\frac{A}{r^2}\right]_{r=a} = -4\pi A \tag{32.28b}$$

so we find $A = -\dfrac{1}{4\pi}$ and therefore

$$G(\mathbf{x},\mathbf{x}') = -\frac{1}{4\pi}\frac{1}{\|\mathbf{x}-\mathbf{x}'\|}\,. \tag{32.29}$$

Ex. 32.4. Wave equation

$$\nabla^2\psi(t,\mathbf{x}) - \frac{1}{c^2}\frac{\partial\psi(t,\mathbf{x})}{\partial t^2} = 0 \tag{32.30}$$

over an infinite domain.

The Green function is a solution to the inhomogeneous equation

$$\nabla^2\psi(t,\mathbf{x}) - \frac{1}{c^2}\frac{\partial\psi(t,\mathbf{x})}{\partial t^2} = \delta(t-t')\delta(\mathbf{x}-\mathbf{x}'). \tag{32.31}$$

Note: the solution only depends on $t-t'$ and $\mathbf{x}-\mathbf{x}'$, so we have translational invariance in t and $\mathbf{x}$. Therefore, without loss of generality, set $t'=0$ and $\mathbf{x}'=0$.

Let

$$\psi(t,\mathbf{x}) = \frac{1}{(2\pi)^4}\iiiint \Psi(\omega,\mathbf{k})e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\,d\omega\,dk_x\,dk_y\,dk_z \tag{32.32a}$$

$$\Psi(\omega,\mathbf{k}) = \iiiint \psi(t,\mathbf{x})e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\,dt\,dx\,dy\,dz\,. \tag{32.32b}$$

The Fourier transform of the inhomogeneous equation is

$$\left(-k^2+\frac{\omega^2}{c^2}\right)\Psi = 1 \tag{32.33a}$$

$$\implies \quad \Psi(\omega,\mathbf{k}) = \frac{c^2}{\omega^2-c^2k^2} \tag{32.33b}$$

where $k=\|\mathbf{k}\|$, and we want

$$\psi(t,\mathbf{x}) = \frac{c^2}{(2\pi)^4}\iiiint \frac{e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}}{\omega^2-c^2k^2}\,d\omega\,dk_x\,dk_y\,dk_z\,. \tag{32.34}$$

To do this integral, choose the axis of spherical polar coordinates in $\mathbf{k}$ space along $\mathbf{x}$. Then $\mathbf{k}\cdot\mathbf{x} = kr\cos\theta$. Also let $\mu = \cos\theta$ so $d\mu = \sin\theta\, d\theta$. Then

$$\psi(t,\mathbf{x}) = \frac{c^2}{(2\pi)^4}\int_{\phi=0}^{2\pi}\int_{\mu=-1}^{1}\int_{k=0}^{\infty}\int_{\omega=-\infty}^{\infty}\frac{e^{i(kr\cos\theta-\omega t)}}{\omega^2-c^2k^2}k^2\, d\omega\, dk\, d\mu\, d\phi \tag{32.35a}$$

$$= \frac{c^2}{(2\pi)^3}\int_{k=0}^{\infty}\int_{\omega=-\infty}^{\infty}\underbrace{\left[\int_{\mu=-1}^{1} e^{ikr\cos\theta}\, d\mu\right]}_{\frac{1}{ikr}(e^{ikr}-e^{-ikr})}\frac{e^{-i\omega t}}{\omega^2-c^2k^2}k^2\, d\omega\, dk \tag{32.35b}$$

$$= \frac{c^2}{(2\pi)^3}\frac{1}{ir}\int_{k=0}^{\infty}\int_{\omega=-\infty}^{\infty}\frac{e^{-i\omega t}}{\omega^2-c^2k^2}(e^{ikr}-e^{-ikr})k\, d\omega\, dk \tag{32.35c}$$

$$= \frac{c^2}{(2\pi)^3}\frac{1}{ir}\int_{k=-\infty}^{\infty}\left[\int_{\omega=-\infty}^{\infty}\frac{e^{-i\omega t}}{\omega^2-c^2k^2}\, d\omega\right]e^{ikr}k\, dk\,. \tag{32.35d}$$

We evaluate the integral over ω

$$\int_{\omega=-\infty}^{\infty}\frac{e^{-i\omega t}}{\omega^2-c^2k^2}\, d\omega\,. \tag{32.36}$$

Note that the integrand has two poles on the real axis, $\omega = -|ck|$ and $\omega = +|ck|$. We therefore modify the integral to be

$$\int_{\omega=-\infty+i\epsilon}^{\infty+i\epsilon}\frac{e^{-i\omega t}}{\omega^2-c^2k^2}\, d\omega \tag{32.37}$$

where we will eventually take the limit $\epsilon \to 0$.

- When $t < 0$, close contour in upper half plane as in Fig. 32.4. The arc C_R is $\omega = Re^{i\theta}, 0 \le \theta \le \pi$, so

$$e^{-i\omega t} = e^{-iRt\cos\theta}e^{Rt\sin\theta}$$
$$\to 0 \text{ as } R \to \infty \text{ for } t < 0. \tag{32.38}$$

  Therefore the integral is zero since the contour encloses no poles.

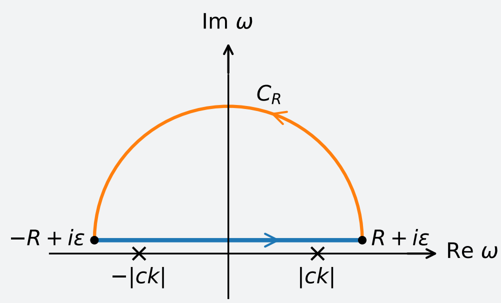


Figure 32.4: Contour Closed in Upper Half Plane

- When $t > 0$, close contour in lower half plane as in Fig. 32.5.
  The arc C_R is $\omega = Re^{-i\theta}$, $0 \le \theta \le \pi$, so

$$\begin{aligned} e^{-i\omega t} &= e^{-iRt\cos\theta} e^{-Rt\sin\theta} \\ &\to 0 \text{ as } R \to \infty \text{ for } t > 0. \end{aligned} \tag{32.39}$$

  Poles are now enclosed!

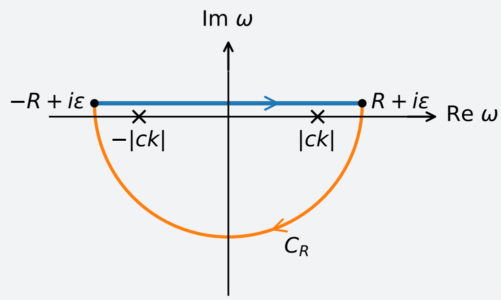


Figure 32.5: Contour Closed in Lower Half Plane

  Now note that

$$\oint_C e^{-i\omega t} \underbrace{\left(\frac{1}{\omega - ck} - \frac{1}{\omega + ck}\right)}_{\frac{2ck}{\omega^2 - c^2k^2}} d\omega = 2\pi i (e^{-ickt} - e^{ickt}) \tag{32.40}$$

  for C enclosing the poles so we find

$$\int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega^2 - c^2k^2} \, d\omega = -\frac{\pi i}{ck}(e^{-ickt} - e^{ickt}) \tag{32.41}$$

  where the negative sign arises because the contour in Fig. 32.5 is traversed clockwise rather than counterclockwise.

Therefore, for $t > 0$, we have

$$\psi(t, \mathbf{x}) = -\frac{c}{8\pi^2 r} \int_{-\infty}^{\infty} e^{ikr}(e^{-ikct} - e^{ikct})\, dk \tag{32.42a}$$

$$= -\frac{c}{4\pi r}[\delta(r - ct) - \delta(r + ct)]. \tag{32.42b}$$

The second term will never contribute because r and t are both positive.

Thus, the Green function for the wave equation is

$$G(t-t',\mathrm{x}-\mathrm{x}') = \begin{cases} 0 & t < t' \\ -\dfrac{c}{4\pi\|\mathrm{x}-\mathrm{x}'\|}\delta\Big(\|\mathrm{x}-\mathrm{x}'\| - c(t-t')\Big) & t > t'\,. \end{cases} \tag{32.43}$$

This is the *causal* or *retarded* Green function.

Had we shifted the contour below the poles we would have found the *advanced* Green function

$$G(t-t',\mathrm{x}-\mathrm{x}') = \begin{cases} -\dfrac{c}{4\pi\|\mathrm{x}-\mathrm{x}'\|}\delta\Big(\|\mathrm{x}-\mathrm{x}'\| + c(t-t')\Big) & t < t' \\ 0 & t > t'\,. \end{cases} \tag{32.44}$$

These different flavors of Green functions correspond to different kinds of boundary conditions. For example, if nothing happens before a disturbance, we use the causal Green function.

Ex. 32.5. Liénard-Wiechert potential.

Consider

$$\nabla^2\varphi - \frac{1}{c^2}\frac{\partial^2\varphi}{\partial t^2} = f(t,\mathrm{x}). \tag{32.45}$$

The solution is

$$\varphi(t,\mathrm{x}) = -\frac{c}{4\pi}\iiiint f(t',\mathrm{x}')\frac{\delta\Big(\|\mathrm{x}-\mathrm{x}'\| - c(t-t')\Big)}{\|\mathrm{x}-\mathrm{x}'\|}\,dt'\,dV' \tag{32.46a}$$

$$= -\frac{1}{4\pi}\iiint \frac{f\Big(t-\frac{1}{c}\|\mathrm{x}-\mathrm{x}'\|,\mathrm{x}'\Big)}{\|\mathrm{x}-\mathrm{x}'\|}\,dV'. \tag{32.46b}$$

This is the **retarded potential** because the source function is evaluated at the retarded time $t-\frac{1}{c}\|\mathrm{x}-\mathrm{x}'\|$.

