Imperial College London

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Mathematics for the Theory of Materials: Lectures 1–13

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Lecture notes may be found on Blackboard (http://bb.imperial.ac.uk)

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Chapter 1

Vector Spaces and Tensors

1.1 Learning Outcomes

To understand the following concepts and be able to apply them to solving problems: vector spaces and their properties; the basic properties and rules of tensor algebra and their transformation laws; suffix notation and Einstein summation convention; the Kronecker and Levi-Civita symbols; principal axes and diagonalisation of symmetric tensors; the application of tensors to the properties of crystals; Neumann's principle; tensor fields; the representation and use of grad, div and curl in suffix notation.

1.2 Further Reading

You are encouraged to read beyond these lecture notes. This has a number of benefits: it allows you to explore material that goes beyond the core concepts included here; it encourages you to develop your skills in assimilating academic literature. Seeing a subject presented in a different ways by different authors can enhance your understanding of it.

1. Riley, Hobson & Bence, *Mathematical Methods for Physics and Engineering, 3rd Ed.*, Chapter 8: Matrices and Vector Spaces; *ibid.* Chapter 9: Normal Modes; *ibid.* Chapter 26: Tensors, Sections 1–9, and 12;

2. Lovett, *Tensor Properties of Crystals*. A nice little book covering crystallography (Ch. 1), tensor algebra (Ch. 2), and applications to materials (Ch. 3–7).

3. Nye, *Physical Properties of Crystals*. Similar to Lovett, but at a much more advanced level.

1.3 Introduction

There are properties of materials that do not depend on the direction in which they are measured. Take, for instance, density: it is the ratio of the mass of an object to its volume, both scalar quantities and, hence, both independent of direction, which means the density itself is a scalar and independent of direction.

There are other properties of crystals that do depend on direction, and this can often be the reason why a material may be scientifically interesting or technologically useful. Electrical conductivity $\underline{\underline{\sigma}}$, for instance, is the ratio of the resultant current density $\underline{J}$ to the applied electric field $\underline{E}$. Both $\underline{J}$ and $\underline{E}$ are quantities which possess a direction as well as a magnitude (i.e., they are vectors). For the same crystal, the result of a measurement of $\underline{\underline{\sigma}}$ will depend on the direction in which $\underline{E}$ is applied and $\underline{J}$ is measured. This means that a single value of $\underline{\underline{\sigma}}$ is not enough to specify the properties of the crystal. In fact, $\underline{\underline{\sigma}}$ is a *second-rank tensor*, which means that it is a quantity that can be represented as a matrix with two suffixes σ_{ij}, $i, j \in \{1, 2, 3\}$, and hence nine components.[1] It turns out that many crystal properties can be thought of as being tensors: elasticity, thermal conductivity, permittivity, magnetic susceptibility, thermal expansivity and many more besides.

This chapter is about the mathematics of such quantities, how to manipulate them, and how to understand what they mean. But first we must review some concepts that you should be familiar with: vectors, vector spaces, matrices, eigenvalues and eigenvectors.

It is worth noting that tensors are not just important in the study of materials. For example, Einstein's theory of general relativity, which describes the force of gravity as being a manifestation of the curvature of spacetime caused by the presence of matter and energy, may be expressed mathematically as a tensor equation.

1.4 Vector Spaces

1.4.1 Introduction

You should be familiar with the concept of a vector[2] to describe quantities that have both a magnitude and a direction in three-dimensional space. Those of you who have studied the theory of Special Relativity will have come across 4-vectors, vectors in four-diomensional space-time. I may not surprise you to learn that the concept of a vector can be extended to an arbitrary number of dimensions and the "space" in which these vectors live can refer to more abstract quantities than, say, one would usually associate with the word "space".

[1] Since the crystal will have some point-group symmetry, not all of these components will be independent.
[2] The word means *carrier*, from the Latin *vehere*, to carry.

1.4.2 Definition of a Vector Space

A set of vectors satisfying the following relations constitute a *linear vector space*:

1. Closed[3] under addition, both commutative and associative:

$$\underline{u} + \underline{v} = \underline{v} + \underline{u} \qquad (\underline{u} + \underline{v}) + \underline{w} = \underline{u} + (\underline{v} + \underline{w})$$

2. Closed under multiplication, both distributive and associative, by a scalar[4]:

$$a(\underline{u} + \underline{v}) = a\underline{u} + a\underline{v} \qquad a(b\underline{u}) = (ab)\underline{u}$$

3. There exists a *null* vector $\underline{0}$:

$$\underline{v} + \underline{0} = \underline{v}$$

4. Multiplication by the unit scalar leaves a vector unaltered:

$$1 \times \underline{v} = \underline{v}$$

5. Each vector $\underline{v}$ has a corresponding negative vector $-\underline{v}$:

$$\underline{v} + (-\underline{v}) = \underline{0}$$

This last property enables subtraction by defining $\underline{u} - \underline{v} \equiv \underline{u} + (-\underline{v})$.

1.4.3 Linear Independence

A set of n non-zero vectors $\{\underline{u}_i\}$ is said to be *linearly independent* if

$$\sum_{i=1}^{n} a_i \underline{u}_i = \underline{0} \Rightarrow a_i = 0 \quad \forall\ i,$$

which implies that no vector in the set can be expressed as a linear combination of all the others.

Conversely, if a set of scalars $\{a_i\}$, at least one of which is non-zero, can be chosen such that the sum on the left-hand side is the null vector, then the set of vectors $\{\underline{u}_i\}$ is said to be *linearly dependent*.

Linear independence can be used to define the dimensionality of a vector space V, which is said to be of dimension n if there exists a set of n linearly independent vectors in V, but all sets of $n + 1$ vectors are linearly dependent.

[3] *Closure* of a set of elements under a given operation implies that the result of the operation is also an element of the set.

[4] A *scalar* is a quantity with magnitude only. The word is derived from the Latin *scala*, which means ladder.

1.4.4 Basis Vectors

Any set of n linearly independent vectors $\{\underline{u}_i\}$ in an n-dimensional vector space V is a *basis* for V. Any vector $\underline{v}$ in V can be represented as a linear combination of the basis vectors:

$$\underline{v} = \sum_{i=1}^{n} a_i \underline{u}_i$$

where the set of scalars $\{a_i\}$ are unique to the given vector $\underline{v}$.

Examples that you will be most familiar with are:

- The three Cartesian basis vectors in three-dimensional Euclidean space ($\mathbb{E}^3$). Any vector $\underline{v} \in \mathbb{E}^3$ can be written uniquely as

  $$\underline{v} = v_1 \hat{\underline{e}}^{(1)} + v_2 \hat{\underline{e}}^{(2)} + v_3 \hat{\underline{e}}^{(3)}$$

  where $\{v_1, v_2, v_3\}$ are the *components* of $\underline{v}$ in the basis $\{\hat{\underline{e}}^{(1)}, \hat{\underline{e}}^{(2)}, \hat{\underline{e}}^{(3)}\}$.

- The two-dimensional representation of the set complex numbers ($\mathbb{C}$) in terms of the basis $\{1, i\}$. Any complex number $z \in \mathbb{C}$ may be expressed uniquely as

  $$z = x + iy$$

  where x and y are the components of z in the basis $\{1, i\}$.

1.4.5 The Inner (or Scalar) Product and Orthogonality

For every pair of vectors $\underline{u}$ and $\underline{v}$ in V, we define the *inner product* $\langle \underline{u} | \underline{v} \rangle \in \mathbb{C}$. The inner product can be thought of as the generalisation of the familiar scalar (or dot) product of three-vectors, $\underline{u} \cdot \underline{v} = uv \cos\theta$ where θ is the angle between $\underline{u}$ and $\underline{v}$. We will use $\underline{u} \cdot \underline{v}$ and $\langle \underline{u} | \underline{v} \rangle$ interchangeably.

The inner product has the following properties

1. $\langle \underline{u} | \underline{v} \rangle = \langle \underline{v} | \underline{u} \rangle^* \quad \Rightarrow \quad \langle \underline{v} | \underline{v} \rangle \in \mathbb{R}$
2. $\langle \underline{u} | a\underline{v}_1 + b\underline{v}_2 \rangle = a \langle \underline{u} | \underline{v}_1 \rangle + b \langle \underline{u} | \underline{v}_2 \rangle$
3. $||\underline{v}||^2 \equiv \langle \underline{v} | \underline{v} \rangle \geq 0$
4. $||\underline{v}|| = 0 \Rightarrow \underline{v} = \underline{0}$

(1) and (2) imply that

$$\langle a\underline{v}_1 + b\underline{v}_2 | \underline{u} \rangle = a^* \langle \underline{v}_1 | \underline{u} \rangle + b^* \langle \underline{v}_2 | \underline{u} \rangle .$$

The *norm* of a vector is defined as $||\underline{v}|| \equiv \langle \underline{v} | \underline{v} \rangle^{1/2}$ and is analogous to the length $|\underline{v}|$ of a three-vector. We will often use $|\underline{v}|$ and $||\underline{v}||$ interchangeably.

Two vectors are said to be *orthogonal* if their inner product is zero. If they each also have unit norm, they are said to be *orthonormal*. The Cartesian basis in three-dimensions is an example of an orthonormal basis since

$$\underline{\hat{e}}^{(i)} \cdot \underline{\hat{e}}^{(j)} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

1.5 Matrices

This section is mainly revision and included to refresh the memory. Knowledge of subsections marked with an asterisk is assumed, therefore they will be skipped over rapidly in lectures.

1.5.1 Notation*

A *matrices* are arrays of numbers, or *elements*, in the form

$$\begin{pmatrix} 3 & 1 \\ 4 & 1 \end{pmatrix} \qquad \begin{pmatrix} 5 & 9 \\ 2 & 6 \\ 5 & 3 \end{pmatrix} \qquad \begin{pmatrix} 5 & 8 & 9 \\ 7 & 9 & 3 \\ 2 & 3 & 8 \end{pmatrix}$$

that obey a special *algebra*, i.e., a special set of rules for their addition, multiplication etc. Lowercase a_{ij} is used to denote the element that is in the i^{th} row and j^{th} column of the matrix $\underline{\underline{A}}$. You will sometimes see the elements of a matrix denoted as $[\underline{\underline{B}}]_{ij}$, which is equivalent to writing b_{ij}.

A subscript used in this way is known as an *index* (plural *indices*) or, equivalently, a *suffix* (plural *suffixes*). Using *suffix notation* is often a very handy way of doing matrix algebra. We shall return to this later.

1.5.2 Basic Matrix Algebra*

The following is a list of the properties of matrix algebra.

1. **Equality**. For two matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ to be equal they must be of the same size, i.e., have the same number of rows and columns, and all their elements must be equal

$$\underline{\underline{A}} = \underline{\underline{B}} \quad \Leftrightarrow \quad a_{ij} = b_{ij} \quad 1 \leq i \leq m,\ 1 \leq j \leq n$$

2. **Multiplication by a scalar**. Multiplying a matrix $\underline{\underline{A}}$ by a scalar λ results in all of the elements $\{a_{ij}\}$ of $\underline{\underline{A}}$ being multiplied by λ

$$\underline{\underline{B}} = \lambda \underline{\underline{A}} \quad \Leftrightarrow \quad b_{ij} = \lambda a_{ij} \quad 1 \leq i \leq m,\ 1 \leq j \leq n$$

3. **Addition and subtraction**. Only matrices of the same size may be added to or subtracted from one another.

$$\underline{\underline{C}} = \underline{\underline{A}} \pm \underline{\underline{B}} \quad \Leftrightarrow \quad c_{ij} = a_{ij} \pm b_{ij} \quad 1 \leq i \leq m,\ 1 \leq j \leq n$$

4. **Matrix addition is commutative and associative:**

$$\underline{\underline{A}} + \underline{\underline{B}} = \underline{\underline{B}} + \underline{\underline{A}}, \qquad \underline{\underline{A}} + (\underline{\underline{B}} + \underline{\underline{C}}) = (\underline{\underline{A}} + \underline{\underline{B}}) + \underline{\underline{C}}$$

5. **Matrix multiplication**. The product $\underline{\underline{C}} = \underline{\underline{A}}\,\underline{\underline{B}}$ exists if and only if the number of columns of $\underline{\underline{A}}$ is equal to the number of rows of $\underline{\underline{B}}$. The matrix product of an $m \times p$ matrix $\underline{\underline{A}}$ and a $p \times n$ matrix $\underline{\underline{B}}$ is defined as

$$\underline{\underline{C}} = \underline{\underline{A}}\,\underline{\underline{B}} \quad \Leftrightarrow \quad c_{ij} = \sum_{k=1}^{p} a_{ik} b_{kj} \quad 1 \leq i \leq m,\ 1 \leq j \leq n$$

6. **Matrix multiplication is associative and distributive, but in general not commutative:**

$$(\underline{\underline{A}}\,\underline{\underline{B}})\underline{\underline{C}} = \underline{\underline{A}}(\underline{\underline{B}}\,\underline{\underline{C}}), \qquad (\underline{\underline{A}} + \underline{\underline{B}})\underline{\underline{C}} = \underline{\underline{A}}\,\underline{\underline{C}} + \underline{\underline{B}}\,\underline{\underline{C}}, \qquad \underline{\underline{A}}\,\underline{\underline{B}} \neq \underline{\underline{B}}\,\underline{\underline{A}}$$

1.5.3 Suffix Notation and Summation Convention

Suffix notation is a powerful tool for the manipulation of tensors. Although we will be mainly concerned with three-dimensions, i.e., all suffixes take values 1, 2 or 3, the notation is much more general and equally well may be applied to N-dimensions.

When using suffix notation, a shorthand that is often used involves ommitting the summation symbol when there is a repeated suffix. For example, the expression for the elements of $\underline{\underline{C}} = \underline{\underline{A}}\,\underline{\underline{B}}$ is

$$c_{ij} = [\underline{\underline{A}}\,\underline{\underline{B}}]_{ij} = \sum_{k} a_{ik} b_{kj} \tag{1.1}$$

and this may be written as

$$c_{ij} = a_{ik} b_{kj} \tag{1.2}$$

where it is implicitly assumed that there is a summation over the repeated index k. This shorthand is known as the *Einstein summation convention*.

There are three basic rules to suffix notation:

1. In any one term of an expression, suffixes may appear only once, twice or not at all.
2. A suffix that appears only once on one side of an expression must also appear once on the other side. It is called a *free suffix* or *free index*.
3. A suffix that appears twice is summed over. It is called a *dummy suffix* or *dummy index*.

The scalar (dot) product of two vectors may, for example, be expressed as

$$\underline{a} \cdot \underline{b} = a_1 b_1 + a_2 b_2 + a_3 b_3 = a_i b_i$$

A matrix-vector multiplication, for example,

$$\underline{y} = \underline{\underline{\mathrm{M}}}\underline{x} = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} m_{11}x_1 + m_{12}x_2 + m_{13}x_3 \\ m_{21}x_1 + m_{22}x_2 + m_{23}x_3 \\ m_{31}x_1 + m_{32}x_2 + m_{33}x_3 \end{pmatrix}$$

may be expressed in suffix notation as

$$y_i = M_{ik} x_k,$$

where i is the free suffix and k is the dummy suffix. Dummy suffixes are so-called because it does not matter what symbol we use to represent them, as long as they always occur in pairs and as long as we do not use a symbol that already appears elsewhere in the expression. Hence,

$$a_i = M_{ij} b_j = M_{i\xi} b_\xi = M_{i\bullet} b_\bullet.$$

Free suffixes must match on both sides of the equation, and indeed in *every term* of the equation. Hence,

$$a_i = M_{ij} b_j - Q_{ip} c_p \quad \text{and} \quad a_\zeta = M_{\zeta j} b_j - Q_{\zeta k} c_k$$

are equivalent (and valid) expressions, whereas

$$a_i = M_{kj} b_j + Q_{ip} c_p$$

is an incorrect use of suffix notation as the left hand side has a free suffix i which is not matched in the first term on the right hand side (which has a free suffix k).

Some more examples are given below:

- $\underline{y} = \underline{\underline{\mathrm{A}}}\underline{x} + \underline{z} \quad \Leftrightarrow \quad y_i = a_{ij} x_j + z_i$
- $\underline{\underline{\mathrm{C}}} = \underline{\underline{\mathrm{A}}}\,\underline{\underline{\mathrm{B}}} \quad \Leftrightarrow \quad c_{ij} = a_{ik} b_{kj}$
- $\underline{\underline{\mathrm{D}}} = \underline{\underline{\mathrm{C}}}^{\mathsf{T}} \quad \Leftrightarrow \quad d_{ij} = c_{ji}$
- $\underline{\underline{\mathrm{C}}} = \underline{\underline{\mathrm{A}}}^{\mathsf{T}}\,\underline{\underline{\mathrm{B}}} \quad \Leftrightarrow \quad c_{ij} = a_{ki} b_{kj}$
- $\mathrm{tr}[\underline{\underline{\mathrm{A}}}] = a_{ii}$
- $\mathrm{tr}[\underline{\underline{\mathrm{A}}}\,\underline{\underline{\mathrm{B}}}\,\underline{\underline{\mathrm{C}}}] = a_{ip} b_{pq} c_{qi}$

The action of replacing two different free suffixes by a single dummy suffix (which is then summed over) is known as *contraction*. For example, c_{ij} represents the ij^{th} element of matrix $\underline{\underline{C}}$. *Contracting* the two free suffixes gives c_{ii} (or, equivalently c_{jj}, or indeed any other choice of symbol for the dummy suffix) which is then just $\mathrm{tr}[\underline{\underline{\mathrm{C}}}]$.

1.5.4 Special Types of Matrix*

1. **Transpose**. The transpose of a matrix $\underline{\underline{\mathrm{M}}}$ is obtained by swapping the rows and columns and is denoted with a superscript "T".

$$[\underline{\underline{\mathrm{A}}}^{\mathsf{T}}]_{ij} = [\underline{\underline{\mathrm{A}}}]_{ji}.$$

   The transpose of a product is equal to the product of the transposes in reverse order:

$$(\underline{\underline{\mathrm{AB}}})^{\mathsf{T}} = \underline{\underline{\mathrm{B}}}^{\mathsf{T}}\underline{\underline{\mathrm{A}}}^{\mathsf{T}},$$

   and, of course, $(\underline{\underline{\mathrm{A}}}^{\mathsf{T}})^{\mathsf{T}} = \underline{\underline{\mathrm{A}}}$.

2. **Hermitian conjugate**. The Hermitian conjugate of a matrix is denoted by a superscript dagger † and is defined as

$$\underline{\underline{\mathrm{M}}}^{\dagger} \equiv (\underline{\underline{\mathrm{M}}}^{*})^{\mathsf{T}} \equiv (\underline{\underline{\mathrm{M}}}^{\mathsf{T}})^{*}$$

   where "*" represents complex conjugation. For real matrices $\underline{\underline{\mathrm{M}}} \in \mathbb{R}$, the operations of Hermitian conjugation and transposing are identical.

3. **Column and row matrices**. A column matrix has m rows and 1 column. A three-vector $\underline{u}$ may be thought of as a column matrix:

$$\underline{u} = \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix}.$$

   A row matrix has 1 row and n columns, e.g., $\underline{u}^{\mathsf{T}}$ is a row matrix

$$\underline{u}^{\mathsf{T}} = \begin{pmatrix} u_x & u_y & u_z \end{pmatrix}.$$

   It is worth noting that the inner product for vectors may be written as a matrix product

$$\underline{a} \cdot \underline{b} = \underline{a}^{\dagger}\underline{b} = (\underline{b}^{\dagger}\underline{a})^{*}$$

4. **Square matrix**. If $\underline{\underline{\mathrm{A}}}$ is a square matrix, then it has the same number of rows as columns. The *trace* of a square $n \times n$ matrix is the sum of its diagonal elements and is denoted

$$\mathrm{tr}(\underline{\underline{\mathrm{A}}}) \equiv \sum_{i=1}^{n} a_{ii} \equiv a_{ii}$$

   The trace has a cyclic property, namely that

$$\mathrm{tr}(\underline{\underline{\mathrm{ABC}}}) = \mathrm{tr}(\underline{\underline{\mathrm{BCA}}}) = \mathrm{tr}(\underline{\underline{\mathrm{CAB}}})$$

5. **Diagonal matrix**. If $\underline{\underline{\Lambda}}$ is diagonal, then $\lambda_{ij} = 0$ if $i \neq j$.

6. **Unit matrix**. The $n \times n$ unit matrix, also known as the *identity* matrix, is conventionally denoted by $\underline{\underline{\mathsf{I}}}^{(n)}$, or just $\underline{\underline{\mathsf{I}}}$ or $\mathbb{1}$, and is a special case of diagonal matrices in which the diagonal elements are all equal to 1:

$$\underline{\underline{\mathsf{I}}} = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

The elements of $\underline{\underline{\mathsf{I}}}$ are usually denoted by δ_{ij} where

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

δ_{ij} is called the *Kronecker delta*[5]. The main properties of the Kronecker delta are

- Symmetric: $\delta_{ij} = \delta_{ji}$
- Trace: $\delta_{ii} = n$ (in n dimensions)
- "Sifting": $x_i = \delta_{ij} x_j$

7. **Inverse matrix**. The inverse matrix $\underline{\underline{\mathsf{A}}}^{-1}$ of $\underline{\underline{\mathsf{A}}}$ satisfies

$$\underline{\underline{\mathsf{A}}}^{-1}\underline{\underline{\mathsf{A}}} = \underline{\underline{\mathsf{A}}}\underline{\underline{\mathsf{A}}}^{-1} = \underline{\underline{\mathsf{I}}}$$

The inverse of a product is equal to the product of the inverses in reverse order

$$(\underline{\underline{\mathsf{A}}}\underline{\underline{\mathsf{B}}})^{-1} = \underline{\underline{\mathsf{B}}}^{-1}\underline{\underline{\mathsf{A}}}^{-1}$$

8. **Tridiagonal matrix**. A matrix in which only the main diagonal and the diagonals immediately above and below it contain non-zero entries. These matrices appear often in the numerical solution of physical problems.

9. **Upper (lower) triangular matrix**. A matrix in which only the main diagonal and all the elements above (below) it are non-zero. The determinant of such a matrix turns out to be equal to the product of the diagonal elements and the inverse of an upper (lower) triangular matrix is also upper (lower) triangular.

10. **Symmetric and anti-symmetric matrices**. If $\underline{\underline{\mathsf{S}}}$ is *symmetric*, then $\underline{\underline{\mathsf{S}}}^{\mathsf{T}} = \underline{\underline{\mathsf{S}}}$ or, alternatively, $s_{ij} = s_{ji}$. If $\underline{\underline{\mathsf{A}}}$ is *anti-symmetric*, then $\underline{\underline{\mathsf{A}}}^{\mathsf{T}} = -\underline{\underline{\mathsf{A}}}$ or, alternatively, $a_{ij} = -a_{ji}$.

    - All anti-symmetric matrices have zeros on the diagonal.
    - Every square matrix may be expressed as the sum of a symmetric and an anti-symmetric matrix.

[5] Named after the German mathematician and logician Leopold Kronecker (1823-1891). He believed that "God made the integers; all else is the work of man".

11. **Orthogonal matrix**. If $\underline{\underline{R}}$ is *orthogonal*, then it satisfies

$$\underline{\underline{R}}\underline{\underline{R}}^{\mathsf{T}} = \underline{\underline{R}}^{\mathsf{T}}\underline{\underline{R}} = \underline{\underline{I}} \quad \Leftrightarrow \quad \underline{\underline{R}}^{-1} = \underline{\underline{R}}^{\mathsf{T}}$$

    It is worth noting that the n columns of any orthogonal matrix form an n-dimensional orthogonal basis of vectors. Why?

12. **Hermitian and anti-Hermitian matrices**. These may be thought of as the complex generalisations of symmetric and anti-symmetric matrices. If $\underline{\underline{H}}$ is *Hermitian*, then $\underline{\underline{H}}^{\dagger} = \underline{\underline{H}}$ or, alternatively, $h_{ij} = h_{ji}^{*}$. If $\underline{\underline{A}}$ is *anti-Hermitian*, then $\underline{\underline{A}}^{\dagger} = -\underline{\underline{A}}$ or, alternatively, $a_{ij} = -a_{ji}^{*}$.

    - All anti-Hermitian matrices have zeros on the diagonal.
    - Every complex square matrix may be expressed as the sum of a Hermitian and an anti-Hermitian matrix.

13. **Unitary matrix**. These may be thought of as complex generalisations of orthogonal matrices. $\underline{\underline{U}}$ is unitary if

$$\underline{\underline{U}}\underline{\underline{U}}^{\dagger} = \underline{\underline{U}}^{\dagger}\underline{\underline{U}} = \underline{\underline{I}} \quad \Leftrightarrow \quad \underline{\underline{U}}^{-1} = \underline{\underline{U}}^{\dagger}$$

1.5.5 Levi-Civita Symbol (Alternating Tensor)

The *Levi-Civita symbol* or *alternating tensor*, is a rank-three isotropic tensor, and is defined as

$$\varepsilon_{ijk} = \begin{cases} 1 & (i,j,k) = (1,2,3),(2,3,1),(3,1,2) \\ -1 & (i,j,k) = (1,3,2),(2,1,3),(3,2,1) \\ 0 & \text{otherwise} \end{cases}$$

In three dimensions, each suffix can take the value 1, 2, or 3, therefore ε_{ijk} has $3^3 = 27$ elements. From the definition, it can be seen that 21 of these are zero (whenever any two suffixes are equal) and the remaining six are ± 1, depending on whether (i,j,k) is a cyclic or anti-cyclic permutation of $(1,2,3)$. In other words,

- $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$
- $\varepsilon_{132} = \varepsilon_{213} = \varepsilon_{321} = -1$
- $\varepsilon_{ijk} = 0$ if $i = j$ or $j = k$ or $i = k$

From the definition follows the cyclic property $\varepsilon_{ijk} = \varepsilon_{jki} = \varepsilon_{kij}$ and $\varepsilon_{ijk} = -\varepsilon_{jik}$ etc.

The alternating tensor can be used to write vector (cross) products in suffix notation:

$$\underline{c} = \underline{a} \times \underline{b} \quad \Leftrightarrow \quad c_i = \varepsilon_{ijk} a_j b_k .$$

A useful identity involving the contraction of two alternating tensors is

$$\varepsilon_{ijk}\varepsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}.$$

For example, we can use it to prove the vector identity

$$\underline{a} \times (\underline{b} \times \underline{c}) = (\underline{a} \cdot \underline{c})\underline{b} - (\underline{a} \cdot \underline{b})\underline{c}$$

as follows

$$\begin{aligned}
[\underline{a} \times (\underline{b} \times \underline{c})]_i &= \varepsilon_{ijk} a_j [\underline{b} \times \underline{c}]_k \\
&= \varepsilon_{ijk} a_j \epsilon_{klm} b_l c_m \\
&= (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}) a_j b_l c_m \\
&= (a_j c_j) b_i - (a_j b_j) c_i \\
&= (\underline{a} \cdot \underline{c})[\underline{b}]_i - (\underline{a} \cdot \underline{b})[\underline{c}]_i
\end{aligned}$$

Note the compactness of the derivation as compared to doing it in Cartesian coordinates and writing out the vector product explicitly.