For example, consider a point source moving on a prescribed path $\mathrm{x}_0(t)$ so that

$$f(t,\mathrm{x}) = \delta^3\Big(\mathrm{x}-\mathrm{x}_0(t)\Big). \tag{32.47}$$

Therefore

$$\varphi(t,\mathrm{x}) = -\frac{1}{4\pi}\iiiint \frac{\delta^3\Big(\mathrm{x}'-\mathrm{x}_0(t')\Big)\delta\Big(t-t'-\frac{1}{c}\|\mathrm{x}-\mathrm{x}'\|\Big)}{\|\mathrm{x}-\mathrm{x}'\|}\,dt'\,dV'. \tag{32.48}$$

First do the integral $\iiint dV'$:

$$\varphi(t,\mathrm{x}) = -\frac{1}{4\pi}\int \frac{\delta\Big(t-t'-\frac{1}{c}\|\mathrm{x}-\mathrm{x}_0(t')\|\Big)}{\|\mathrm{x}-\mathrm{x}_0(t')\|}\,dt'. \tag{32.49}$$

Note: the integrand contains $\delta(g(t'))$ with

$$g(t') = t - t' - \frac{1}{c}\|\mathrm{x}-\mathrm{x}_0(t')\| \tag{32.50a}$$

which has a single root at the **retarded time** t_r where the worldline of the particle passes through the past light cone, see Fig. 32.6,

$$g(t_r) = 0 \qquad \text{for} \qquad t_r = t - \frac{1}{c}\|\mathrm{x}-\mathrm{x}_0(t_r)\| \tag{32.50b}$$

(note that x_0 is evaluated at time t_r in the definition of t_r) and

$$\left.\frac{dg}{dt'}\right|_{t'=t_r} = -1 + \frac{1}{c}\frac{\mathbf{v}_0(t_r)\cdot(\mathrm{x}-\mathrm{x}_0(t_r))}{\|\mathrm{x}-\mathrm{x}_0(t_r)\|} \tag{32.50c}$$

where $\mathbf{v}_0(t) = d\mathrm{x}(t)/dt$ is the velocity of the point source.

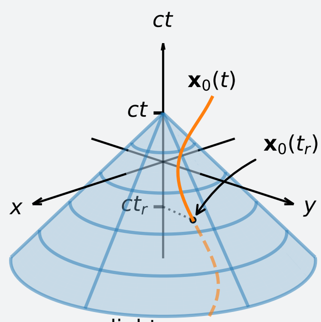


Figure 32.6: Light Cone and Retarded Time

We use the identity of Eq. (14.10) to perform the integral $\int dt'$:

$$\varphi(t,\mathrm{x}) = -\frac{1}{4\pi}\frac{1}{\|\mathrm{x}-\mathrm{x}_0(t_r)\|}\frac{1}{1-\frac{1}{c}\frac{\mathbf{v}_0(t_r)\cdot(\mathrm{x}-\mathrm{x}_0(t_r))}{\|]\mathrm{x}-\mathrm{x}_0(t_r)\|}} \tag{32.51}$$

and thus we obtain the **Liénard-Wiechert potential**

$$\boxed{\begin{aligned}&\varphi(t,\mathrm{x}) = -\frac{1}{4\pi}\frac{1}{\|\mathrm{x}-\mathrm{x}_0(t_r)\| - \frac{1}{c}\mathbf{v}_0(t_r)\cdot(\mathrm{x}-\mathrm{x}_0(t_r))}\\ &\text{with}\quad t_r = t - \frac{1}{c}\|\mathrm{x}-\mathrm{x}_0(t_r)\|.\end{aligned}} \tag{32.52}$$

Integral Equations

Green functions can be used to convert a partial differential equation with boundary conditions into an integral equation.

Consider

$$\nabla^2\varphi(\mathbf{x}) = \rho(\mathbf{x})\varphi(\mathbf{x}) \tag{32.53}$$

in some region with some suitable boundary conditions.
Suppose that $G(\mathbf{x}, \mathbf{x}')$ is the Green function for the Laplace equation in the region with the boundary conditions so that

$$\nabla^2 G(\mathbf{x}, \mathbf{x}') = \delta^3(\mathbf{x} - \mathbf{x}') \tag{32.54}$$

and so the solution of

$$\nabla^2\varphi(\mathbf{x}) = f(\mathbf{x}) \tag{32.55}$$

is

$$\varphi(\mathbf{x}) = \iiint G(\mathbf{x}, \mathbf{x}') f(\mathbf{x}')\, dV'\,. \tag{32.56}$$

Then, with $f(\mathbf{x}) = \rho(\mathbf{x})\varphi(\mathbf{x})$ we have

$$\varphi(\mathbf{x}) = \iiint G(\mathbf{x}, \mathbf{x}')\rho(\mathbf{x}')\varphi(\mathbf{x}')\, dV'\,. \tag{32.57}$$

This **integral equation** for $\varphi(\mathbf{x})$ is equivalent to the differential equation of Eq. (32.53) with the boundary conditions built into it.

The above integral equation is an example of a homogeneous linear integral equation. One example of an inhomogeneous integral equation is **Fredholm integral equation** of the second kind

$$\varphi(\mathbf{x}) = f(\mathbf{x}) + \lambda \iiint K(\mathbf{x}, \mathbf{x}')\varphi(\mathbf{x}')\, dV' \tag{32.58}$$

where $K(\mathbf{x}, \mathbf{x}')$ is called the **kernel**.

We will only briefly touch on solving integral equations.

Neumann series

Consider the Fredholm integral equation of the second kind

$$\varphi(\mathrm{x}) = f(\mathrm{x}) + \lambda \iiint K(\mathrm{x},\mathrm{x}')\varphi(\mathrm{x}')\,dV' \tag{32.59}$$

and solve this by iteration: begin with the approximation

$$\varphi(\mathrm{x}) \approx f(\mathrm{x})\,. \tag{32.60}$$

Now substitute the integral equation into itself to build up successive refinements to this approximation

$$\varphi(\mathrm{x}) = f(\mathrm{x}) + \lambda \iiint K(\mathrm{x},\mathrm{x}')\left[f(\mathrm{x}') + \lambda \iiint K(\mathrm{x}',\mathrm{x}'')\varphi(\mathrm{x}'')\,dV''\right] dV' \tag{32.61a}$$

$$= f(\mathrm{x}) + \lambda \iiint K(\mathrm{x},\mathrm{x}')f(\mathrm{x}')\,dV' \tag{32.61b}$$
$$+\lambda^2 \iiint\!\!\!\iiint K(\mathrm{x},\mathrm{x}')K(\mathrm{x}',\mathrm{x}'')\varphi(\mathrm{x}'')\,dV'\,dV''$$

so our next level of approximation is

$$\varphi(\mathrm{x}) \approx f(\mathrm{x}) + \lambda \iiint K(\mathrm{x},\mathrm{x}')f(\mathrm{x}')\,dV'\,. \tag{32.62}$$

Repeat...

$$\varphi(\mathrm{x}) = f(\mathrm{x}) + \lambda \iiint K(\mathrm{x},\mathrm{x}')f(\mathrm{x}')\,dV' \tag{32.63}$$
$$+\lambda^2 \iiint\!\!\!\iiint K(\mathrm{x},\mathrm{x}')K(\mathrm{x}',\mathrm{x}'')f(\mathrm{x}'')\,dV'\,dV''$$
$$+\cdots\,.$$

This is known as the **Neumann series** and it converges for small λ provided $K(\mathrm{x},\mathrm{x}')$ is bounded.

If we let $\mathcal{L}$ be a linear integral operator defined by

$$\mathcal{L}\, f(\mathbf{x}) = \lambda \iiint K(\mathbf{x},\mathbf{x}')f(\mathbf{x}')\, dV' \tag{32.64}$$

then our integral equation can be written as

$$(1-\mathcal{L})\varphi(\mathbf{x}) = f(\mathbf{x}) \tag{32.65}$$

and the formal solution would be

$$\varphi(\mathbf{x}) = \frac{1}{1-\mathcal{L}} f(\mathbf{x}) \tag{32.66}$$

where $(1-\mathcal{L})^{-1}$ is some operator to be determined.

We now write the Neumann series solution as

$$\varphi(\mathbf{x}) = \sum_{n=0}^{\infty} \mathcal{L}^n f(\mathbf{x}) \tag{32.67}$$

where $\mathcal{L}^0 f(\mathbf{x}) = f(\mathbf{x})$ and $\mathcal{L}^n f(\mathbf{x}) = \mathcal{L}[\mathcal{L}^{n-1} f(\mathbf{x})]$. Therefore

$$\frac{1}{1-\mathcal{L}} = \sum_{n=0}^{\infty} \mathcal{L}^n \,. \tag{32.68}$$

The Neumann series thus generalizes the geometric series and brings us by a commodius vicus of recirculation back to §1.

Ex. 32.6. Scattering in quantum mechanics.

Consider the equation

$$\nabla^2\psi(\mathsf{x}) - \frac{2m}{\hbar}V(\mathsf{x})\psi(\mathsf{x}) + k^2\psi(\mathsf{x}) = 0 \tag{32.69}$$

with boundary conditions that $\psi(\mathsf{x})e^{-iEt/\hbar}$ is an incident plane wave with wave vector $\mathbf{k}_0$ plus outgoing waves as $\|\mathsf{x}\| \to \infty$ and $k^2 = k_0^2 = 2mE/\hbar^2$.