1.5.6 Determinants*

Associated with each square matrix $\underline{\underline{A}}$ there is a scalar quantity called the *determinant* that is denoted

$$\det \underline{\underline{A}} \equiv |\underline{\underline{A}}|$$

For a 2×2 matrix, it is given by $\det \underline{\underline{A}} = a_{11}a_{22} - a_{12}a_{21}$, and for a 3×3 matrix it is

$$\det \underline{\underline{A}} \equiv \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$

The alternating tensor may be used to express the determinant of a 3×3 matrix $\underline{\underline{A}}$:

$$\det \underline{\underline{A}} = \varepsilon_{ijk} a_{1i} a_{2j} a_{3k}$$

The general form for the determinant of an $n \times n$ matrix is given by

$$\det \underline{\underline{A}} = \sum_{k=1}^{n} a_{1k} (-1)^{k-1} \det \underline{\underline{A}}^{(1k)}$$

where $\underline{\underline{A}}^{(1k)}$ is the $(n-1) \times (n-1)$ matrix obtained by deleting the first row and k^{th} column of $\underline{\underline{A}}$. This formula can be repeated until the problem is reduced to just a sum over determinants of 2×2 matrices.

Determinants have the following properties:

1. In the general formula above, the determinant is expanded over the first row of elements, but we may do so over any row or column, as long as we get the signs of the terms correct. E.g., over the i^{th} row we have

$$\det \underline{\underline{A}} = \sum_{k=1}^{n} a_{ik}(-1)^{k-i} \det \underline{\underline{A}}^{(ik)}$$

and over the k^{th} column we have

$$\det \underline{\underline{A}} = \sum_{i=1}^{n} a_{ik}(-1)^{k-i} \det \underline{\underline{A}}^{(ik)}.$$

$\det \underline{\underline{A}}^{(ik)}$ is known as the *minor* of a_{ik}, and $(-1)^{k-i} \det \underline{\underline{A}}^{(ik)}$ is known as the *cofactor* of a_{ik}. Cofactors are just minors that are multiplied by an appropriate sign $(-1)^{k-i}$.

2. $\det \underline{\underline{A}} = 0$ if
   - all the elements of one row (or column) are zero
   - any two rows (or two columns) are identical
   - any two rows (or two columns) are proportional
3. If two rows (or two columns) of a matrix are interchanged, then the sign of the determinant changes.
4. If each element in one row (or column) of a matrix is multiplied by a scalar λ, then the determinant is also multiplied by λ.
5. For an $n \times n$ matrix, $\det(\lambda \underline{\underline{A}}) = \lambda^n \det \underline{\underline{A}}$
6. The determinant is unchanged if a multiple of a particular row (or column) is added to the corresponding elements of another row (or column).
7. Interchanging all the columns and rows does not affect the value of the determinant, i.e., $\det \underline{\underline{A}} = \det \underline{\underline{A}}^{\mathsf{T}}$
8. The determinant of a product is the product of determinants, i.e., $\det(\underline{\underline{A}}\,\underline{\underline{B}}) = \det \underline{\underline{A}} \det \underline{\underline{B}}$

1.5.7 Linear Equations and Inverse Matrices*

An example of a system of linear equations is

$$\begin{array}{rcl} a_{11}x_1 + a_{12}x_2 &=& y_1 \\ a_{21}x_1 + a_{22}x_2 &=& y_2 \end{array} \quad \Leftrightarrow \quad a_{ij}x_j = y_i \quad \Leftrightarrow \quad \underline{\underline{A}}\,\underline{x} = \underline{y}$$

If $\underline{y} = \underline{0}$, then the equations are said to be *homogeneous*. Otherwise they are known as *inhomogeneous*. Knowledge of the inverse of $\underline{\underline{A}}$ enables solution of the equations. If and inverse exists, then it is unique.

The general expression for the inverse of an $n \times n$ matrix $\underline{\underline{A}}$ is

$$[A^{-1}]_{ij} = \frac{(-1)^{i-j} \det \underline{\underline{A}}^{(ji)}}{\det \underline{\underline{A}}} \equiv \frac{\text{adj } \underline{\underline{A}}}{\det \underline{\underline{A}}}$$

where $\underline{\underline{A}}^{(ji)}$ is the matrix $\underline{\underline{A}}$ with the j^{th} row and i^{th} column removed. Notice the interchange between i and j. The numerator is known as the *adjoint* of $\underline{\underline{A}}$ and is obtained by replacing each element of $\underline{\underline{A}}$ with its cofactor and taking the transpose of the result.

If $\det \underline{\underline{A}} = 0$, then $\underline{\underline{A}}^{-1}$ does not exist and $\underline{\underline{A}}$ is said to be *singular*. If a matrix $\underline{\underline{A}}$ is singular, then the vectors composed of the rows (or columns) of $\underline{\underline{A}}$ must be linearly dependent. In other words, one row (or column) can be written as a linear combination of the others. If a matrix is non-singular, then its rows (or columns) are linearly independent and $\underline{\underline{A}}^{-1}$ exists.

Consider the homogeneous linear equations given by

$$\underline{\underline{A}}\underline{x} = \underline{0} \quad \Leftrightarrow \quad a_{ij}x_j = 0$$

1. If $\underline{\underline{A}}$ is non-singular, then $\det \underline{\underline{A}} \neq 0$, $\underline{\underline{A}}^{-1}$ exists, and there is one unique solution $\underline{x} = \underline{0}$.
2. If $\underline{\underline{A}}$ is singular, then $\det \underline{\underline{A}} = 0$ and $\underline{\underline{A}}^{-1}$ does not exist. There are two possibilities, either
   - $\underline{x} = \underline{0}$, or
   - there is a family of solutions

Now consider the inhomogeneous equation

$$\underline{\underline{A}}\underline{x} = \underline{y} \quad \Leftrightarrow \quad a_{ij}x_j = y_i$$

1. If $\underline{\underline{A}}$ is non-singular, then $\underline{\underline{A}}^{-1}$ exists and there is a unique solution $\underline{x} = \underline{\underline{A}}^{-1}\underline{y}$.
2. If $\underline{\underline{A}}$ is singular, then $\det \underline{\underline{A}} = 0$ and $\underline{\underline{A}}^{-1}$ does not exist. There are two possibilities, either
   - there is a family of solutions, or
   - the equations are inconsistent and there is no solution

1.5.8 Eigenvalues and Eigenvectors*

An eigenvalue equation takes the form

$$a_{ij}x_j = \lambda x_i$$

where a_{ij} are the componenets of a rank-two tensor, and $\underline{x}$ is an *eigenvector* with corresponding *eigenvalue* λ. For an $n \times n$ symmetric tensor there will be n distinct eigenvectors and corresponding eigenvalues.

In the context of material properties, eigenvectors are also known as *principal directions* and eigenvalues as *principal values*.

Rearranging the eigenvalue equation gives

$$(a_{ij} - \lambda \delta_{ij}) x_j = 0$$

which has non-trivial solutions ($\underline{x} \neq \underline{0}$) if

$$\det(\underline{\underline{A}} - \lambda \underline{\underline{I}}) = \underline{0}$$

This condition, when expanded out, gives an n^{th}-order polynomial in λ, known as the *characteristic equation*, whose n roots $\{\lambda^{(i)}\}$, $i \in \{1, \ldots, n\}$, are the n eigenvalues of $\underline{\underline{A}}$. Substituting each eigenvalue back into the original eigenvalue equation enables the eigenvector $\underline{x}^{(i)}$ corresponding to each eigenvalue $\lambda^{(i)}$ to be found.

Three important properties of symmetric tensors are that:

1. They are always diagonalisable
2. Their eigenvalues are real
3. Their eigenvectors are orthogonal

For proofs see, e.g., Riley, Hobson and Bence.

1.5.9 Normal Modes*

Consider the arrangement of masses and springs shown in Fig. 1.1. The force F exerted by a spring of spring-constant k that is extended from equilibrium by a displacement x is given by Hooke's law: $F = kx$. Newton's second law tells us that the acceleration of an object of mass m is related to the net force F that acts upon it by $F = m\ddot{x}$. Considering the net force on each mass, the equations of motion for the system shown in Fig. 1.1 are

$$\begin{aligned} m\ddot{x}_1 &= -k_1 x_1 + k_2(x_2 - x_1) \\ m\ddot{x}_2 &= -k_2(x_2 - x_1) \end{aligned}$$

This pair of coupled second order differential equations may be written in matrix form as

$$m \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix} = \begin{pmatrix} -k_1 - k_2 & k_2 \\ k_2 & -k_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

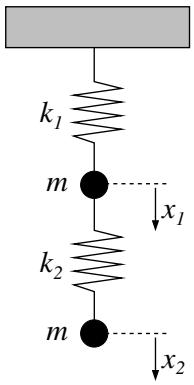

Figure 1.1: Two equal masses m and springs with spring-constants k_1 and k_2. Displacements from equilibrium are denoted by x_1 and x_2.

Physical intuition tells us that when the system is set in motion, the masses are going to undergo some sort of oscillation. So we try to find special solutions such that both masses oscillate with the same, pure frequency ω, i.e., solutions that look like

$$x_k(t) = \alpha_k e^{i\omega t}$$

where $\boldsymbol{\alpha}$ is a constant vector. Such solutions are called *normal modes*. Differentiating twice we find

$$\ddot{\underline{x}} = (i\omega)^2 \boldsymbol{\alpha} e^{i\omega t} = -\omega^2 \underline{x},$$

which we substitute back into the coupled differential equations above to obtain

$$-m\omega^2 \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -k_1 - k_2 & k_2 \\ k_2 & -k_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

which we may rearrange to give

$$\frac{1}{m} \begin{pmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \omega^2 \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}.$$

It may be seen that these equations are of the general form of an eigenvalue[6] equation:

$$\underline{\underline{A}} \underline{x} = \lambda \underline{x}$$

where $\lambda = \omega^2$ and

$$\underline{\underline{A}} = \frac{1}{m} \begin{pmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 \end{pmatrix}.$$

The eigenvectors are in some sense very special, because applying the matrix $\underline{\underline{A}}$ to an eigenvector does not change its direction – the result $\lambda \underline{x}$ is simply $\underline{x}$ scaled by the eigenvalue λ.

[6] *Eigen* is a German word meaning *same*. You can see why: in the case of the masses on springs, if the masses all oscillate with the *same* frequency ω, then that is an *eigen*frequency of the system, related to the eigenvalue λ by $\lambda = \omega^2$.

1.6 Scalars, Vectors and Tensors

Scalars have magnitude and are independent of the any direction. Examples of scalar physical quantities include density, temperature, mass, volume. As we shall see, scalars are also *rank-zero tensors*.

Vectors have magnitude and direction. Physical examples include velocity, force, temperature gradient, electric field, current density. Given a set of basis vectors $\{\underline{\hat{e}}\}$, any vector $\underline{v}$ may be described in terms of its *components* $\{v_i\}$ in that basis

$$\underline{v} = \sum_{i=1}^{3} v_i \underline{\hat{e}}^{(i)} \equiv \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}.$$

Vectors are examples of *rank-one tensors*.

Rank-two tensors are an extension of the concept of a vector. Consider the following example. For the special case of an isotropic[7] crystal, no matter what direction in which an electric field $\underline{E}$ is applied, the resulting current density $\underline{J}$ will be in the same direction as the field and given by

$$\underline{J} = \sigma_{\text{iso}} \underline{E}$$

or, in suffix notation,

$$J_i = \sigma_{\text{iso}} E_i = \sigma_{\text{iso}} \delta_{ij} E_j$$

where the scalar σ_{iso} is the *conductivity* of the isotropic crystal[8]. In other words, $\underline{J}$ and $\underline{E}$ are parallel. In general, however, electrical conductivity in most crystals is not isotropic and $\underline{J}$ and $\underline{E}$ will not be parallel. The general relationship between $\underline{J}$ and $\underline{E}$ is given by

$$\underline{J} = \underline{\underline{\sigma}}\,\underline{E} \quad \Leftrightarrow \quad J_i = \sigma_{ij} E_j.$$

$\underline{\underline{\sigma}}$ is the electrical conductivity *tensor*, and is an example of a rank-two tensor. Thus, if I were to apply an electric field of the form $\underline{E} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, the resulting current density would be $\underline{J} = \begin{pmatrix} \sigma_{12} \\ \sigma_{22} \\ \sigma_{32} \end{pmatrix}$, i.e., not only does current flow in the direction $\underline{\hat{e}}^{(2)}$ in which the field was applied, but also along the transverse directions $\underline{\hat{e}}^{(1)}$ and $\underline{\hat{e}}^{(3)}$.

A tensor is a mathematical representation of a physical quantity. The rank of a tensor is equal to the number of its free suffixes. Examples of rank-two tensors:

[7] Isotropic means identical in all directions.
[8] Cubic crystals are an example for which the conductivity is isotropic.

Property	Equation
Permittivity	$D_i = \varepsilon_{ij} E_j$
Dielectric susceptibility	$P_i = \varepsilon_0 \chi^{\mathrm{e}}_{ij} E_j$
Permeability	$B_i = \mu_{ij} H_j$
Magnetic susceptibility	$M_i = \chi^{\mathrm{m}}_{ij} H_j$
Electrical conductivity	$J_i = \sigma_{ij} E_j$
Thermal conductivity	$h_i = -\kappa_{ij} \nabla_j T$
Thermal expansion	$\epsilon_{ij} = \alpha_{ij} \Delta T$
Stress	$F_i = \sigma_{ij} A_j$
Strain	$u_i - (u_0)_i = \epsilon_{ij} x_j + \omega_{ij} x_j$

1.7 Transformations

When we talk about *transformations*, what we mean is a change of basis from one orthogonal set $\{\underline{\hat{e}}\}$ to another $\{\underline{\hat{e}}'\}$.

Measurement of a physical property (such as polarisation, conductivity, susceptibility etc.) is made with respect to a particular basis. When we change basis, the physical property itself does not change, but the way in which we represent it does, i.e., the components of the tensor that we use to describe the physical property change.

1.7.1 Revision: Transformation of Vectors

Consider a physical property that has magnitude and direction and hence may be represented by a vector (i.e., a rank-one tensor). This property can be described by its components in the basis $\{\underline{\hat{e}}\}$, or by its components in the rotated basis $\{\underline{\hat{e}}'\}$,

$$\underline{p} = p_1 \underline{\hat{e}}^{(1)} + p_2 \underline{\hat{e}}^{(2)} + p_3 \underline{\hat{e}}^{(3)} = p'_1 \underline{\hat{e}}'^{(1)} + p'_2 \underline{\hat{e}}'^{(2)} + p'_3 \underline{\hat{e}}'^{(3)}$$

as shown in Fig. 1.2. If we denote the components with respect to the basis $\{\underline{\hat{e}}\}$ by the vector $\underline{p}$ and the components with respect to the basis $\{\underline{\hat{e}}'\}$ by $\underline{p}'$, i.e.,

$$\underline{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \quad \text{and} \quad \underline{p}' = \begin{pmatrix} p'_1 \\ p'_2 \\ p'_3 \end{pmatrix},$$

then the two sets of components are related by an orthogonal transformation[9], which in the case shown in Fig. 1.2, is described by

$$\begin{aligned} p'_1 &= p_1 \cos\theta + p_2 \sin\theta \\ p'_2 &= -p_1 \sin\theta + p_2 \cos\theta \\ p'_3 &= p_3 \end{aligned}$$

[9] Recall that an orthogonal matrix is one for which $\underline{R}^{\mathsf{T}} \underline{R} = \underline{R} \underline{R}^{\mathsf{T}} = \underline{I}$.

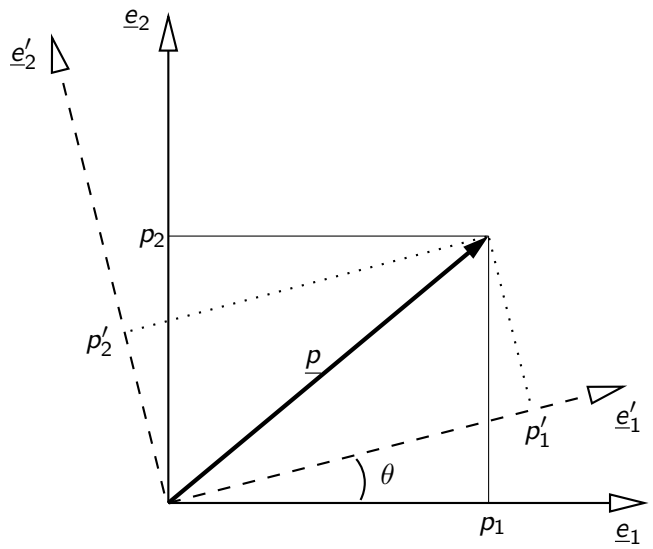

Figure 1.2: The vector $\underline{p}$ may be described by its components in the basis $\{\underline{\hat{e}}\}$ or $\{\underline{\hat{e}}'\}$. In the case drawn $\underline{\hat{e}}^{(3)} = \underline{\hat{e}}'^{(3)}$ points out of the page.

or, in suffix notation

$$\underline{p}' = \underline{\underline{\mathrm{L}}}\,\underline{p} \quad \Leftrightarrow \quad p'_i = l_{ij} p_j \tag{1.3}$$

where in this particular example

$$\underline{\underline{\mathrm{L}}} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Eqn. 1.3 is the **transformation law for a rank-one tensor**. The matrix $\underline{\underline{\mathrm{L}}}$ defines the transformation between two coordinate systems and is orthogonal:

$$l_{ki} l_{kj} = l_{ik} l_{jk} = \delta_{ij}$$

In general, the transformation matrix $\underline{\underline{\mathrm{L}}}$ is given by

$$l_{ij} = \underline{\hat{e}}'^{(i)} \cdot \underline{\hat{e}}^{(j)} \tag{1.4}$$

It is worth noting that the elements in the i^{th} row of $\underline{\underline{\mathrm{L}}}$ are the *direction cosines* (Fig. 1.3) of $\underline{\hat{e}}'^{(i)}$ with respect to the basis $\{\underline{\hat{e}}\}$.

Exercise: The polarisation of a crystal is measured in the basis $\{\underline{\hat{e}}\}$ to be $\underline{P} = \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix}$ (in SI units[10]). Find the polarisation $\underline{P}'$ as measured in a different basis $\{\underline{\hat{e}}'\}$ where

$$\underline{\hat{e}}^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \underline{\hat{e}}^{(3)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \underline{\hat{e}}^{(2)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

[10] The SI unit of polarisation is Cm^{-2}.

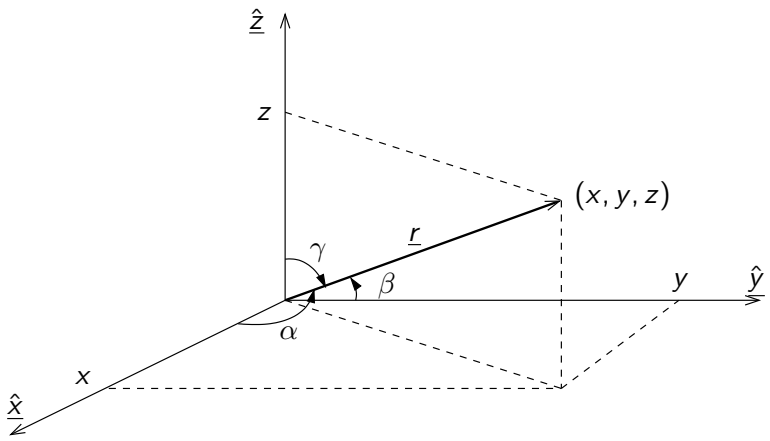

Figure 1.3: Revision: the direction cosines of vector $\underline{r}$ are $\cos\alpha$, $\cos\beta$ and $\cos\gamma$.

and

$$\hat{\underline{e}}'^{(1)} = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix} \quad \hat{\underline{e}}'^{(2)} = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\0\\1\end{pmatrix} \quad \hat{\underline{e}}'^{(3)} = \frac{1}{\sqrt{6}}\begin{pmatrix}1\\-2\\1\end{pmatrix}.$$

1.7.2 Transformation of Rank-Two Tensors

An example of a rank-two tensor is the conductivity $\underline{\underline{\sigma}}$ of a crystal, which connects the applied electric field $\underline{E}$ and the resulting current density $\underline{J}$:

$$J_i = \sigma_{ij} E_j \tag{1.5}$$

As mentioned before, these quantities have a physical reality. Only their representation changes, depending on the choice of basis. So, what happens to the above relation when we change our basis from $\{\hat{\underline{e}}\}$ to $\{\hat{\underline{e}}'\}$? There is no reason to expect that the physical laws of Nature should undergo any change, therefore we would expect that the current, conductivity and electric field, as measured in the new basis, would obey the same relationship, i.e.,

$$J'_i = \sigma'_{ik} E'_k, \tag{1.6}$$

where, as we saw in the previous section, the transformation law for rank-one tensors is such that

$$J'_i = l_{ip} J_p \quad \text{and} \quad E'_k = l_{kq} E_q.$$

Substituting these expressions into Eqn. 1.6 we have

$$\begin{aligned} J'_i &= \sigma'_{ik} E'_k \\ l_{ip} J_p &= \sigma'_{ik} l_{kq} E_q \\ l_{ij} l_{ip} J_p &= l_{ij} \sigma'_{ik} l_{kq} E_q \\ \delta_{jp} J_p &= l_{ij} l_{kq} \sigma'_{ik} E_q \\ J_j &= l_{ij} l_{kq} \sigma'_{ik} E_q \end{aligned}$$

Hence, comparing with Eqn. 1.5,

$$\begin{aligned} l_{ij} l_{kq} \sigma'_{ik} &= \sigma_{jq} \\ l_{pj} l_{ij} l_{rq} l_{kq} \sigma'_{ik} &= l_{pj} l_{rq} \sigma_{jq} \\ \delta_{pi} \delta_{rk} \sigma'_{ik} &= l_{pj} l_{rq} \sigma_{jq} \\ \sigma'_{pr} &= l_{pj} l_{rq} \sigma_{jq} \end{aligned}$$

which provides us with the **transformation law for a rank-two tensor**:

$$\boxed{A'_{ij} = l_{ip} l_{jq} A_{pq} \quad \Leftrightarrow \quad \underline{\underline{A}}' = \underline{\underline{L}} \underline{\underline{A}} \underline{\underline{L}}^{\mathsf{T}}} \tag{1.7}$$

This equation gives us the components A'_{ij} of a rank-two tensor in a basis $\{\underline{\hat{e}}'\}$, given its components A_{ij} in the basis $\{\underline{\hat{e}}\}$. In other words, it tells us how the components of the tensor transform from one basis to another.

Exercise: The conductivity of a crystal is measured in the basis $\{\underline{\hat{e}}\}$ to be

$$\underline{\underline{\sigma}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

(in SI units[11]). Find the conductivity $\underline{\underline{\sigma}}'$ as measured in a different basis $\{\underline{\hat{e}}'\}$ where

$$\underline{\hat{e}}^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \underline{\hat{e}}^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \underline{\hat{e}}^{(3)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

and

$$\underline{\hat{e}}'^{(1)} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad \underline{\hat{e}}'^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \quad \underline{\hat{e}}'^{(3)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}.$$

There are a number of checks one can use to help verify that you've transformed your tensor correctly:

1. $\mathrm{tr}\, \underline{A}' = \mathrm{tr}\, \underline{A}$ (why?)
2. $\det \underline{A}' = \det \underline{A}$ (why?)
3. Symmetry is preserved by the transformation (why?)

[11] The SI unit of conductivity is $(\Omega \mathrm{m})^{-1}$.

1.7.3 Definition of a Tensor

Above we discussed and derived the transformation of scalars (rank-zero tensors), vectors (rank-one tensors) and rank-two tensors. Scalars are, of course, invariant with respect to transformations – for example, when we measure the temperature of a sample, the result does not depend on our choice of axes:

$$T' = T$$

The components of a vector transform according to Eqn. 1.3:

$$T'_i = l_{ip} T_p$$

and the components of rank-two tensors transform according to Eqn. 1.7:

$$T'_{ij} = l_{ip} l_{jq} T_{pq}$$

We can keep going and write down the **transformation law** for a tensor of *any* rank in the same way:

$$\boxed{T'_{ijk\ldots} = l_{ip} l_{jq} l_{kr} \ldots T_{pqr\ldots}} \tag{1.8}$$

Eqn. 1.8 actually serves as the *definition* of a tensor:

A tensor is a physical quantity whose components transform according to the transformation law of Eq. 1.8.

The power and usefulness of suffix notation becomes more apparent when we start dealing with tensors of rank greater than two. Examples of such higher-rank tensors are given below.

Property	Equation	Notes
Piezoelectric modulus	$P_i = d_{ijk}\sigma_{jk}$	Polarisation $\underline{P}$, stress $\underline{\underline{\sigma}}$
Elastic compliance	$\epsilon_{ij} = s_{ijkl}\sigma_{kl}$	Strain $\underline{\underline{\epsilon}}$, stress $\underline{\underline{\sigma}}$
Elastic stiffness	$\sigma_{ij} = c_{ijkl}\epsilon_{kl}$	as above

1.7.4 Tensors vs Matrices

As we have seen, the components of a rank-two tensor can be represented as an array of numbers $[T_{ij}]$, much in the same way the transformation matrix $[l_{ij}]$ is represented as an array of numbers. However, this is where the analogy ends, for these quantities are fundamentally very different. $[T_{ij}]$ is the representation of a physical quantity in a particular basis $\{\hat{\underline{e}}\}$; $[l_{ij}]$ is rather an array of coefficients that tells us how one basis $\{\hat{\underline{e}}\}$ is related to another $\{\hat{\underline{e}}'\}$. It makes sense to talk about transforming $[T_{ij}]$ from one basis to another; it makes no such sense for $[l_{ij}]$. This is why $[T_{ij}]$ is a tensor, while $[l_{ij}]$ is not.

1.8 Diagonalisation of Rank-Two Tensors

We have seen that the transformation law for a rank-2 tensor is given by Eq. 1.7. In general, a rank-two tensor has nine components. If the tensor is symmetric, as is usually the case, the number of independent components is reduced to six. A question worth asking is "Is there a basis in which the representation of the tensor is actually diagonal?", i.e., is there a special basis in which there are just three non-zero components along the diagonal? The answer is yes! Any symmetric rank-two tensor can be diagonalised by a suitable rotation of basis, and the basis in which the tensor is diagonal is the basis of eigenvectors (the *principal directions*).

Exercise: The components of a tensor in the basis $\{\hat{\underline{e}}\}$ are given by

$$\underline{\underline{\mathrm{T}}} = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix}.$$

Find the principal values $\{\lambda\}$ and principal directions $\{\hat{\underline{e}}'\}$. Draw the orientation of the principal directions relative to the basis $\{\hat{\underline{e}}\}$.

The *normalised* principal directions are simply the basis vectors $\{\hat{\underline{e}}'\}$ of the new basis in which the representation of the tensor is diagonal, i.e., the transformation matrix is given by $l_{ij} = \hat{\underline{e}}'^{(i)} \cdot \hat{\underline{e}}^{(j)}$. The transformed tensor is then given by the usual transformation law, and is diagonal (i.e., all off-diagonal components are zero), with the eigenvalues $\lambda^{(i)}$ along the diagonal:

$$\underline{\underline{\mathrm{T}}}' = \underline{\underline{\mathrm{L}}}\,\underline{\underline{\mathrm{T}}}\,\underline{\underline{\mathrm{L}}}^{\mathsf{T}} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

Exercise: For the tensor $\underline{\underline{\mathrm{T}}}$ in the previous exercise, calculate the transformation matrix $\underline{\underline{\mathrm{L}}}$ and hence show that $\underline{\underline{\mathrm{T}}}'$ is diagonal with the eigenvalues along the diagonal. What is the angle of rotation in this transformation? Verify that the determinant and trace are invariant with respect to the transformation.