The Helmholtz equation

$$\nabla^2\psi(\mathsf{x}) + k^2\psi(\mathsf{x}) = f(\mathsf{x}) \tag{32.70}$$

with outgoing wave boundary condition has the Green function

$$G(\mathsf{x},\mathsf{x}') = -\frac{1}{4\pi}\frac{e^{ik\|\mathsf{x}-\mathsf{x}'\|}}{\|\mathsf{x}-\mathsf{x}'\|} \tag{32.71}$$

so the differential equation can be transformed into the integral equation

$$\psi(\mathsf{x}) = \underbrace{e^{i\mathbf{k}_0\cdot\mathsf{x}}}_{\text{incident wave}} - \underbrace{\frac{2m}{4\pi\hbar^2}\iiint\frac{e^{ik\|\mathsf{x}-\mathsf{x}'\|}}{\|\mathsf{x}-\mathsf{x}'\|}V(\mathsf{x}')\psi(\mathsf{x}')\,dV'}_{\text{outgoing wave}}\,. \tag{32.72}$$

The first iteration in the Neumann series gives the **Born approximation**

$$\psi(\mathsf{x}) \approx e^{i\mathbf{k}_0\cdot\mathsf{x}} - \frac{m}{2\pi\hbar^2}\iiint\frac{e^{ik\|\mathsf{x}-\mathsf{x}'\|}}{\|\mathsf{x}-\mathsf{x}'\|}V(\mathsf{x}')e^{i\mathbf{k}_0\cdot\mathsf{x}'}\,dV'\,. \tag{32.73}$$

Problems

Problem 37.

Find the lowest frequency of oscillation of acoustic waves in a hollow sphere of radius a. The boundary condition is $\psi = 0$ at $r = a$ and ψ obeys the differential equation

$$\nabla^2\psi = \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}\,.$$

Problem 38.

A sphere of radius a is at temperature $T = 0$ throughout. At time $t = 0$ it is immersed in a liquid bath at temperature T_0. Find the subsequent temperature distribution $T(r, t)$ inside the sphere. This distribution satisfies:

$$\nabla^2 T - \frac{1}{\alpha}\frac{\partial T}{\partial t} = 0\,.$$

Problem 39.

Find the three lowest eigenvalues of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

for a particle confined in a cylindrical box of radius a and height b where $\psi = 0$ on the walls and $a \approx b$.

Zeros of the Bessel functions:
$J_0(x) = 0$ for $x = 2.404, 5.520, \quad 8.654, \ldots$
$J_1(x) = 0$ for $x = 3.832, 7.016, 10.173, \ldots$
$J_2(x) = 0$ for $x = 5.135, 8.417, 11.619, \ldots.$

Appendix

A Series Expansions

Binomial series

$$(1+x)^{\alpha} = 1 + \alpha x + \frac{\alpha(\alpha-1)}{2!}x^2 + \frac{\alpha(\alpha-1)(\alpha-2)}{3!}x^3 + \cdots$$
$$= 1 + \binom{\alpha}{1}x + \binom{\alpha}{2}x^2 + \binom{\alpha}{3}x^3 + \cdots . \qquad \text{(A.1)}$$

Special cases:

$$(1+x)^2 = 1 + 2x + x^2 \qquad \text{(A.2)}$$
$$(1+x)^3 = 1 + 3x + 3x^2 + x^3 \qquad \text{(A.3)}$$
$$(1+x)^{-1} = 1 - x + x^2 - x^3 + x^4 - \cdots \qquad -1 < x < 1 \qquad \text{(A.4)}$$
$$(1+x)^{-2} = 1 - 2x + 3x^2 - 4x^3 + 5x^4 - \cdots \qquad -1 < x < 1 \qquad \text{(A.5)}$$
$$(1+x)^{-3} = 1 - 3x + 6x^2 - 10x^3 + 15x^4 - \cdots \qquad -1 < x < 1 \qquad \text{(A.6)}$$
$$(1+x)^{1/2} = 1 + \frac{1}{2}x - \frac{1}{2\cdot 4}x^2 + \frac{1\cdot 3}{2\cdot 4\cdot 6}x^3 - \cdots \qquad -1 < x \le 1 \qquad \text{(A.7)}$$
$$(1+x)^{-1/2} = 1 - \frac{1}{2}x + \frac{1\cdot 3}{2\cdot 4}x^2 - \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}x^3 + \cdots \qquad -1 < x \le 1 \qquad \text{(A.8)}$$
$$(1+x)^{1/3} = 1 + \frac{1}{3}x - \frac{2}{3\cdot 6}x^2 + \frac{2\cdot 5}{3\cdot 6\cdot 9}x^3 - \cdots \qquad -1 < x \le 1 \qquad \text{(A.9)}$$
$$(1+x)^{-1/3} = 1 - \frac{1}{3}x + \frac{1\cdot 4}{3\cdot 6}x^2 - \frac{1\cdot 4\cdot 7}{3\cdot 6\cdot 9}x^3 - \cdots \qquad -1 < x \le 1 \qquad \text{(A.10)}$$

Series for exponential and logarithmic functions

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \qquad -\infty < x < \infty \qquad \text{(A.11)}$$
$$\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \cdots \qquad -1 < x \le 1 \qquad \text{(A.12)}$$
$$\frac{1}{2}\ln\left(\frac{1+x}{1-x}\right) = x + \frac{x^3}{3} + \frac{x^5}{5} + \frac{x^7}{7} + \cdots \qquad -1 < x < 1 \qquad \text{(A.13)}$$
$$\ln x = 2\left\{\left(\frac{x-1}{x+1}\right) + \frac{1}{2}\left(\frac{x-1}{x+1}\right)^3 + \frac{1}{5}\left(\frac{x-1}{x+1}\right)^5 + \cdots\right\} \qquad x > 0 \qquad \text{(A.14)}$$

Series for trigonometric functions

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots \qquad -\infty < x < \infty \qquad \text{(A.15)}$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \qquad -\infty < x < \infty \qquad \text{(A.16)}$$

$$\tan x = x + \frac{x^3}{3} + \frac{2x^5}{15} + \cdots + \frac{2^{2n}(2^{2n}-1)B_n x^{2n-1}}{(2n)!} + \cdots \qquad |x| < \frac{\pi}{2} \qquad \text{(A.17)}$$

$$\cot x = \frac{1}{x} - \frac{x}{3} - \frac{x^3}{45} - \cdots - \frac{2^{2n}B_n x^{2n-1}}{(2n)!} - \cdots \qquad 0 < |x| < \pi \qquad \text{(A.18)}$$

$$\arcsin x = x + \frac{1}{2}\frac{x^3}{3} + \frac{1\cdot 3}{2\cdot 4}\frac{x^5}{5} + \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}\frac{x^7}{7} + \cdots \qquad |x| < 1 \qquad \text{(A.19)}$$

$$\arccos x = \frac{\pi}{2} - \arcsin x \qquad \text{(A.20)}$$

$$\arctan x = x - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} \qquad |x| < 1 \qquad \text{(A.21)}$$

$$\arctan x = \pm\frac{\pi}{2} - \frac{1}{x} + \frac{1}{3x^3} - \frac{1}{5x^5} + \cdots \qquad x \gtrless 0,\ |x| \geq 1 \qquad \text{(A.22)}$$

$$\operatorname{arccot} x = \frac{\pi}{2} - \arctan x \qquad \text{(A.23)}$$

Series for hyperbolic functions

$$\sinh x = x + \frac{x^3}{3!} + \frac{x^5}{5!} + \frac{x^7}{7!} + \cdots \qquad -\infty < x < \infty \qquad \text{(A.24)}$$

$$\cosh x = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \frac{x^6}{6!} + \cdots \qquad -\infty < x < \infty \qquad \text{(A.25)}$$

$$\tanh x = x - \frac{x^3}{3} + \cdots + \frac{(-1)^{n-1}2^{2n}(2^{2n}-1)B_n x^{2n-1}}{(2n)!} + \cdots \qquad |x| < \frac{\pi}{2} \qquad \text{(A.26)}$$

$$\coth x = \frac{1}{x} + \frac{x}{3} - \cdots + \frac{(-1)^{n-1}2^{2n}B_n x^{2n-1}}{(2n)!} - \cdots \qquad 0 < |x| < \pi \qquad \text{(A.27)}$$

$$\operatorname{arcsinh} x = x - \frac{1}{2}\frac{x^3}{3} + \frac{1\cdot 3}{2\cdot 4}\frac{x^5}{5} - \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}\frac{x^7}{7} + \cdots \qquad |x| < 1 \qquad \text{(A.28)}$$

$$\operatorname{arcsinh} x = \ln(2x) + \frac{1}{2}\frac{1}{2x^2} - \frac{1\cdot 3}{2\cdot 4}\frac{1}{4z^4} + \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}\frac{1}{6z^6} - \cdots \qquad x > 1 \qquad \text{(A.29)}$$

$$\operatorname{arccosh} x = \ln(2x) - \frac{1}{2}\frac{1}{2x^2} - \frac{1\cdot 3}{2\cdot 4}\frac{1}{4z^4} - \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}\frac{1}{6z^6} - \cdots \qquad x > 1 \qquad \text{(A.30)}$$

$$\operatorname{arctanh} x = x + \frac{x^3}{3} + \frac{x^5}{5} + \frac{x^7}{7} + \cdots \qquad |x| < 1 \qquad \text{(A.31)}$$

$$\operatorname{arccoth} x = \frac{1}{x} + \frac{1}{3x^3} + \frac{1}{5x^5} + \frac{1}{7x^7} + \cdots \qquad |x| > 1 \qquad \text{(A.32)}$$

B Special Functions

Gamma Function

Definition (positive arguments)

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t}\, dt \qquad x > 0 \tag{B.1}$$

Recursion formula

$$\Gamma(x+1) = x\Gamma(x) \tag{B.2}$$
$$\Gamma(n+1) = n! \quad \text{for} \quad n = 0, 1, 2, \cdots \tag{B.3}$$