1.8.1 Representation Quadric

The representation quadric of a rank-two tensor is given by the equation

$$x_i T_{ij} x_j = c \quad \Leftrightarrow \quad \underline{x}^{\mathsf{T}} \underline{\underline{\mathsf{T}}} \underline{x} = c,$$

where c is a constant. When expanded out, this gives us a general quadratic form

$$t_{11}x_1^2 + t_{22}x_2^2 + t_{33}x_3^2 + 2t_{12}x_1x_2 + 2t_{23}x_2x_3 + 2t_{13}x_1x_3 = c,$$

where we have assumed that the tensor is symmetric $t_{ij} = t_{ji}$. The equation above is difficult to visualise in three-dimensions, so let us consider the plane $x_3 = 0$, in which case it becomes

$$t_{11}x_1^2 + t_{22}x_2^2 + +2t_{12}x_1x_2 = c.$$

The great benefit of tensor diagonalisation becomes clear when we notice that in the basis in which the tensor is diagonal, the representation quadric also becomes diagonal. Performing a rotation of basis we find

$$\begin{aligned} \underline{x}^{\mathsf{T}} \underline{\underline{\mathsf{T}}} \underline{x} &= c \\ \underline{x}^{\mathsf{T}} (\underline{\underline{\mathsf{L}}}^{\mathsf{T}} \underline{\underline{\mathsf{L}}}) \underline{\underline{\mathsf{T}}} (\underline{\underline{\mathsf{L}}}^{\mathsf{T}} \underline{\underline{\mathsf{L}}}) \underline{x} &= c \\ (\underline{x}^{\mathsf{T}} \underline{\underline{\mathsf{L}}}^{\mathsf{T}}) (\underline{\underline{\mathsf{L}}} \underline{\underline{\mathsf{T}}} \underline{\underline{\mathsf{L}}}^{\mathsf{T}}) (\underline{\underline{\mathsf{L}}} \underline{x}) &= c \\ \underline{x'}^{\mathsf{T}} \underline{\underline{\mathsf{T}}}' \underline{x'} &= c \end{aligned}$$

where we have used $\underline{\underline{\mathsf{L}}}^{\mathsf{T}} \underline{\underline{\mathsf{L}}} = I$ and the transformation laws for rank-one and rank-two tensors

$$x'_i = l_{ip} x_p \quad \text{and} \quad t'_{ij} = l_{ip} l_{jq} t_{pq}.$$

If $\underline{\underline{\mathsf{L}}}$ is chosen such that $\underline{\underline{\mathsf{T}}}'$ is diagonal, with principal values $\{\lambda'\}$, then, in the new basis, the cross-terms in the quadratic form disappear:

$$\underline{x'}^{\mathsf{T}} \underline{\underline{\mathsf{T}}}' \underline{x'} = \lambda'^{(1)} x'^2_1 + \lambda'^{(2)} x'^2_2 + \lambda'^{(3)} x'^2_3 = c.$$

Whereas in the original basis, the quadratic form may have been difficult to visualise (due to the x_1x_2 cross-term), in the basis of eigenvectors, in which the quadratic form is diagonal, it is much easier.

In Fig. 1.4 we plot the representation quadric for the tensor

$$\underline{\underline{T}} = \begin{pmatrix} 5 & 1 & 0 \\ 1 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

in the plane $x_3 = 0$.

Exercise: Write down the expression for the quadratic form. Find the eigenvalues and eigenvectors of $\underline{\underline{\mathsf{T}}}$. Express the quadratic form in the basis of eigenvectors. Draw the eigenvectors on Fig. 1.4 and label the lengths of the axes of the ellipse.

Things to note:

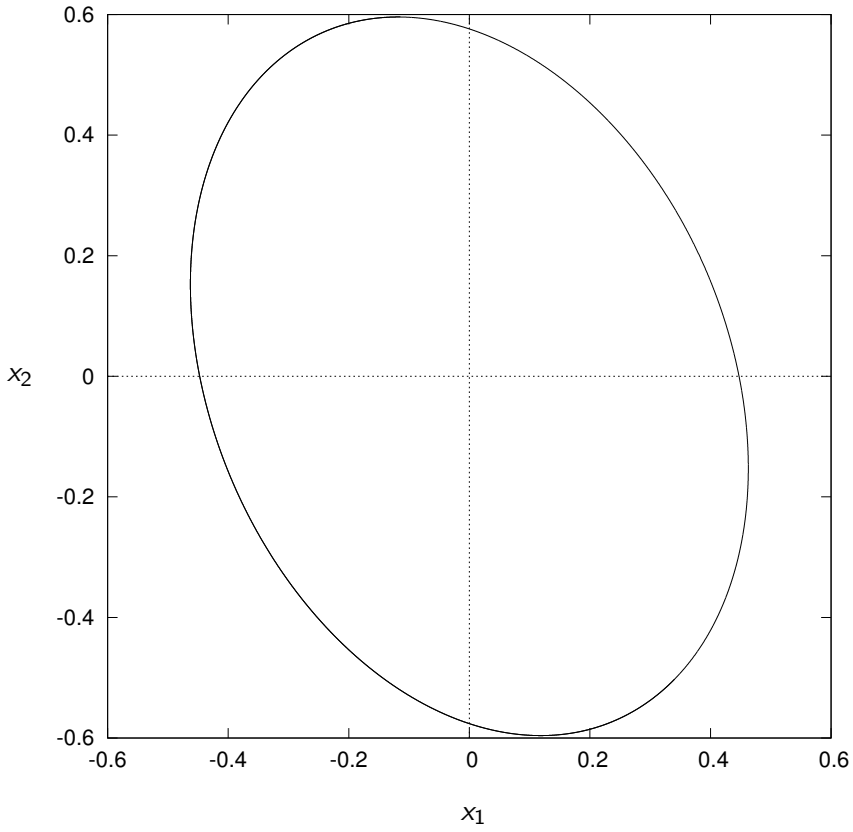

Figure 1.4: Quadric surface $x_i t_{ij} x_j = 1$ in the plane $x_3 = 0$.

1. The symmetry axes are aligned along the principal directions, which is why they are called the *principal axes*.

2. The i^{th} principal axis of the quadric surface has length $\sqrt{\dfrac{c}{\lambda_i}}$, where λ_i is the corresponding principal value.

3. Depending on the signs of the principal values, the quadric surface may be an ellipsoid or a hyperboloid (or other interesting shapes).

1.8.2 Stationary Property of Eigenvalues

The squared distance from the origin to the quadric surface, normalised to the scale of the surface, is given by

$$\mathrm{d}^2(\underline{x}) = \frac{\underline{x}^{\mathsf{T}}\underline{x}}{c} = \frac{\underline{x}^{\mathsf{T}}\underline{x}}{\underline{x}^{\mathsf{T}}\underline{\underline{\mathsf{T}}}\underline{x}},$$

and from what was discussed above about the principal axes being aligned with the symmetry axes of the surface, it must be the case that the principal axes are the directions for which d^2

is stationary. Conversely, we can show that the inverse of this quantity, $1/d^2(\underline{x})$, which we will denote by $\lambda(\underline{x})$, is stationary when $\underline{x}$ is in the direction of a principal axis:

$$\begin{aligned}\delta(\lambda(\underline{x})) &= \frac{2(\delta\underline{x}^{\mathsf{T}})\underline{\underline{\mathsf{T}}}\underline{x}}{\underline{x}^{\mathsf{T}}\underline{x}} - \frac{\underline{x}^{\mathsf{T}}\underline{\underline{\mathsf{T}}}\underline{x}}{(\underline{x}^{\mathsf{T}}\underline{x})^2}\cdot 2(\delta\underline{x}^{\mathsf{T}})\underline{x} \\ &= \frac{2}{\underline{x}^{\mathsf{T}}\underline{x}}\left[(\delta\underline{x}^{\mathsf{T}})\underline{\underline{\mathsf{T}}}\underline{x} - \frac{\underline{x}^{\mathsf{T}}\underline{\underline{\mathsf{T}}}\underline{x}}{\underline{x}^{\mathsf{T}}\underline{x}}(\delta\underline{x}^{\mathsf{T}})\underline{x}\right] \\ &= \frac{2}{\underline{x}^{\mathsf{T}}\underline{x}}(\delta\underline{x}^{\mathsf{T}})\left[\underline{\underline{\mathsf{T}}}\underline{x} - \lambda(\underline{x})\underline{x}\right],\end{aligned}$$

where, in the first step, we have used the fact that $\underline{x}^{\mathsf{T}}\underline{\underline{\mathsf{T}}}(\delta\underline{x}) = (\delta\underline{x}^{\mathsf{T}}\underline{\underline{\mathsf{T}}}\underline{x})$. Now we see that λ is stationary, i.e., $\delta\lambda(\underline{x}) = 0$, when $\underline{\underline{\mathsf{T}}}\underline{x} = \lambda(\underline{x})\underline{x}$. In other words, when $\underline{x}$ is aligned with a principal axis. It is also worth noting that the eigenvalues of $\underline{\underline{\mathsf{T}}}$ are the values of $\lambda(\underline{x})$ at its stationary points.

To summarise, the eigenvalues of a Hermitian matrix $\underline{\underline{\mathsf{H}}}$ are the values of the function

$$\lambda(\underline{x}) = \frac{\underline{x}^{\mathsf{T}}\underline{\underline{\mathsf{H}}}\underline{x}}{\underline{x}^{\mathsf{T}}\underline{x}}$$

at its stationary points which occur when $\underline{x}$ is aligned with an eigenvector of $\underline{\underline{\mathsf{H}}}$. This is the basis of the Rayleigh-Ritz method[12] for estimating eigenvalues and the quotient in the equation above is often called the Rayleigh quotient.

1.9 Tensor Properties of Crystals

1.9.1 Matter Tensors

Many tensors are a measure of the properties of a crystal, such as electrical and thermal conductivity, $[\sigma_{ij}]$ and $[\kappa_{ij}]$, electric and magnetic susceptibility, $[\chi^{\mathrm{e}}_{ij}]$ and $[\chi^{\mathrm{m}}_{ij}]$, etc. Such tensors are known as *matter tensors*.

Most rank-two matter tensors are symmetric. Symmetric rank-two tensors, as we saw earlier, have six independent components when expressed in some arbitrary basis. The number of independent components is further reduced due to the inherent symmetry of the crystal.

1.9.2 Neumann's Principle

It is a fundamental postulate of crystal theory that matter tensors must conform to the point group symmetry of the crystal. This is the basis of *Neumann's Principle*[13], which states that

[12] See Riley, Hobson and Bence, Ch. 9.3 for more details.

[13] Franz Ernst Neumann (1798–1895), German mineralogist, physicist and mathematician.

The symmetry elements of any physical property of a crystal must include the symmetry elements of the point group of the crystal.

Neumann's Principle enables us to simplify matter tensors if we know the point group symmetry of the crystal[14]. For example, it tells us that symmetric rank-two matter tensors must take a specific form for each of the seven distinct crystal systems when the tensor is represented in the conventional Cartesian co-ordinate basis for that crystal system. These forms are given in Table 1.1, and the conventional Cartesian co-ordinate axes $\{x_i\}$ for each crystal system are given in Table 1.2.

The representation quadric, discussed earlier, represents a rank-two matter tensor completely. When it is expressed in the basis of the crystal axes, the equation of the representation quadric has as many independent coefficients as there are independent elements in the matter tensor and its symmetry is the symmetry of the crystal property it describes. The quadric can be thought of as being an object whose orientation is fixed with respect to the crystal axes.

For example, a crystal with cubic symmetry is characterised by having four three-fold symmetry axes, also known as *triad* axes, that are arranged like the body diagonals of a cube. By Neumann's principal, the representation quadric of a cubic crystal must also have four triad axes and the only way in which this can be achieved is if the quadric surface is spherical. As such, all the principal values are equal and the associated matter tensor is isotropic and takes the same form no matter which basis it is represented in.

At the other extreme, a triclinic crystal has no symmetry axes and therefore there are no restrictions on the representation quadric, possibly other than a centre of symmetry which, as we're only considering symmetric tensors, it already has. Therefore the number of independent elements of the associated tensor is equal to the number of independent elements possessed by any symmetric tensor, i.e., six. These can be thought of as being three for specifying the dimensions of the quadric and three for specifying its orientation with respect to the crystal axes.

1.9.3 Thermal Conductivity as an Example

You are familiar with the concept of heat flow in a one-dimensional solid

$$h_x = -k\frac{\partial T}{\partial x}$$

where h_x is the quantity of heat per unit time per unit area of cross-section flowing in the x-direction due to a temperature gradient $\partial T/\partial x$ in that direction, and k is the *thermal conductivity*[15] of the solid.

[14] Note that the physical property need not have the *same* symmetries as the crystal point group, but must *include* them. Often matter tensors have more symmetries than the point group.

[15] The SI units of thermal conductivity are $\mathrm{Wm^{-1}K^{-1}}$.

Optical Class	Crystal System	N	Tensor†
Isotropic	Cubic	1	$\begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & s \end{pmatrix}$
Uniaxial	Tetragonal Hexagonal Trigonal	2	$\begin{pmatrix} s_1 & 0 & 0 \\ 0 & s_1 & 0 \\ 0 & 0 & s_2 \end{pmatrix}$
Biaxial	Orthorhombic	3	$\begin{pmatrix} s_1 & 0 & 0 \\ 0 & s_2 & 0 \\ 0 & 0 & s_3 \end{pmatrix}$
	Monoclinic	4	$\begin{pmatrix} s_{11} & 0 & s_{13} \\ 0 & s_2 & 0 \\ s_{13} & 0 & s_{33} \end{pmatrix}$
	Triclinic	6	$\begin{pmatrix} s_{11} & s_{12} & s_{13} \\ s_{12} & s_{22} & s_{23} \\ s_{13} & s_{23} & s_{33} \end{pmatrix}$

Table 1.1: Symmetric rank-two matter tensors in each of the seven crystal classes. N refers to the number of independent elements. †Referred to conventional axes for the crystal system.

In a three-dimensional, isotropic solid, this equation generalises to

$$\underline{h} = -k\nabla T \quad \Rightarrow \quad h_i = -k\frac{\partial T}{\partial x_i}$$

but we now know that only cubic crystals are isotropic, therefore, in general, the form of the equation is

$$h_i = -k_{ij}\frac{\partial T}{\partial x_j} \tag{1.9}$$

where $[k_{ij}]$ is the *thermal conductivity tensor*, a rank-two tensor. The physical meaning of k_{ij} is clear from the equation above: consider setting up a unit temperature gradient in the x_1 direction

$$\nabla T = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \underline{h} = -\begin{pmatrix} k_{11} \\ k_{21} \\ k_{31} \end{pmatrix},$$

i.e., the heat flow along the temperature gradient is $-k_{11}$, while in the two transverse directions it is $-k_{21}$ and $-k_{31}$.

Crystal system	Conventional axes
Cubic Orthorhombic	x_1, x_2 and x_3 along $\underline{a}$, $\underline{b}$ and $\underline{c}$, respectively
Tetragonal Hexagonal Trigonal	x_1 along $\underline{a}$, x_3 along $\underline{c}$
Monoclinic	x_2 along $\underline{b}$
Triclinic	No fixed relation to crystallographic directions

Table 1.2: The conventional Cartesian co-ordinate axes $\{x_i\}$ for each of the seven distinct crystal systems. $\underline{a}$, $\underline{b}$ and $\underline{c}$ are the lattice vectors of the unit cell of the crystal.

Expressing Eq. 1.9 in the basis of principle axes $\{x_i'\}$ gives, e.g., for an orthorhombic crystal

$$h_i' = -\kappa^{(i)} \frac{\partial T}{\partial x_i'}$$

where $\{\kappa^{(i)}\}$ are the principal values of $\underline{\underline{\mathrm{k}}}$ and h_i' are the components of the heat flow in the basis of principal axes.

Experimentally, it is found that $\underline{\underline{\mathrm{k}}}$ is symmetric[16], and that its principal values $\{\kappa^{(i)}\}$ are always positive. As such, its quadric surface

$$\kappa^{(1)} x_1'^2 + \kappa^{(2)} x_2'^2 + \kappa^{(3)} x_3'^2 = 1$$

is always ellipsoidal.

Inverting Eq. 1.9 gives

$$\frac{\partial T}{\partial x_i} = -r_{ij} h_j, \tag{1.10}$$

where the quantity $[r_{ij}]$ is the *thermal resistivity tensor*. In matrix form, $\underline{\underline{\mathrm{r}}}$ is the inverse of $\underline{\underline{\mathrm{k}}}$:

$$\underline{\underline{\mathrm{r}}} = \underline{\underline{\mathrm{k}}}^{-1}$$

This does not mean that $r_{ij} = (k_{ij})^{-1}$! However, it does imply that the *principal values* $\{\rho^{(i)}\}$ of the resistivity tensor are related to the principal values of the conductivity tensor by $\rho_i = \dfrac{1}{\kappa_i}$.

[16] There are also good theoretical grounds for this being the case. The interested should look up references to Onsager's Principle.

1.9.4 Steady-State Heat Flow in Crystals

The phrase "steady-state" means that the heat flow and temperature at any point in the system do not vary with time. We will consider two special cases of steady-state heat flow.

Heat Flow in a Thin, Wide Sample

The geometry of this situation is shown in Fig. 1.5. A thin, wide sample of a crystal is held between conducting plates that maintain a steady temperature on either side of the crystal. Due to the geometry of the sample, the isotherms (lines of constant temperature) must lie parallel to the surfaces of the crystal (aside from effects at the ends). The temperature gradient $-\nabla T$ must be perpendicular to the isotherms and must therefore be along the x_1 direction, as shown in the diagram, i.e.,

$$\frac{\partial T}{\partial x_2} = \frac{\partial T}{\partial x_3} = 0.$$

The heat flow $\underline{h}$ is then given by Eq. 1.9, which reduces to

$$h_i = -k_{1i}\frac{\partial T}{\partial x_1}, \quad i \in \{1, 2, 3\}.$$

In general, the direction of heat flow will be different to that of the temperature gradient. In fact, the rate of heat flow across the sample (which is what might be measured in an experiment) is not $|\underline{h}|$, but rather h_1.

Heat Flow in a Long, Narrow Sample

Consider a long, narrow sample held between two conductors that maintain a constant temperature difference, as shown in Fig. 1.6. If the walls of the rod are insulated, or the sample is held in vacuum, then the direction of heat flow must be parallel to the axis of the rod (again, there will always be end effects). As a result, the temperature gradient will, in general, be at an angle to the direction of heat flow and will be given by Eq. 1.10. Since $h_2 = h_3 = 0$, we have

$$\frac{\partial T}{\partial x_i} = -r_{1i}h_1.$$

The temperature gradient along the axis of the rod (which is what might be measured in an experiment) is therefore given by $-r_{11}h_1$.

1.10 Tensor Differential Operators

1.10.1 Tensor Fields

A scalar field $\phi(\underline{x})$ is a quantity that has a magnitude at every point $\underline{x}$ in space, e.g., the temperature $T(\underline{x})$ inside this room. A vector field is a quantity that has a magnitude and direction at

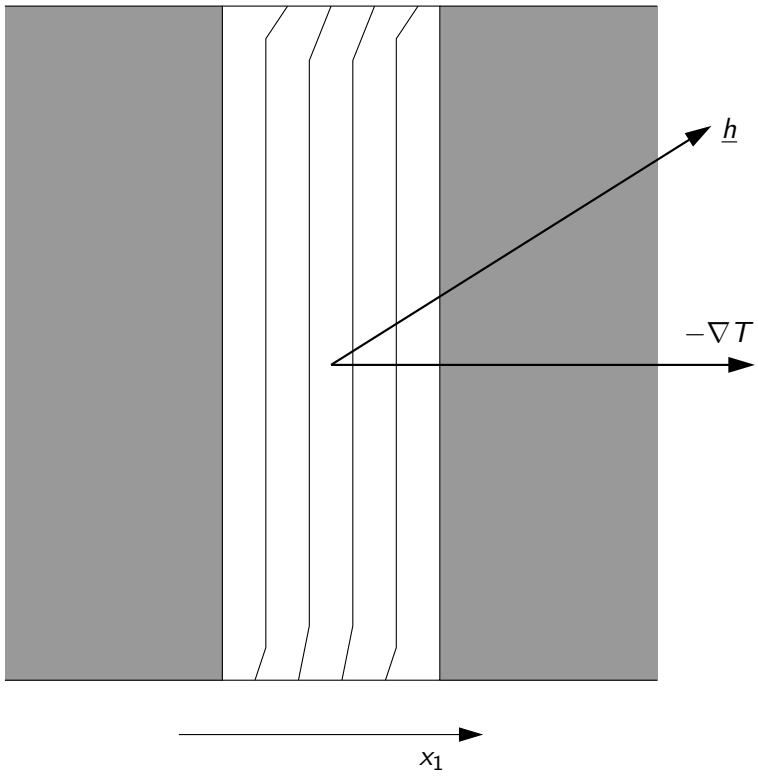

Figure 1.5: Heat flow in a thin, wide sample.

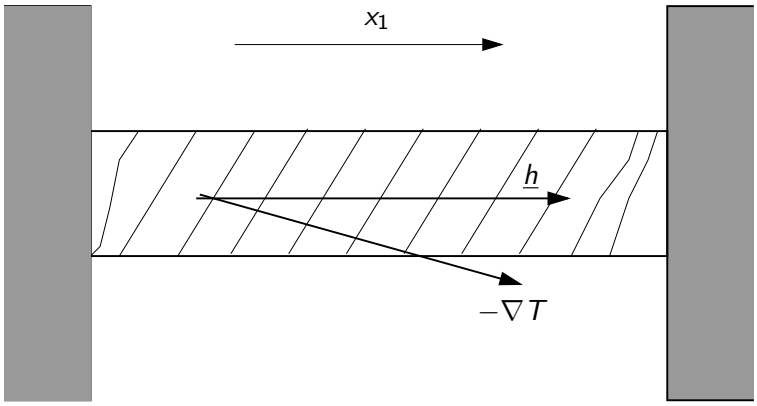

Figure 1.6: Heat flow in a long, narrow sample.

every point in space, e.g., the velocity $\underline{v}(\underline{x})$ of the air flow in this room. Similarly, one can extend this concept to tensor fields of higher-rank. An example is the stress field $[\sigma_{ij}(\underline{x})]$ in a crystal, which can depend on position.

When dealing with tensor fields, whatever the rank of the tensor, it is important to know *how the field varies with position*. In other words, one needs to know derivatives of the field with respect to position, which brings us onto the topic of the gradient operator ∇.

1.10.2 Suffix Notation for ∇

The definitions of grad, div and curl in Cartesian co-ordinates may be expressed using suffix notation:

$$[\nabla\phi]_i = \partial_i\phi$$
$$\nabla \cdot \underline{F} = \partial_i F_i$$
$$[\nabla \times \underline{F}]_i = \varepsilon_{ijk}\partial_j F_k$$

where we have used the convenient shorthand $\partial_i \equiv \dfrac{\partial}{\partial x_i}$.

1.10.3 ∇ as a Rank-One Tensor

In fact, it turns out that ∂_i is a rank-one tensor as it can be shown to satisfy the transformation law for rank-one tensors,

$$\partial'_i = l_{ip}\partial_p$$

where $\partial'_i \equiv \frac{\partial}{\partial x'_i}$.

Proof: For any quantity T, which may be a scalar, vector or tensor field, from the chain rule

$$\partial'_i T = (\partial_p T)\frac{\partial x_p}{\partial x'_i}.$$

$[x_i]$ is a rank-one tensor, therefore

$$\begin{aligned} x_p &= l_{jp}x'_j \\ \Rightarrow \quad \frac{\partial x_p}{\partial x'_i} &= \frac{\partial}{\partial x'_i}(l_{jp}x'_j) \\ &= l_{jp}\frac{\partial x'_j}{\partial x'_i} \\ &= l_{jp}\delta_{ji} = l_{ip} \end{aligned}$$

Hence, substituting into our expression above we obtain $\partial'_i T = l_{ip}\partial_p T$. Since T is arbitrary, $\partial'_i = l_{ip}\partial_p$, as required.

An important point to note is that previous tensors that we have come across in this course, when written in suffux notation, were just numbers whose order in an expression could be changed without affecting the result. For example

$$a_i b_{ij} c_j d_k = d_k b_{ij} a_i c_j = c_j b_{ij} d_k a_i \quad \text{etc.}$$

The same is not true for ∂_i. ∂_i is a *differential operator* and, by convention, acts to everything appearing to its right. Therefore for vector fields $\underline{u}(\underline{x})$ and $\underline{v}(\underline{x})$, for instance,

$$\partial_i u_i v_j = \partial_i(u_i v_j) = u_i(\partial_i v_j) + (\partial_i u_i)v_j$$

where we have used product rule to expand the differential of the product $u_i v_j$.

- Proof that $\nabla \cdot (\phi \underline{u}) = \underline{u} \cdot \nabla\phi + \phi \nabla \cdot \underline{u}$:

$$\begin{aligned} [\nabla \cdot (\phi \underline{u})]_i &= \partial_i(\phi u_i) \\ &= u_i(\partial_i \phi) + \phi(\partial_i u_i) \qquad \text{(using product rule)} \\ &= [\underline{u} \cdot \nabla\phi]_i + [\phi \nabla \cdot \underline{u}]_i \end{aligned}$$

- Proof that $\nabla \times (\underline{u} \times \underline{v}) = (\nabla \cdot \underline{v})\underline{u} - (\nabla \cdot \underline{u})\underline{v} + (\underline{v} \cdot \nabla)\underline{u} - (\underline{u} \cdot \nabla)\underline{v}$:

$$\begin{aligned} [\nabla \times (\underline{u} \times \underline{v})]_i &= \varepsilon_{ijk}\partial_j(\varepsilon_{klm}u_l v_m) \qquad \text{(using } [\underline{a} \times \underline{b}]_i = \varepsilon_{ijk}a_j b_k\text{)} \\ &= \varepsilon_{ijk}\varepsilon_{klm}\partial_j(u_l v_m) \qquad \text{(since } \varepsilon_{klm} \text{ is a constant)} \\ &= (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})\partial_j(u_l v_m) \\ &= \partial_j(u_i v_j) - \partial_j(u_j v_i) \\ &= u_i \partial_j v_j + v_j \partial_j u_i - u_j \partial_j v_i - v_i \partial_j u_j \qquad \text{(using product rule)} \\ &= [(\nabla \cdot \underline{v})\underline{u}]_i + [(\underline{v} \cdot \nabla)\underline{u}]_i - [(\underline{u} \cdot \nabla)\underline{v}]_i - [(\nabla \cdot \underline{u})\underline{v}]_i \end{aligned}$$

Chapter 2

Green Functions

2.1 Learning Outcomes

To understand and be able to use the methods of variation of parameters and Green functions to solve problems involving inhomogeneous linear differential equations.

2.2 Further Reading

1. Riley, Hobson & Bence, *Mathematical Methods for Physics and Engineering, 3rd Ed.*, Chapter 15: Higher-Order Differential Equations, Sections 2.4 and 2.5.
2. Arfken & Weber, *Mathematical Methods for Physicists, 4th (Intl.) Ed.*, Chapter 9: Sturm-Liouville Theory–Orthogonal Functions, Section 5.

2.3 Introduction

Green functions[1] are an invaluable tool for the solution of inhomogeneous differential equations and also have applications in other, unrelated branches of mathematics and physics such as quantum field theory and statistical field theory.

We begin by considering the general, second-order linear ordinary differential equation (ODE):

$$\mathcal{L}[y] \equiv \left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + p(x)\frac{\mathrm{d}}{\mathrm{d}x} + q(x)\right] y(x) = f(x), \tag{2.1}$$

subject to certain boundary conditions that must be specified. These may be *fixed point* boundary conditions, e.g., $y(0) = y(L) = \alpha$, or they may be *initial value* boundary conditions, e.g., $y(0) =$

[1] Named after George Green (1793–1841), a British mathematician and physicist, a Nottinghamshire miller who was entirely self-taught.

$y'(0) = \alpha$. If $\alpha = 0$, the boundary or initial conditions are said to be *homogeneous*, otherwise they are termed *inhomogeneous*. Similarly, the differential equation itself is called *homogeneous* if $f(x) = 0$ and *inhomogeneous* otherwise.