Negative arguments

Use repeated application of the recursion formula

$$\Gamma(x) = \frac{\Gamma(x+1)}{x} \tag{B.4}$$

Special values

$$\Gamma(\tfrac{1}{2}) = \sqrt{\pi} \tag{B.5}$$
$$\Gamma(n+\tfrac{1}{2}) = \frac{1\cdot 3\cdot 5 \cdots (2n-1)}{2^n}\sqrt{\pi} \qquad n = 1, 2, 3, \ldots \tag{B.6}$$
$$\Gamma(-n+\tfrac{1}{2}) = \frac{(-1)^n 2^n}{1\cdot 3\cdot 5 \cdots (2n-1)}\sqrt{\pi} \qquad n = 1, 2, 3, \ldots \tag{B.7}$$

Relationships

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin x\pi} \qquad \text{Euler's reflection formula} \tag{B.8}$$
$$2^{2x-1}\Gamma(x)\Gamma(x+\tfrac{1}{2}) = \sqrt{\pi}\,\Gamma(2x) \qquad \text{Legendre's duplication formula} \tag{B.9}$$

Asymptotic expansions

$$\Gamma(x) \sim \sqrt{2\pi x}\, x^{x-1/2} e^{-x} \left\{ 1 + \frac{1}{12x} + \frac{1}{288x^2} - \frac{139}{51\,840x^3} + \cdots \right\} \tag{B.10}$$

$$\ln \Gamma(x) \sim x \ln x - x - \frac{1}{2} \ln\left(\frac{x}{2\pi}\right) + \frac{1}{12x} - \frac{1}{360x^3} + \cdots \tag{B.11}$$

$$n! \sim \sqrt{2\pi n}\, n^n e^{-n} \qquad \text{Stirling's formula} \tag{B.12}$$

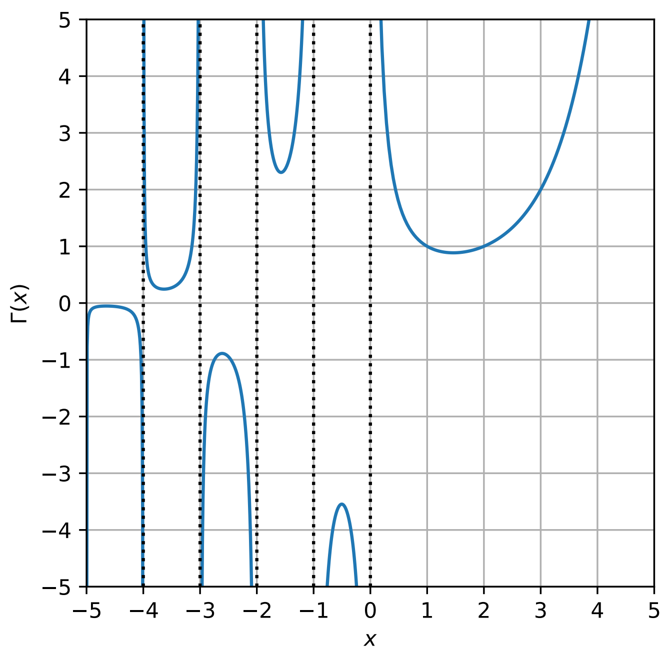


Figure B.1: Gamma Function

Bessel Functions

Bessel differential equation

$$x^2 y'' + xy' + (x^2 - \nu^2)y = 0 \qquad \nu \geq 0 \tag{B.13}$$

Solutions are called Bessel functions of order ν.

Bessel functions of the first kind

$$J_\nu(x) = \frac{x^\nu}{2^\nu \Gamma(\nu+1)} \left\{ 1 - \frac{x^2}{2(2\nu+2)} + \frac{x^4}{2\cdot 4(2\nu+2)(2\nu+4)} - \cdots \right\} \tag{B.14}$$

$$= \sum_{k=0}^{\infty} \frac{(-1)^k (x/2)^{\nu+2k}}{k!\Gamma(\nu+k+1)} \tag{B.15}$$

$$J_{-\nu}(x) = \frac{x^{-\nu}}{2^{-\nu} \Gamma(1-\nu)} \left\{ 1 - \frac{x^2}{2(2-2\nu)} + \frac{x^4}{2\cdot 4(2-2\nu)(4-2\nu)} - \cdots \right\} \tag{B.16}$$

$$= \sum_{k=0}^{\infty} \frac{(-1)^k (x/2)^{2k-\nu}}{k!\Gamma(k+1-\nu)} \tag{B.17}$$

$$J_{-n}(x) = (-1)^n J_n(x) \qquad n = 0, 1, 2, \ldots \tag{B.18}$$

If $\nu \neq 0, 1, 2, \ldots$, $J_\nu(x)$ and $J_{-\nu}(x)$ are linearly independent.
For $\nu = 0, 1$

$$J_0(x) = 1 - \frac{x^2}{2^2} + \frac{x^4}{2^2 \cdot 4^2} - \frac{x^6}{2^2 \cdot 4^2 \cdot 6^2} + \cdots \tag{B.19}$$

$$J_1(x) = \frac{x}{2} - \frac{x^3}{2^2 \cdot 4} + \frac{x^5}{2^2 \cdot 4^2 \cdot 6} - \frac{x^7}{2^2 \cdot 4^2 \cdot 6^2 \cdot 8} + \cdots \tag{B.20}$$

Bessel functions of the second kind

$$Y_\nu(x) = \frac{J_\nu(x)\cos\nu\pi - J_{-\nu}(x)}{\sin\nu\pi} \qquad \nu \neq 0, 1, 2, \ldots \tag{B.21}$$

$$Y_n(x) = \lim_{\nu \to n} Y_\nu(x) \qquad n = 0, 1, 2, \ldots \tag{B.22}$$

$$Y_{-n}(x) = (-1)^n Y_n(x) \qquad n = 0, 1, 2, \ldots \tag{B.23}$$

Hankel functions

$$H_\nu^{(1)}(x) = J_\nu(x) + i\,Y_\nu(x) \tag{B.24}$$

$$H_\nu^{(2)}(x) = J_\nu(x) - i\,Y_\nu(x) \tag{B.25}$$

Limiting forms

As $x \to 0$,

$$J_0(x) \to 1 \tag{B.26}$$

$$J_\nu(x) \sim \frac{1}{\Gamma(\nu+1)}\left(\frac{x}{2}\right)^\nu \qquad \nu \neq -1,-2,-3,\ldots \tag{B.27}$$

$$Y_0(x) \sim \frac{2}{\pi}\ln x \tag{B.28}$$

$$Y_\nu(x) \sim -\frac{\Gamma(\nu)}{\pi}\left(\frac{x}{2}\right)^{-\nu} \qquad \nu > 0 \text{ or } \nu = -\tfrac{1}{2},-\tfrac{3}{2},-\tfrac{5}{2},\ldots \tag{B.29}$$

$$Y_{-\nu}(x) \sim -\frac{\Gamma(\nu)}{\pi}\cos\nu\pi\left(\frac{x}{2}\right)^{-\nu} \qquad \nu > 0,\ \nu \neq \tfrac{1}{2},\tfrac{3}{2},\tfrac{5}{2},\ldots \tag{B.30}$$

$$H_\nu^{(1)}(x) \sim -H_\nu^{(2)}(x) \sim -i\frac{\Gamma(\nu)}{\pi}\left(\frac{x}{2}\right)^{-\nu} \qquad \nu > 0 \tag{B.31}$$

As $x \to \infty$,

$$J_\nu(x) \sim \sqrt{\frac{2}{\pi x}}\cos\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right) \tag{B.32}$$

$$Y_\nu(x) \sim \sqrt{\frac{2}{\pi x}}\sin\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right) \tag{B.33}$$

$$H_\nu^{(1)}(x) \sim \sqrt{\frac{2}{\pi x}}\exp\left[i\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right)\right] \tag{B.34}$$

$$H_\nu^{(2)}(x) \sim \sqrt{\frac{2}{\pi x}}\exp\left[-i\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right)\right] \tag{B.35}$$

Recurrence relations

For $\mathcal{C}_\nu$ denoting J_ν, Y_ν, $H_\nu^{(1)}$, or $H_\nu^{(2)}$

$$\mathcal{C}_{\nu-1}(x) + \mathcal{C}_{\nu+1}(x) = \frac{2\nu}{x}\mathcal{C}_\nu(x) \tag{B.36}$$

$$\mathcal{C}_{\nu-1}(x) - \mathcal{C}_{\nu+1}(x) = 2\mathcal{C}'_\nu(x) \tag{B.37}$$

$$\mathcal{C}'_\nu(x) = \mathcal{C}_{\nu-1}(x) - \frac{\nu}{x}\mathcal{C}_n(\nu) \tag{B.38}$$

$$\mathcal{C}'_\nu(x) = \frac{\nu}{x}\mathcal{C}_\nu(x) - \mathcal{C}_{\nu+1}(x) \tag{B.39}$$

Bessel Functions of Integer Order

Generating function

$$\exp\left[\left(\frac{x}{2}\right)\left(t-\frac{1}{t}\right)\right] = \sum_{n=-\infty}^{\infty} J_n(x)t^n \tag{B.40}$$