2.4 Variation of Parameters

You should recall from elementary courses on solving ODEs, that the general solution to Eqn. (2.1) is of the form

$$y(x) = y_0(x) + ay_1(x) + by_2(x), \tag{2.2}$$

where $y_1(x)$ and $y_2(x)$ are solutions of the homogeneous equation $\mathcal{L}[y] = 0$ and $y_0(x)$ is called the *particular integral*, which is any (non-trivial) solution that satisfies $\mathcal{L}[y] = f(x)$ subject to the specified boundary conditions. Finding the solutions to the homogeneous equation is usually the easier part. To find the particular integral, the method of variation of parameters may be used, in which we make an *ansatz*[2] for the particular integral:

$$y_0(x) = u(x)y_1(x) + v(x)y_2(x). \tag{2.3}$$

If $u(x)$ and $v(x)$ were constants, then $y_0(x)$ would be, by the principle of superposition, just a solution of the homogeneous equation. Therefore, we will vary these parameters subject to the constraint

$$u'(x)y_1(x) + v'(x)y_2(x) = 0, \tag{2.4}$$

such that $y_0(x)$ satisfies the inhomogeneous equation. Taking the first and second derivatives of Eqn. (2.3), making use of Eqn. (2.4) to simplify things, gives

$$\begin{aligned} y_0' &= uy_1' + u'y_1 + vy_2' + v'y_2 \\ &= uy_1' + vy_2' \\ y_0'' &= uy''_1 + u'y_1' + vy''_2 + v'y_2'. \end{aligned}$$

Substituting these expressions into the differential equation, after some rearrangement, gives

$$\mathcal{L}[y_0] \equiv y_0'' + py_0' + qy_0 = u'y_1' + v'y_2'$$

Hence, $y_0(x)$ is a particular solution to the differential equation if

$$u'(x)y_1'(x) + v'(x)y_2'(x) = f(x). \tag{2.5}$$

Eqns. (2.4) and (2.5) may be solved simultaneously to give

$$u'(x) = -\frac{f(x)y_2(x)}{W(x)} \quad \text{and} \quad v'(x) = \frac{f(x)y_1(x)}{W(x)} \tag{2.6}$$

where

$$W(x) \equiv \begin{vmatrix} y_1 & y_2 \\ y_1' & y_2' \end{vmatrix} = y_1y_2' - y_2y_1' \tag{2.7}$$

[2] An educated guess which will later turn out to have been a good one. From the German word meaning *onset* or *starting-point*.

is known as the *Wronskian*[3] of y_1 and y_2. It can be shown that if y_1 and y_2 are linearly independent solutions to the homogeneous equation, then $W \neq 0$.

Eqn. (2.6) may be solved to obtain $u(x)$ and $v(x)$, and hence $y_0(x)$. It is important to make sure that $y(x)$ satisfies the boundary or initial conditions that are appropriate to the problem. Examples are given below.

2.4.1 Homogeneous Initial Conditions

Integrating Eqn. (2.6) gives

$$u(x) = -\int_\alpha^x \frac{f(x')y_2(x')}{W(x')}\,\mathrm{d}x' \quad \text{and} \quad v(x) = \int_\alpha^x \frac{f(x')y_1(x')}{W(x')}\,\mathrm{d}x',$$

where the lower limit in each integral is chosen such that the expression for the particular integral

$$y_0(x) = \int_\alpha^x \left[\frac{y_1(x')y_2(x) - y_2(x')y_1(x)}{W(x')}\right] f(x')\,\mathrm{d}x'$$

satisfies the homogeneous initial conditions $y_0(\alpha) = y_0'(\alpha) = 0$. The solution to the ODE that satisfies the initial conditions is then just $y(x) = y_0(x)$, which can be expressed as

$$y(x) = \int_\alpha^\infty G(x, x')f(x')\,\mathrm{d}x'$$

where we have defined the *Green function*

$$G(x, x') = \begin{cases} 0 & x' > x \\ \frac{y_1(x')y_2(x) - y_2(x')y_1(x)}{W(x')} & x' < x \end{cases}.$$

2.4.2 Inhomogeneous Initial Conditions

Consider more general initial conditions of the form $y(\alpha) = c_1$, $y'(\alpha) = c_2$. We can convert the problem into a homogeneous one by defining

$$y(x) = \tilde{y}(x) + g(x),$$

where $g(x)$ is any function chosen to satisfy the inhomogeneous initial conditions $g(\alpha) = c_1$, $g'(\alpha) = c_2$. Then it can be seen that

$$\mathcal{L}[\tilde{y}] = \tilde{f}(x),$$

where

$$\tilde{f} \equiv f - g'' - pg' - qg,$$

and $\tilde{y}(x)$ now satisfies homogeneous initial conditions $\tilde{y}(\alpha) = \tilde{y}'(\alpha) = 0$.

[3] Named after the Polish mathematician Józef Maria Hoene-Wroński (1778–1853).

2.4.3 Homogeneous Two-Point Boundary Conditions

An example of homogeneous two-point boundary conditions is $y(\alpha) = y(\beta) = 0$. A solution to Eqn. (2.1) that satisfies $y(\alpha) = 0$ is

$$y(x) = \int_\alpha^x \left[\frac{y_1(x')y_2(x) - y_2(x')y_1(x)}{W(x')}\right] f(x')\,\mathrm{d}x' + k\left[y_1(\alpha)y_2(x) - y_1(x)y_2(\alpha)\right],$$

where k is an arbitrary constant. Setting $y(\beta) = 0$ gives

$$k\left[y_1(\alpha)y_2(\beta) - y_1(\beta)y_2(\alpha)\right] = -\int_\alpha^\beta \left[\frac{y_1(x')y_2(\beta) - y_2(x')y_1(\beta)}{W(x')}\right] f(x')\,\mathrm{d}x',$$

which enables the constant k to be determined if and only if neither $y_1(x)$ nor $y_2(x)$ vanish at both α and β[4]. To simplify the algebra, it is expedient to choose y_1 and y_2 such that

$$y_1(\alpha) = y_2(\beta) = 0,$$

which implies that

$$k = -\frac{1}{y_2(\alpha)}\int_\alpha^\beta \frac{y_2(x')f(x')}{W(x')}\,\mathrm{d}x',$$

which may be substituted into the solution to give

$$\begin{aligned} y(x) &= \int_\alpha^x \left[\frac{y_1(x')y_2(x) - y_2(x')y_1(x)}{W(x')}\right] f(x')\,\mathrm{d}x' + \int_\alpha^\beta \frac{y_2(x')y_1(x)}{W(x')} f(x')\,\mathrm{d}x' \\ &= \int_\alpha^x \frac{y_1(x')y_2(x)}{W(x')} f(x')\,\mathrm{d}x' + \int_x^\beta \frac{y_2(x')y_1(x)}{W(x')} f(x')\,\mathrm{d}x' \qquad (2.8) \\ &\equiv \int_\alpha^\beta G(x,x')f(x')\,\mathrm{d}x', \qquad (2.9) \end{aligned}$$

where we have defined the Green function

$$G(x,x') = \begin{cases} \frac{y_1(x')y_2(x)}{W(x')} & \alpha \le x' < x \\ \frac{y_1(x)y_2(x')}{W(x')} & x < x' \le \beta \end{cases}, \qquad (2.10)$$

and the solution satisfies the required boundary conditions.

Let us consider the properties of the Green function $G(x,x')$.

1. Continuity at $x = x'$

$$\begin{aligned} \left[G(x,x')\right]_{x=x'} &\equiv \lim_{\epsilon\to 0}\left[G(x,x')\right]_{x=x'-\epsilon}^{x=x'+\epsilon} \\ &= \lim_{\epsilon\to 0}\left[\frac{y_1(x')y_2(x'+\epsilon)}{W(x')} - \frac{y_1(x'-\epsilon)y_2(x')}{W(x')}\right] \\ &= 0 \end{aligned}$$

[4] In other words, a solution to the inhomogeneous differential equation exists if and only if there is no solution to the homogeneous differential equation that satisfies both boundary conditions.

2. Unit discontinuity of $\frac{\partial G}{\partial x}$ at $x = x'$

$$\begin{aligned}\left[\frac{\partial G}{\partial x}\right]_{x=x'} &\equiv \lim_{\epsilon\to 0}\left[\frac{y_1(x')y_2'(x'+\epsilon)}{W(x')} - \frac{y_1'(x'-\epsilon)y_2(x')}{W(x')}\right] \\ &= \frac{W(x')}{W(x')} \\ &= 1\end{aligned}$$

We derived above the form of the Green function for the differential operator of Eqn. (2.1) using the method of variation of parameters. Below we consider Green functions via a more formal approach and derive the same results, but first we have to meet the Dirac delta-function.

2.5 Dirac Delta-Function

The Dirac delta-function[5] $\delta(x - x')$ has the fundamental, defining property

$$\int_a^b g(x')\,\delta(x - x')\,\mathrm{d}x' = g(x) \quad \text{for } x \in [a, b]. \tag{2.11}$$

What this shows is that under integration the delta-function "picks out" the value of $g(x)$ at the point on which the delta-function is centred.

It may be thought of as a "spike", centred on $x = x'$, with zero width, infinite height and unit area underneath[6]

$$\delta(x - x') = \begin{cases} \infty & x = x' \\ 0 & \text{otherwise} \end{cases}$$

2.5.1 Properties of $\delta(x)$

- $\delta(x) = \delta(-x)$ is an even function
- $\delta^*(x) = \delta(x)$ is a real function
- The area under $\delta(x)$ is 1
$$\int_{-\eta}^{\eta} \delta(x)\,\mathrm{d}x = 1 \quad \forall\ \eta > 0$$
- The Fourier transform of $\delta(x)$ is a constant
$$\tilde{\delta}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \delta(x)\,\mathrm{e}^{-ikx}\,\mathrm{d}x = \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{-ikx}\Big|_{x=0} = \frac{1}{\sqrt{2\pi}}$$

[5] Paul Adrien Maurice Dirac (1902–1984), British theoretical physicist. Dirac shared the Nobel Prize in Physics (1933) with Erwin Schrödinger, for his work on Quantum Theory.

[6] Technically, this definition is only heuristic as $\delta(x)$ can not really be called a *function*, rather it is a *distribution* which is defined only under integration, as in Eqn. 2.11.

2.5.2 $\delta(x)$ as the Limit of a Top-Hat Function

$\delta(x)$ may be thought of as the limit of a top-hat function of width ϵ and height $\frac{1}{\epsilon}$ as $\epsilon \to 0$:

$$\delta(x) = \lim_{\epsilon \to 0} \delta_\epsilon(x)$$

where

$$\delta_\epsilon(x) = \begin{cases} \epsilon^{-1} & |x| < \epsilon/2 \\ 0 & \text{otherwise} \end{cases}$$

$\delta_\epsilon(x)$ is sketched for different values of ϵ in Fig. 2.1.

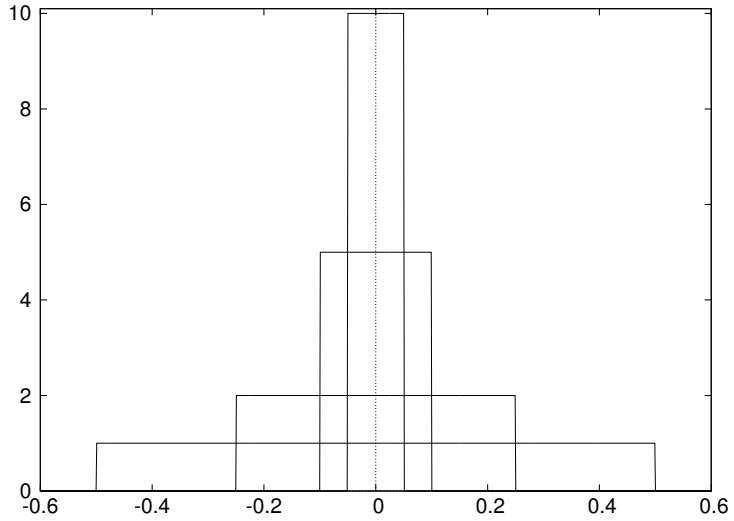

Figure 2.1: $\delta_\epsilon(x)$ for $\epsilon \in \{1, 0.5, 0.2, 0.1\}$.

Using Fig. 2.2 as a guide, consider the limit

$$\begin{aligned}
\lim_{\epsilon \to 0} \int_{x-\epsilon/2}^{x+\epsilon/2} f(x')\, \delta_\epsilon(x - x')\, \mathrm{d}x' &= \lim_{\epsilon \to 0} \int_{x-\epsilon/2}^{x+\epsilon/2} f(x')\, \frac{1}{\epsilon}\, \mathrm{d}x' \\
&= \lim_{\epsilon \to 0} f(a) \int_{x-\epsilon/2}^{x+\epsilon/2} \frac{1}{\epsilon}\, \mathrm{d}x' \quad a \in [x - \frac{\epsilon}{2}, x + \frac{\epsilon}{2}] \\
&= \lim_{\epsilon \to 0} f(a) \left[\frac{x'}{\epsilon} \right]_{x-\epsilon/2}^{x+\epsilon/2} \\
\Rightarrow \int f(x')\, \delta(x - x')\, \mathrm{d}x' &= f(x),
\end{aligned}$$

which is exactly Eqn. 2.11.