Integral forms

$$J_0(x) = \frac{1}{\pi}\int_0^{\pi} \cos(x\sin\theta)\,d\theta \tag{B.41}$$

$$J_n(x) = \frac{1}{\pi}\int_0^{\pi} \cos(n\theta - x\sin\theta)\,d\theta \tag{B.42}$$

$$Y_0(x) = -\frac{2}{\pi}\int_0^{\infty} \cos(x\cosh t)\,dt \tag{B.43}$$

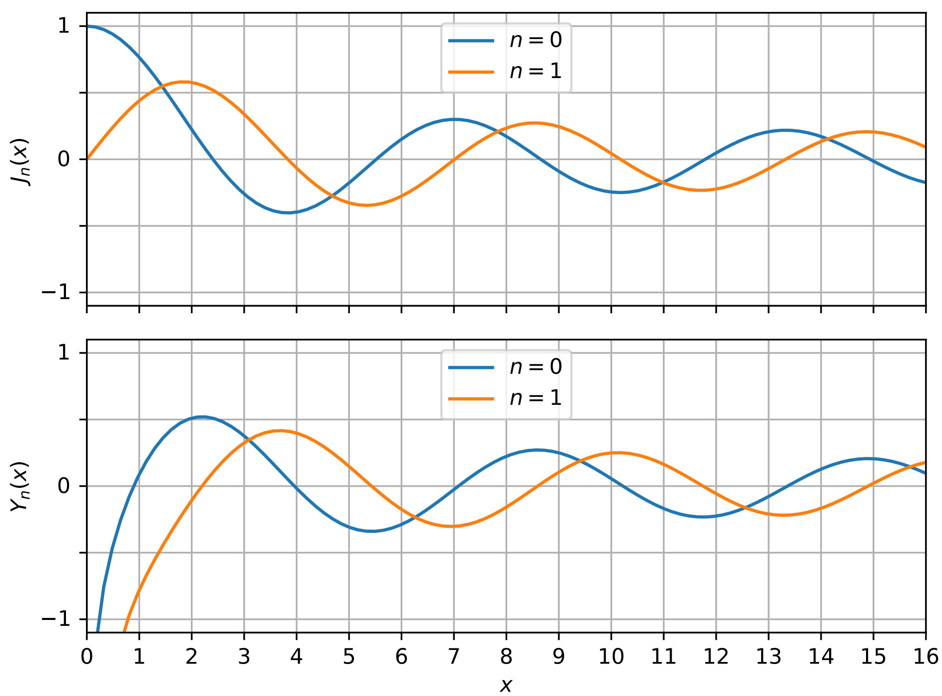


Figure B.2: Bessel Functions of the First and Second Kinds

Definite integrals

$$\int_0^1 [J_n(\alpha t)]^2 \, t \, dt = \tfrac{1}{2}[J_n'(\alpha)]^2 - \tfrac{1}{2}(1 - n^2/\alpha^2)[J_n(\alpha)]^2 \tag{B.44}$$

$$\int_0^1 J_n(\alpha t) J_n(\beta t) \, t \, dt = \frac{\alpha J_n(\beta) J_n'(\alpha) - \beta J_n(\alpha) J_n'(\beta)}{\beta^2 - \alpha^2} \qquad \alpha \neq \beta \tag{B.45}$$

$$\int_0^\infty J_n(xt) J_n(x' t) \, t \, dt = \frac{\delta(x - x')}{x} \tag{B.46}$$

Note in Eq. (B.45) that if α and β are zeros of the Bessel function J_n or of the derivative of the Bessel function J_n' then we have

$$\int_0^1 J_n(x_{np} t) J_n(x_{nq} t) \, t \, dt = 0 \qquad p \neq q \tag{B.47}$$

$$\int_0^1 J_n(y_{np} t) J_n(y_{nq} t) \, t \, dt = 0 \qquad p \neq q \tag{B.48}$$

where x_{np} is the pth zero of J_n and y_{np} is the pth zero of J_n'.

Zeros of Bessel functions

If $J_n(x_{np}) = 0$ and $J_n'(y_{np}) = 0$ for $p = 1, 2, 3, \ldots$ then

$$x_{0p} = 2.4048, \quad 5.5201, \quad 8.6537, \quad \ldots \tag{B.49}$$

$$x_{1p} = 3.8317, \quad 7.0156, \quad 10.1735, \quad \ldots \tag{B.50}$$

$$x_{2p} = 5.1356, \quad 8.4172, \quad 11.6198, \quad \ldots \tag{B.51}$$

$$y_{0p} = 3.8317, \quad 7.0156, \quad 10.1735, \quad \ldots \tag{B.52}$$

$$y_{1p} = 1.8412, \quad 5.3314, \quad 8.5363, \quad \ldots \tag{B.53}$$

$$y_{2p} = 3.0542, \quad 6.7061, \quad 9.9695, \quad \ldots \tag{B.54}$$

Bessel Functions of Half-Integer Order

$$J_{1/2}(x) = \left(\frac{2}{\pi x}\right)^{1/2} \sin x \tag{B.55}$$

$$J_{-1/2}(x) = \left(\frac{2}{\pi x}\right)^{1/2} \cos x \tag{B.56}$$

$$J_{3/2} = \left(\frac{2}{\pi x}\right)^{1/2} \left(\frac{1}{x} \sin x - \cos x\right) \tag{B.57}$$

$$J_{-3/2} = \left(\frac{2}{\pi x}\right)^{1/2} \left(-\frac{1}{x} \cos x - \sin x\right) \tag{B.58}$$

Spherical Bessel Functions

Spherical Bessel differential equation

$$x^2 y''(x) + 2xy'(x) + [x^2 - \ell(\ell+1)]y(x) = 0 \tag{B.59}$$

Spherical Bessel functions of the first, second, and third kind

$$j_\ell(x) = \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x) \tag{B.60}$$

$$y_\ell(x) = \sqrt{\frac{\pi}{2x}} Y_{\ell+1/2}(x) = (-1)^{\ell+1} \sqrt{\frac{\pi}{2x}} J_{-\ell-1/2}(x) \tag{B.61}$$

$$h_\ell^{(1)}(x) = j_\ell(x) + i y_\ell(x) \tag{B.62}$$

$$h_\ell^{(2)}(x) = [h_\ell^{(1)}(x)]^* = j_\ell(x) - i y_\ell(x)\,. \tag{B.63}$$

For $\ell = 0, 1$

$$j_0(x) = \frac{\sin x}{x} \qquad y_0(x) = -\frac{\cos x}{x} \qquad h_0^{(1)}(x) = -i\frac{e^{ix}}{x} \tag{B.64}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad y_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x} \qquad h_1^{(1)}(x) = -\frac{e^{ix}}{x^2}(i + x) \tag{B.65}$$

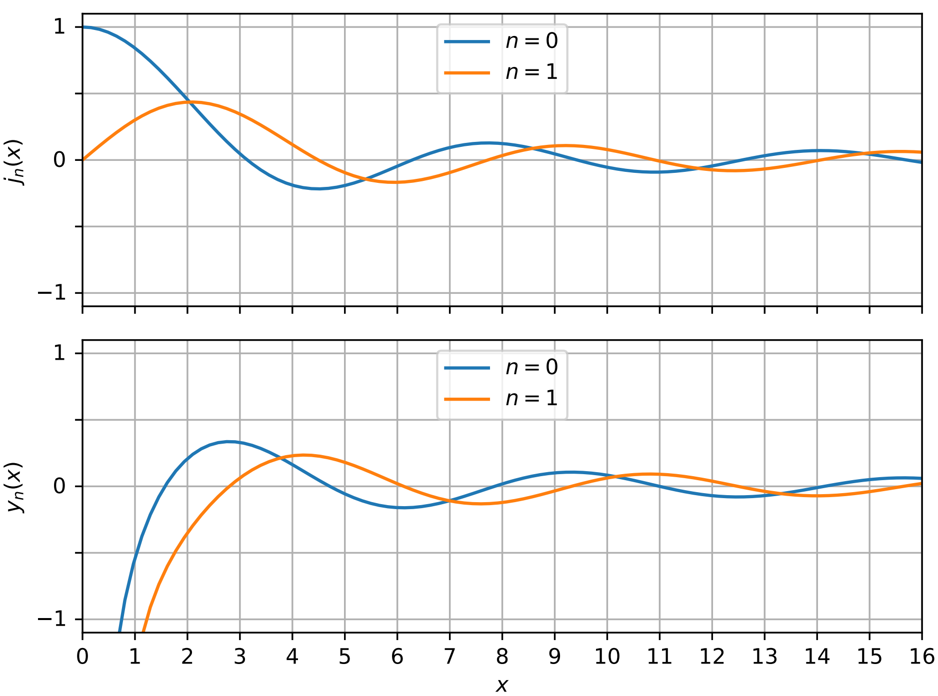


Figure B.3: Spherical Bessel Functions of the First and Second Kinds

Modified Bessel Functions

Modified Bessel differential equation

$$x^2 y''(x) + x y'(x) - (x^2 + \nu^2) y(x) = 0 \tag{B.66}$$

Modified Bessel functions of the first and second kind

$$I_\nu(x) = \frac{J_\nu(ix)}{i^\nu} \tag{B.67}$$

$$K_\nu(x) = \frac{\pi}{2} i^{\nu+1} H_\nu^{(1)}(ix) \tag{B.68}$$

For $\nu = 0, 1$

$$I_0(x) = 1 + \frac{x^2}{2^2} + \frac{x^4}{2^2 \cdot 4^2} + \frac{x^6}{2^2 \cdot 4^2 \cdot 6^2} + \cdots \tag{B.69}$$

$$I_1(x) = \frac{x}{2} + \frac{x^3}{2^2 \cdot 4} + \frac{x^5}{2^2 \cdot 4^2 \cdot 6} + \frac{x^7}{2^2 \cdot 4^2 \cdot 6^2 \cdot 8} + \cdots \tag{B.70}$$

Limiting forms

$$I_\nu(x) \sim \frac{1}{\Gamma(\nu+1)} \left(\frac{x}{2}\right)^\nu \qquad \text{as } x \to 0 \qquad \nu \neq -1, -2, -3, \ldots \tag{B.71}$$

$$K_\nu(x) \sim \frac{1}{2} \Gamma(\nu) \left(\frac{x}{2}\right)^{-\nu} \qquad \text{as } x \to 0 \qquad \nu > 0 \tag{B.72}$$

$$K_0(x) \sim -\ln x \qquad \text{as } x \to 0 \tag{B.73}$$

$$I_\nu(x) \sim \frac{1}{\sqrt{2\pi x}} e^x \qquad \text{as } x \to \infty \tag{B.74}$$

$$K_\nu(x) \sim \sqrt{\frac{\pi}{2x}} e^{-x} \qquad \text{as } x \to \infty \tag{B.75}$$

Modified Bessel Functions of Integer Order

Generating function

$$\exp\left[\left(\frac{x}{2}\right)\left(t+\frac{1}{t}\right)\right] = \sum_{n=-\infty}^{\infty} I_n(x)t^n \tag{B.76}$$

Integral forms

$$I_0(x) = \frac{1}{\pi}\int_0^{\pi} \cosh(x\sin\theta)\,d\theta = \frac{1}{\pi}\int_0^{\pi} e^{x\cos\theta}\,d\theta \tag{B.77}$$

$$K_0(x) = \int_0^{\infty} \cos(x\sinh t)\,dt \tag{B.78}$$

$$I_n(x) = \frac{1}{\pi}\int_0^{\pi} e^{x\cos\theta}\cos(n\theta)\,d\theta \qquad n = 0, 1, 2, \ldots \tag{B.79}$$

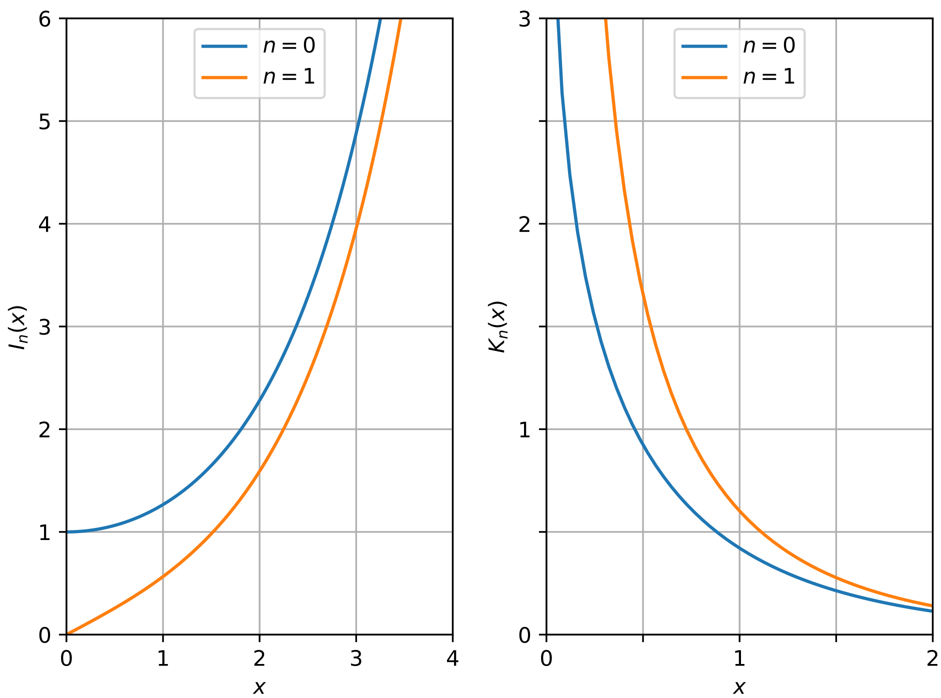


Figure B.4: Modified Bessel Functions of the First and Second Kinds

Legendre Functions

Legendre differential equation

$$(1-x^2)y'' - 2xy' + \ell(\ell+1)y = 0 \tag{B.80}$$

Legendre polynomials

$$P_\ell(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n \qquad \text{Rodrigues's formula} \tag{B.81}$$

For $\ell = 0, 1, 2, 3$

$$P_0(x) = 1 \tag{B.82}$$
$$P_1(x) = x \tag{B.83}$$
$$P_2(x) = \tfrac{1}{2}(3x^2-1) \tag{B.84}$$
$$P_3(x) = \tfrac{1}{2}(5x^3-3x) \tag{B.85}$$

Generating function

$$\frac{1}{\sqrt{1-2tx+t^2}} = \sum_{\ell=0}^{\infty} P_\ell(x)t^\ell \tag{B.86}$$

Recurrence formulas

$$P'_{\ell+1}(x) + P'_{\ell-1}(x) = 2xP'_\ell(x) + P_\ell(x) \tag{B.87}$$
$$P'_{\ell+1}(x) - P'_{\ell-1}(x) = (2\ell+1)P_\ell(x) \tag{B.88}$$
$$P'_{\ell+1}(x) = (\ell+1)P_n(x) + xP'_\ell(x) \tag{B.89}$$
$$P'_{\ell-1}(x) = -\ell P_\ell(x) + xP'_\ell(x) \tag{B.90}$$

Orthogonality and completeness

$$\int_{-1}^{1} P_\ell(x)P_{\ell'}(x)\,dx = \frac{2}{2\ell+1}\delta_{\ell\ell'} \tag{B.91}$$
$$\sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}P_\ell(x)P_\ell(x') = \delta(x-x') \tag{B.92}$$

Special values

$$P_\ell(1) = 1 \tag{B.93}$$
$$P_\ell(-1) = (-1)^n \tag{B.94}$$
$$P_\ell(-x) = (-1)^n P_\ell(x) \tag{B.95}$$
$$P_\ell(0) = \begin{cases} 0 & \ell \text{ odd} \\ (-1)^{\ell/2} \dfrac{1 \cdot 3 \cdot 5 \cdots (\ell - 1)}{2 \cdot 4 \cdot 6 \cdots \ell} & \ell \text{ even} \end{cases} \tag{B.96}$$

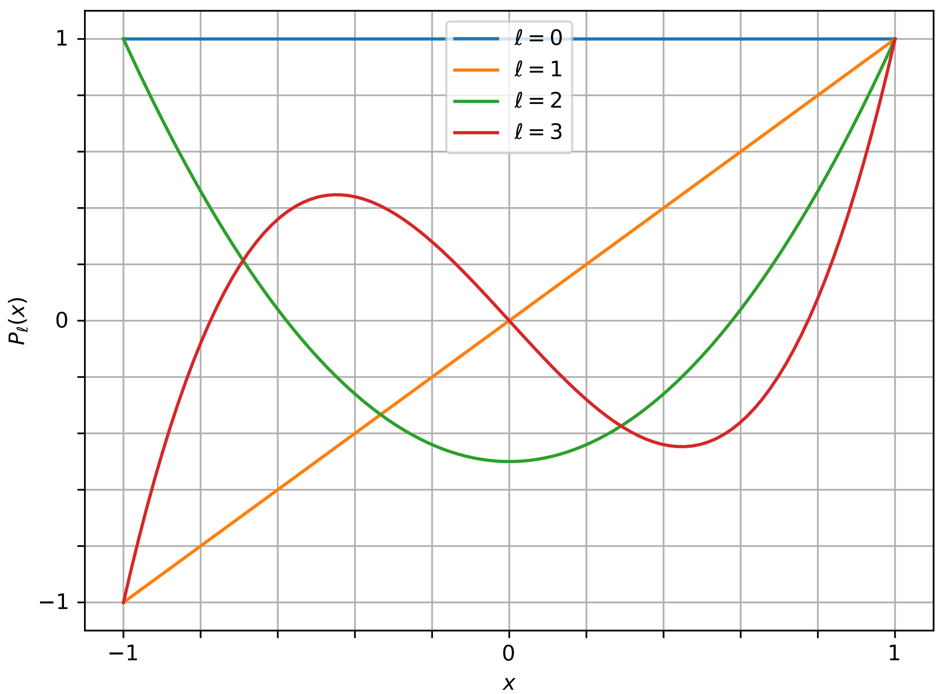


Figure B.5: Legendre Polynomials

Legendre functions of the second kind

$$Q_\ell(x) = \begin{cases} U_\ell(1)V_\ell(x) & \ell = 0,2,4,\ldots \\ -V_\ell(1)U_\ell(x) & \ell = 1,3,5,\ldots \end{cases} \tag{B.97}$$

$$U_\ell(x) = 1 - \frac{\ell(\ell+1)}{2!}x^2 + \frac{\ell(\ell-2)(\ell+1)(\ell+3)}{4!}x^4 - \cdots \tag{B.98}$$

$$V_\ell(x) = x - \frac{(\ell-1)(\ell+2)}{3!}x^3 + \frac{(\ell-1)(\ell-3)(\ell+2)(\ell+4)}{5!}x^5 - \cdots \tag{B.99}$$

$$U_\ell(1) = (-1)^{\ell/2}\frac{2^\ell}{\ell!}\{(\ell/2)!\}^2 \qquad \ell = 0,2,4,\ldots \tag{B.100}$$

$$V_\ell(1) = (-1)^{(\ell-1)/2}\frac{2^{\ell-1}}{\ell!}\{[(\ell-1)/2]!\}^2 \qquad \ell = 1,3,5,\ldots \tag{B.101}$$

For $\ell = 0,1$

$$Q_0(x) = \frac{1}{2}\ln\left(\frac{1+x}{1-x}\right) \tag{B.102}$$

$$Q_1(x) = \frac{x}{2}\ln\left(\frac{1+x}{1-x}\right) - 1 \tag{B.103}$$

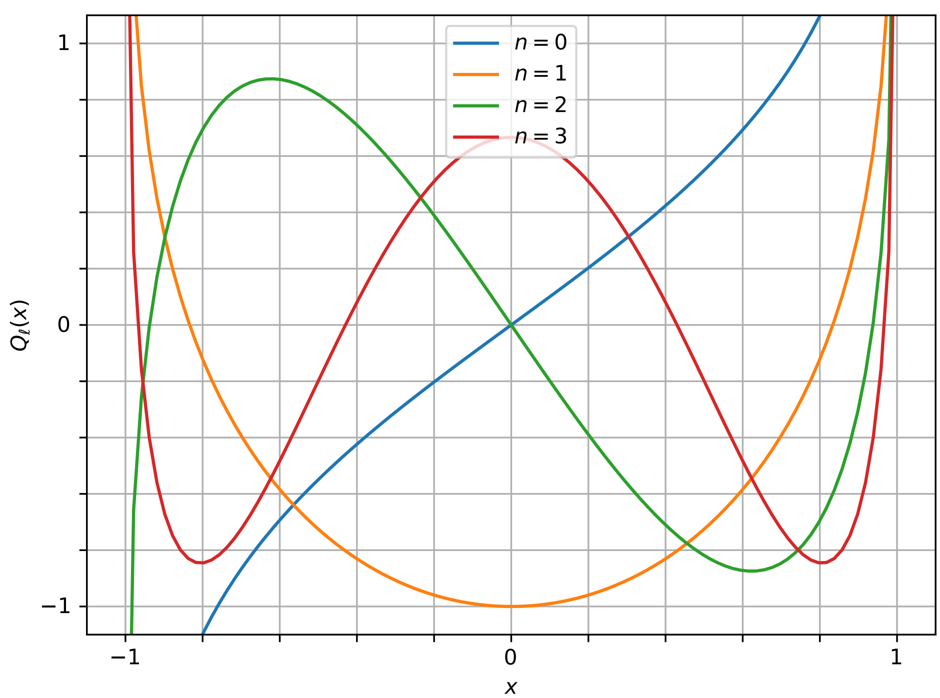


Figure B.6: Legendre Functions of the Second Kind

Associated Legendre Functions

Associated Legendre differential equation

$$(1-x^2)y'' - 2xy' + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right]y = 0 \tag{B.104}$$

Associated Legendre functions of the first kind

$$P_\ell^m = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x) \tag{B.105}$$

$$= \frac{(-1)^m}{2^\ell \ell!} (1-x^2)^{m/2} \frac{d^{\ell+m}}{dx^{\ell+m}} (x^2-1)^\ell \tag{B.106}$$

$$P_\ell^0(x) = P_\ell(x) \tag{B.107}$$

$$P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(x) \tag{B.108}$$

$$P_\ell^m(x) = 0 \qquad \text{if } m > n \tag{B.109}$$

For $\ell = 1, 2$

$$P_1^1(x) = -\sqrt{1-x^2} \tag{B.110}$$

$$P_2^1(x) = -3x\sqrt{1-x^2} \tag{B.111}$$

$$P_2^2(x) = 3(1-x^2) \tag{B.112}$$

Orthogonality

$$\int_{-1}^{1} P_\ell^m(x) P_{\ell'}^m(x)\, dx = \frac{2}{2\ell+1} \frac{(\ell+m)!}{(\ell-m)!} \delta_{\ell\ell'} \tag{B.113}$$

Associated Legendre functions of the second kind

$$Q_\ell^m = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} Q_\ell(x) \tag{B.114}$$

Spherical Harmonics

$$Y_\ell^m(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}P_\ell^m(\cos\theta)e^{im\phi} \tag{B.115}$$

$$Y_\ell^{-m}(\theta,\phi) = (-1)^m[Y_\ell^m(\theta,\phi)]^* \tag{B.116}$$

$$Y_\ell^0(\theta,\phi) = \sqrt{\frac{(2\ell+1)}{4\pi}}P_\ell(\cos\theta) \tag{B.117}$$

For $\ell = 0,1,2$

$$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}} \tag{B.118}$$

$$Y_1^0(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta \tag{B.119}$$

$$Y_1^1(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{i\phi} \tag{B.120}$$

$$Y_2^0(\theta,\phi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta-1) \tag{B.121}$$

$$Y_2^1(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta e^{i\phi} \tag{B.122}$$

$$Y_2^2(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2i\phi} \tag{B.123}$$

Orthogonality and completeness

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} Y_\ell^m(\theta,\phi)[Y_{\ell'}^{m'}(\theta,\phi)]^* \sin\theta\, d\theta\, d\phi = \delta_{\ell\ell'}\delta_{mm'} \tag{B.124}$$

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi)[Y_\ell^m(\theta',\phi')]^* = \frac{1}{\sin\theta}\delta(\theta-\theta')\delta(\phi-\phi') \tag{B.125}$$

Addition theorem

$$\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi)[Y_\ell^m(\theta',\phi')]^* = \frac{2\ell+1}{4\pi}P_\ell(\cos\gamma) \tag{B.126}$$

where

$$\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi') \tag{B.127}$$

With $\theta = \theta'$ and $\phi = \phi'$, $\cos\gamma = 1$ so

$$\sum_{m=-\ell}^{\ell} |Y_\ell^m(\theta,\phi)|^2 = \frac{2\ell+1}{4\pi} \tag{B.128}$$

C Vector Identities

$$\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = \mathbf{b}\cdot(\mathbf{c}\times\mathbf{a}) = \mathbf{c}\cdot(\mathbf{a}\times\mathbf{b}) = \det\begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{bmatrix} \tag{C.1}$$

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = (\mathbf{a}\cdot\mathbf{c})\mathbf{b} - (\mathbf{a}\cdot\mathbf{b})\mathbf{c} \tag{C.2}$$

$$(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d}) = (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d}) - (\mathbf{a}\cdot\mathbf{d})(\mathbf{b}\cdot\mathbf{c}) \tag{C.3}$$

$$\boldsymbol{\nabla}\cdot(\psi\mathbf{a}) = \psi\boldsymbol{\nabla}\cdot\mathbf{a} + (\boldsymbol{\nabla}\psi)\cdot\mathbf{a} \tag{C.4}$$

$$\boldsymbol{\nabla}\times(\psi\mathbf{a}) = \psi\boldsymbol{\nabla}\times\mathbf{a} + (\boldsymbol{\nabla}\psi)\times\mathbf{a} \tag{C.5}$$

$$\boldsymbol{\nabla}(\mathbf{a}\cdot\mathbf{b}) = (\mathbf{a}\cdot\boldsymbol{\nabla})\mathbf{b} + (\mathbf{b}\cdot\boldsymbol{\nabla})\mathbf{a} + \mathbf{a}\times(\boldsymbol{\nabla}\times\mathbf{b}) + \mathbf{b}\times(\boldsymbol{\nabla}\times\mathbf{a}) \tag{C.6}$$

$$\boldsymbol{\nabla}\cdot(\mathbf{a}\times\mathbf{b}) = (\boldsymbol{\nabla}\times\mathbf{a})\cdot\mathbf{b} - (\boldsymbol{\nabla}\times\mathbf{b})\cdot\mathbf{a} \tag{C.7}$$

$$\boldsymbol{\nabla}\times(\mathbf{a}\times\mathbf{b}) = \mathbf{a}(\boldsymbol{\nabla}\cdot\mathbf{b}) - \mathbf{b}(\boldsymbol{\nabla}\cdot\mathbf{a}) + (\mathbf{b}\cdot\boldsymbol{\nabla})\mathbf{a} - (\mathbf{a}\cdot\boldsymbol{\nabla})\mathbf{b} \tag{C.8}$$

$$\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\mathbf{a}) = 0 \tag{C.9}$$

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\psi) = \mathbf{0} \tag{C.10}$$

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{a}) = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{a}) - \nabla^2\mathbf{a} \tag{C.11}$$

$$\oint_{\partial S} \mathsf{A}\cdot d\mathbf{s} = \iint_S (\boldsymbol{\nabla}\times\mathsf{A})\cdot d\mathbf{S} \qquad \text{Stokes's theorem} \tag{C.12}$$

$$\oiint_{\partial V} \mathsf{A}\cdot d\mathbf{S} = \iiint_V \boldsymbol{\nabla}\cdot\mathsf{A}\, dV \qquad \text{Gauss's theorem} \tag{C.13}$$

$$\oiint_{\partial V} \psi\boldsymbol{\nabla}\varphi\cdot d\mathbf{S} = \iiint_V (\psi\nabla^2\varphi + \boldsymbol{\nabla}\varphi\cdot\boldsymbol{\nabla}\psi)\, dV \qquad \text{Green's 1st identity} \tag{C.14}$$

$$\oiint_{\partial V} (\psi\boldsymbol{\nabla}\varphi - \varphi\boldsymbol{\nabla}\psi)\cdot d\mathbf{S} = \iiint_V (\psi\nabla^2\varphi - \varphi\nabla^2\psi)\, dV \qquad \text{Green's 2nd identity} \tag{C.15}$$

$$\oiint_{\partial V} \varphi\, d\mathbf{S} = \iiint_V \boldsymbol{\nabla}\varphi\, dV \tag{C.16}$$

$$\oiint_{\partial V} \mathsf{A}\times d\mathbf{S} = -\iiint_V \boldsymbol{\nabla}\times\mathsf{A}\, dV \tag{C.17}$$

$$\oint_{\partial S} \varphi\, d\mathbf{s} = -\iint_S \boldsymbol{\nabla}\varphi\times d\mathbf{S} \tag{C.18}$$

$$\iiint_V \mathsf{A}\cdot\boldsymbol{\nabla}\varphi\, dV = \oiint_{\partial V} \varphi\mathsf{A}\cdot d\mathbf{S} - \iiint_V \varphi\boldsymbol{\nabla}\cdot\mathsf{A}\, dV \tag{C.19}$$

Helmholtz's theorem

$$\mathbf{A}(\mathbf{x}) = \nabla\times\frac{1}{4\pi}\iiint\frac{\nabla'\times\mathbf{A}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV' - \nabla\frac{1}{4\pi}\iiint\frac{\nabla'\cdot\mathbf{A}(\mathbf{x}')}{\|\mathbf{x}-\mathbf{x}'\|}\,dV' \tag{C.20}$$

If $\mathbf{x}$ is a position vector, $r = \|\mathbf{x}\|$, and $\mathbf{n} = \mathbf{x}/r$

$$\nabla\cdot\mathbf{x} = 3 \tag{C.21}$$

$$\nabla\times\mathbf{x} = \mathbf{0} \tag{C.22}$$

$$\nabla\cdot[\mathbf{n}f(r)] = \frac{2}{r}f(r) + \frac{\partial f(r)}{\partial r} \tag{C.23}$$

$$\nabla\times[\mathbf{n}f(r)] = \mathbf{0} \tag{C.24}$$

$$(\mathbf{a}\cdot\nabla)[\mathbf{n}f(r)] = \frac{f(r)}{r}[\mathbf{a}-\mathbf{n}(\mathbf{a}\cdot\mathbf{n})] + \mathbf{n}(\mathbf{a}\cdot\mathbf{n})\frac{\partial f(r)}{\partial r} \tag{C.25}$$

$$\nabla(\mathbf{x}\cdot\mathbf{a}) = \mathbf{a} + \mathbf{x}(\nabla\cdot\mathbf{a}) + (\mathbf{x}\times\nabla)\times\mathbf{a} \tag{C.26}$$

$$\nabla^2\frac{1}{r} = -4\pi\delta^3(\mathbf{x}) \tag{C.27}$$

$$\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}\frac{1}{r} = \frac{3x_i x_j - r^2\delta_{ij}}{r^5} - \frac{4\pi}{3}\delta_{ij}\delta^3(\mathbf{x}) \tag{C.28}$$

Unit vector relations

$$\mathbf{e}_\rho = \cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y \tag{C.29}$$

$$\mathbf{e}_\phi = -\sin\phi\,\mathbf{e}_x + \cos\phi\,\mathbf{e}_y \tag{C.30}$$

$$\mathbf{e}_x = \cos\phi\,\mathbf{e}_\rho - \sin\phi\,\mathbf{e}_\phi \tag{C.31}$$

$$\mathbf{e}_y = \sin\phi\,\mathbf{e}_\rho + \cos\phi\,\mathbf{e}_\phi \tag{C.32}$$

$$\mathbf{e}_r = \sin\theta\cos\phi\,\mathbf{e}_x + \sin\theta\sin\phi\,\mathbf{e}_y + \cos\theta\,\mathbf{e}_z \tag{C.33}$$

$$\mathbf{e}_\theta = \cos\theta\cos\phi\,\mathbf{e}_x + \cos\theta\sin\phi\,\mathbf{e}_y - \sin\theta\,\mathbf{e}_z \tag{C.34}$$

$$\mathbf{e}_\phi = -\sin\phi,\mathbf{e}_x + \cos\phi\,\mathbf{e}_y \tag{C.35}$$

$$\mathbf{e}_x = \sin\theta\cos\phi\,\mathbf{e}_r + \cos\theta\cos\phi\,\mathbf{e}_\theta - \sin\phi\,\mathbf{e}_\phi \tag{C.36}$$

$$\mathbf{e}_y = \sin\theta\sin\phi\,\mathbf{e}_r + \cos\theta\sin\phi\,\mathbf{e}_\theta + \cos\phi\,\mathbf{e}_\phi \tag{C.37}$$

$$\mathbf{e}_z = \cos\theta\,\mathbf{e}_r - \sin\theta\,\mathbf{e}_\theta \tag{C.38}$$

Line, area, and volume elements

$$d\mathbf{s} = dx\,\mathbf{e}_x + dy\,\mathbf{e}_y + dz\,\mathbf{e}_z \tag{C.39}$$

$$= d\rho\,\mathbf{e}_\rho + \rho\,d\phi\,\mathbf{e}_\phi + dz\,\mathbf{e}_z \tag{C.40}$$

$$= dr\,\mathbf{e}_r + r\,d\theta\,\mathbf{e}_\theta + r\sin\theta\,d\phi\,\mathbf{e}_\phi \tag{C.41}$$

$$d\boldsymbol{\mathcal{A}} = dy\,dz\,\mathbf{e}_x + dz\,dx\,\mathbf{e}_y + dx\,dy\,\mathbf{e}_z \tag{C.42}$$

$$= \rho\,d\phi\,dz\,\mathbf{e}_\rho + dz\,d\rho\,\mathbf{e}_\phi + \rho\,d\rho\,d\phi\,\mathbf{e}_z \tag{C.43}$$

$$= r^2\sin\theta\,d\theta\,d\phi\,\mathbf{e}_r + r\sin\theta\,d\phi\,dr\,\mathbf{e}_\theta + r\,dr\,d\theta\,\mathbf{e}_\phi \tag{C.44}$$

$$dV = dx\,dy\,dz = \rho\,d\rho\,d\phi\,dz = r^2\sin\theta\,dr\,d\theta\,d\phi \tag{C.45}$$

Rectilinear Coordinates (x, y, z)

$$\boldsymbol{\nabla}\psi = \frac{\partial\psi}{\partial x}\mathbf{e}_x + \frac{\partial\psi}{\partial y}\mathbf{e}_y + \frac{\partial\psi}{\partial z}\mathbf{e}_z \tag{C.46}$$

$$\boldsymbol{\nabla}\cdot\mathbf{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \tag{C.47}$$

$$\boldsymbol{\nabla}\times\mathbf{A} = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right)\mathbf{e}_x + \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)\mathbf{e}_y + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\mathbf{e}_z \tag{C.48}$$

$$\nabla^2\psi = \frac{\partial^2 A_x}{\partial x^2} + \frac{\partial^2 A_y}{\partial y^2} + \frac{\partial^2 A_z}{\partial z^2} \tag{C.49}$$

$$\nabla^2\mathbf{A} = \nabla^2 A_x\,\mathbf{e}_x + \nabla^2 A_y\,\mathbf{e}_y + \nabla^2 A_z\,\mathbf{e}_z \tag{C.50}$$

Cylindrical Coordinates (ρ, ϕ, z)

$$\boldsymbol{\nabla}\psi = \frac{\partial\psi}{\partial\rho}\mathbf{e}_\rho + \frac{1}{\rho}\frac{\partial\psi}{\partial\phi}\mathbf{e}_\phi + \frac{\partial\psi}{\partial z}\mathbf{e}_z \tag{C.51}$$

$$\boldsymbol{\nabla}\cdot\mathbf{A} = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho A_\rho) + \frac{1}{\rho}\frac{\partial A_\phi}{\partial\phi} + \frac{\partial A_z}{\partial z} \tag{C.52}$$

$$\boldsymbol{\nabla}\times\mathbf{A} = \left(\frac{1}{\rho}\frac{\partial A_z}{\partial\phi} - \frac{\partial A_\phi}{\partial z}\right)\mathbf{e}_\rho + \left(\frac{\partial A_\rho}{\partial z} - \frac{\partial A_z}{\partial\rho}\right)\mathbf{e}_\phi + \frac{1}{\rho}\left(\frac{\partial}{\partial\rho}(\rho A_\phi) - \frac{\partial A_\rho}{\partial\phi}\right)\mathbf{e}_z \tag{C.53}$$

$$\nabla^2\psi = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2} \tag{C.54}$$

$$\nabla^2\mathbf{A} = \left(\nabla^2 A_\rho - \frac{1}{\rho^2}A_\rho - \frac{2}{\rho^2}\frac{\partial A_\phi}{\partial\phi}\right)\mathbf{e}_\rho + \left(\nabla^2 A_\phi - \frac{1}{\rho^2}A_\phi - \frac{2}{\rho^2}\frac{\partial A_\rho}{\partial\phi}\right)\mathbf{e}_\phi + \nabla^2 A_z\,\mathbf{e}_z \tag{C.55}$$

Spherical Polar Coordinates (r, θ, ϕ)

$$\boldsymbol{\nabla}\psi = \frac{\partial\psi}{\partial r}\mathbf{e}_r + \frac{1}{r}\frac{\partial\psi}{\partial\theta}\mathbf{e}_\theta + \frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}\mathbf{e}_\phi \tag{C.56}$$

$$\boldsymbol{\nabla}\cdot\mathbf{A} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 A_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_\theta) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial\phi} \tag{C.57}$$

$$\boldsymbol{\nabla}\times\mathbf{A} = \frac{1}{r\sin\theta}\left(\frac{\partial}{\partial\theta}(\sin\theta A_\phi) - \frac{\partial A_\theta}{\partial\phi}\right)\mathbf{e}_r + \frac{1}{r}\left(\frac{1}{\sin\theta}\frac{\partial A_r}{\partial\phi} - \frac{\partial}{\partial r}(rA_\phi)\right)\mathbf{e}_\theta + \frac{1}{r}\left(\frac{\partial}{\partial r}(rA_\theta) - \frac{\partial A_r}{\partial\theta}\right)\mathbf{e}_\phi \tag{C.58}$$

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} \tag{C.59}$$

$$\begin{aligned}\nabla^2\mathbf{A} = {}&\left[\nabla^2 A_r - \frac{2}{r^2}A_r - \frac{2}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_\theta) - \frac{2}{r^2\sin\theta}\frac{\partial A_\phi}{\partial\phi}\right]\mathbf{e}_r + \left[\nabla^2 A_\theta - \frac{1}{r^2\sin^2\theta}A_\theta + \frac{2}{r^2}\frac{\partial A_r}{\partial\theta} - \frac{2\cos\theta}{r^2\sin^2\theta}\frac{\partial A_\phi}{\partial\phi}\right]\mathbf{e}_\theta\\ &+\left[\nabla^2 A_\phi - \frac{1}{r^2\sin^2\theta}A_\phi + \frac{2}{r^2\sin^2\theta}\frac{\partial A_r}{\partial\phi} + \frac{2\cos\theta}{r^2\sin^2\theta}\frac{\partial A_\theta}{\partial\phi}\right]\mathbf{e}_\phi\,.\end{aligned} \tag{C.60}$$

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