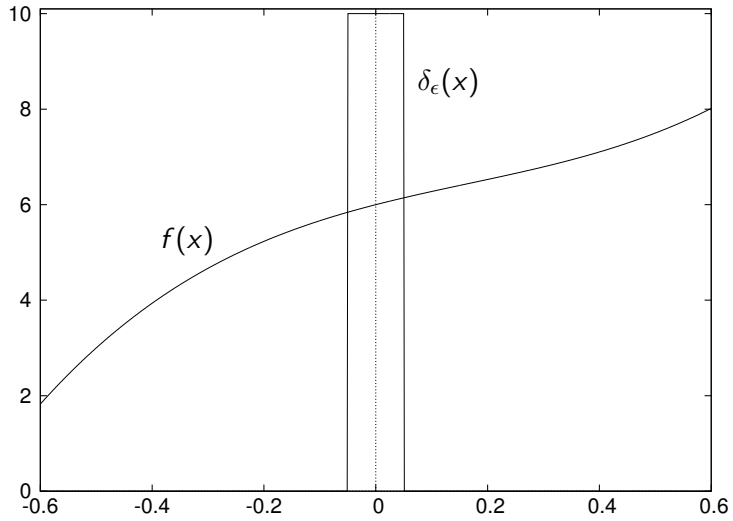

Figure 2.2: Generic sketch of $f(x)$ and $\delta_\epsilon(x)$.

2.5.3 $\delta(x)$ as the Limit of a Sinc Function

Consider the integral:

$$\delta_\epsilon(x) = \frac{1}{2\pi}\int_{-1/\epsilon}^{1/\epsilon} \mathrm{e}^{ikx}\,\mathrm{d}k.$$

We can integrate the expression for $\delta_\epsilon(x)$:

$$\begin{aligned} \delta_\epsilon(x) &= \frac{1}{2\pi}\left[\frac{\mathrm{e}^{ikx}}{ix}\right]_{k=-1/\epsilon}^{1/\epsilon} \\ &= \frac{1}{\epsilon\pi}\frac{\sin(x/\epsilon)}{x/\epsilon} \\ \Rightarrow \qquad \delta_\epsilon(x) &= \frac{\mathrm{sinc}(x/\epsilon)}{\epsilon\pi} \end{aligned}$$

Where $\mathrm{sinc}(x) \equiv \dfrac{\sin x}{x}$. $\delta_\epsilon(x)$ is plotted in Fig. 2.3 for different values of ϵ.

Show that[7]

$$f(x) = \lim_{\epsilon\to 0}\int f(x')\delta_\epsilon(x-x')\,\mathrm{d}x'. \tag{2.12}$$

[7] You may find the Riemann-Lebesque lemma helpful: $\lim_{\lambda\to\pm\infty}\int g(t)\sin(\lambda t)\,\mathrm{d}t = 0$.

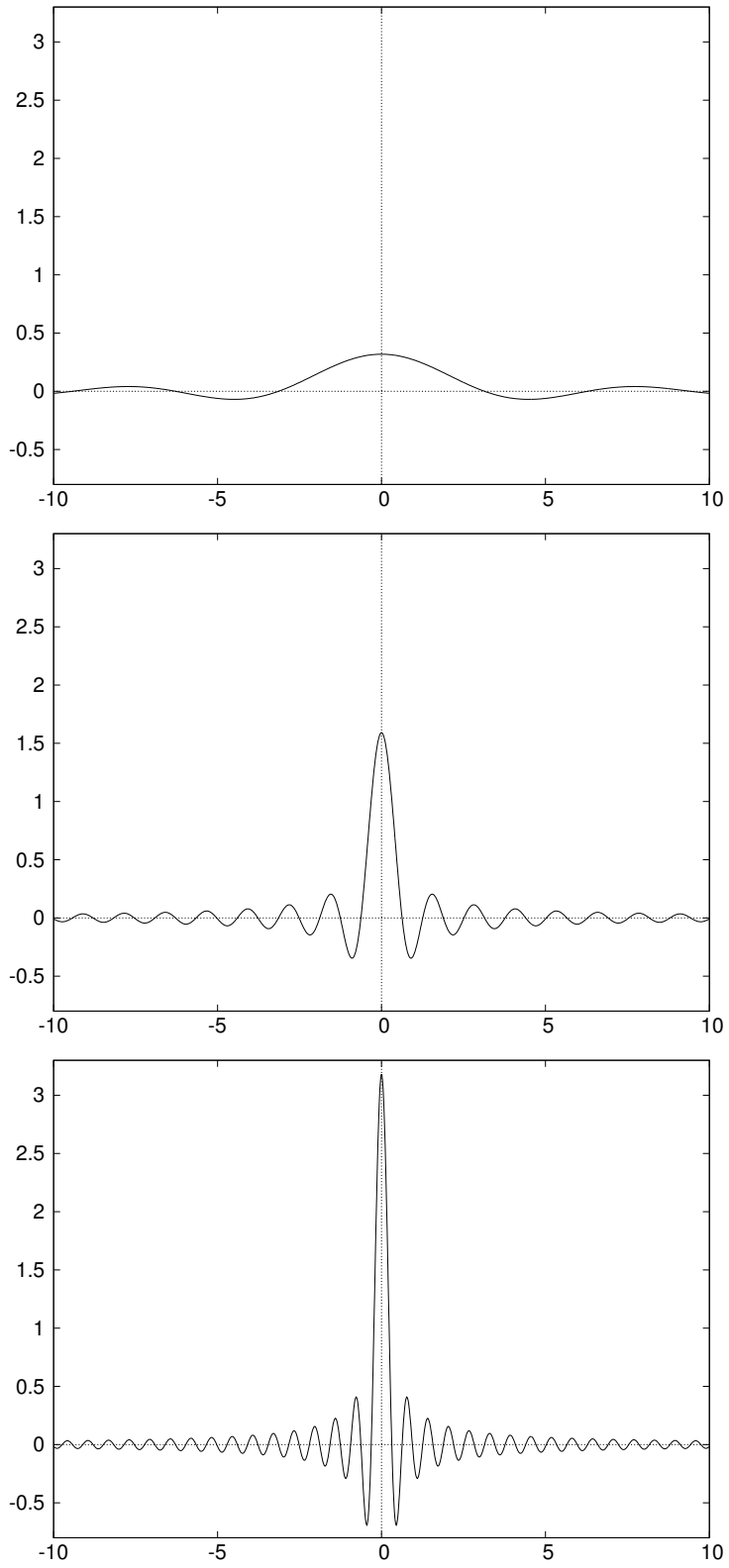

Figure 2.3: $\delta_\epsilon(x) = \dfrac{\mathrm{sinc}(x/\epsilon)}{\epsilon\pi}$ for $\epsilon \in \{1, 0.2, 0.1\}$.

2.5.4 $\delta(x)$ as the Continuous Analogue of δ_{ij}

The Dirac delta-function can also be thought of as the continuous analogue of the discrete Krönecker-delta δ_{ij} which has a property analogous to Eqn. 2.11, but for discrete variables

$$\sum_j \delta_{ij} g_j = g_i.$$

2.6 Green Functions

Consider a second order differential operator of the form

$$\mathcal{L} = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + p(x)\frac{\mathrm{d}}{\mathrm{d}x} + q(x),$$

and the associated inhomogeneous equation

$$\mathcal{L}[y(x)] = f(x),$$

subject to, e.g., two-point boundary conditions $y(\alpha) = y(\beta) = 0$. The Green function $G(x, x')$ is defined by

$$\mathcal{L}[G(x, x')] = \delta(x - x'),$$

where $\delta(x)$ is the Dirac delta-function. $G(x, x')$ is subject to the same boundary conditions as $y(x)$, namely $G(\alpha, x') = G(\beta, x') = 0$. The solution to the original inhomogeneous equation is then given by

$$y(x) = \int_\alpha^\beta G(x, x') f(x')\,\mathrm{d}x',$$

which is easily verified by operating on both sides with $\mathcal{L}$:

$$\begin{aligned}\mathcal{L}[y] &= \int_\alpha^\beta \mathcal{L}[G(x, x')] f(x')\,\mathrm{d}x' \\ &= \int_\alpha^\beta \delta(x - x') f(x')\,\mathrm{d}x' \\ &= f(x).\end{aligned}$$

For $x \neq x'$, $\delta(x - x') = 0$, therefore

$$\mathcal{L}[G(x, x')] = 0 \quad x \neq x',$$

i.e., the Green function satisfies the homogenoeus equation with solutions $y_1(x)$ and $y_2(x)$. Therefore, by the principle of superposition, we may write

$$G(x, x') = \begin{cases} A(x')y_1(x) + B(x')y_2(x) & \alpha < x < x' \\ C(x')y_1(x) + D(x')y_2(x) & x' < x < \beta \end{cases}$$

To find the parameters $A(x')$, $B(x')$, $C(x')$ and $D(x')$, we use the boundary conditions on $G(x, x')$, the continuity of $G(x, x')$, and the unit discontinuity of $\frac{\partial G}{\partial x}$ at $x = x'$:

1. Boundary conditions: $G(\alpha, x') = G(\beta, x') = 0$.

$$A(x')y_1(\alpha) + B(x')y_2(\alpha) = 0 \tag{2.13}$$
$$C(x')y_1(\beta) + D(x')y_2(\beta) = 0 \tag{2.14}$$

2. Continuity of G and unit discontinuity of $\frac{\partial G}{\partial x}$.

$$\begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} C - A \\ D - B \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{2.15}$$

which, if $W \neq 0$, may be inverted to give

$$C - A = -\frac{y_2(x')}{W(x')} \quad \text{and} \quad D - B = \frac{y_1(x')}{W(x')}. \tag{2.16}$$

We can simplify the algebra considerably by choosing $y_1(x)$ and $y_2(x)$ such that

$$y_1(\alpha) = y_2(\beta) = 0.$$

It then follows from Eqns. (2.13) and (2.14) that

$$B(x') = C(x') = 0,$$

Hence, from Eqns. (2.16) we have

$$A(x') = \frac{y_2(x')}{W(x')} \quad \text{and} \quad D(x') = \frac{y_1(x')}{W(x')},$$

giving us the final result

$$G(x, x') = \begin{cases} \frac{y_1(x')y_2(x)}{W(x')} & \alpha \leq x' < x \\ \frac{y_1(x)y_2(x')}{W(x')} & x < x' \leq \beta \end{cases},$$

which is the same result derived using the variation of parameters method (Eqn. (2.10)). Hence the final solution that satisfies the differential equation and the boundary conditions $y(\alpha) = y(\beta) = 0$ is given, as before, by

$$y(x) = \int_\alpha^\beta G(x, x')f(x')\,\mathrm{d}x' \tag{2.17}$$
$$= \int_\alpha^x \frac{y_1(x')y_2(x)}{W(x')} f(x')\,\mathrm{d}x' + \int_x^\beta \frac{y_2(x')y_1(x)}{W(x')} f(x')\,\mathrm{d}x'. \tag{2.18}$$

Chapter 3

Hilbert Spaces

3.1 Learning Outcomes

To understand and be able to use the following concepts in solving problems: Hilbert spaces, linear dependence of functions, orthogonality of functions; Sturm-Liouville theory, self-adjoint differential operators, eigenfunctions and eigenvalues; eigenfunction expansions and completeness.

3.2 Further Reading

1. Riley, Hobson & Bence, *Mathematical Methods for Physics and Engineering, 3rd Ed.*, Chapter 17: Eigenfunction Methods for Differential Equations; Chapter 18: Special Functions.
2. Arfken & Weber, *Mathematical Methods for Physicists, 4th (Intl.) Ed.*, Chapter 9: Sturm-Liouville Theory–Orthogonal Functions.

3.3 Introduction

By analogy with finite-dimensional spaces of vectors that were discussed in Ch. 1, we may think of functions as objects in an infinite-dimensional space, known as a *Hilbert space*[1]. All of the characteristics of vector spaces carry over to the concept of Hilbert spaces, including the important idea of *orthogonality*. We will see a deep connection between Hermitian matrices and a particular class of differential operators known as self-adjoint operators. The eigenfunctions of self-adjoint operators, much like the eigenvectors of Hermitian matrices, turn out to be orthogonal and these orthogonal functions, much like orthogonal vectors, may be used as a complete basis set for the Hilbert space. In this chapter we will introduce everything rather pedagogically and for the case of problems in one spatial dimension only. The concepts generalise to higher numbers of dimensions in a straightforward way as you will see later in the course.

[1] Named after German mathematician David Hilbert (1862–1943).

3.4 Hilbert Spaces

3.4.1 Definition

A set of functions $\{u(x), v(x), w(x), ...\}$ on the interval $x \in [a, b]$ satisfying the same conditions outlined for finite-dimensional vectors in Section 1.4.2, constitute an (infinte-dimensional) Hilbert space.

3.4.2 Properties

In the same way that a set of linearly independent vectors can be used to uniquely express a arbitrary vector in the vector space, any (reasonable) function $f(x)$ on the interval $x \in [a, b]$ may be expressed in terms of a set of linearly independent basis functions $\{y_i(x)\}$

$$f(x) = \sum_{i=1}^{\infty} a_i y_i(x).$$

The inner product on an interval $x \in [a, b]$ is defined as

$$\langle f|g\rangle = \int_a^b f^*(x) w(x) g(x)\, \mathrm{d}x,$$

where $w(x)$ is a real-valued *weight function*[2] that is positive on the interval $x \in [a, b]$. Functions $f(x)$ and $g(x)$ are said to be orthogonal with respect to $w(x)$ on the interval $x \in [a, b]$ if $\langle f|g\rangle = 0$. The *norm* of $f(x)$ is given by $||f|| = \langle f|f\rangle^{1/2}$, and $f(x)$ may be normalised in the usual way: $\hat{f}(x) = f(x)/||f||$.

A set of functions is called *orthogonal* if

$$\langle y_i|y_j\rangle = 0 \quad \text{for } i \neq j,$$

and *orthonormal* if

$$\langle y_i|y_j\rangle = \delta_{ij}.$$

Given a set of linearly independent functions $\{f_n(x)\}$, one may construct an orthonormal set of functions $\{g_n(x)\}$ by the procedure of *Gram-Schmidt orthogonalisation*, which is explored further in the problem sets.

3.5 Sturm-Liouville Theory

Sturm-Liouville theory[3] is the theory of inhomogeneous equations of the from $\mathcal{L}y = f$ for second-order differential operators that are *self-adjoint*. In particular, it is concerned with $f = \lambda y$, where $y(x)$ is called an *eigenfunction* of $\mathcal{L}$ with associated eigenvalue λ.

[2] We will turn our attention to its origin in the next section.

[3] Named after Jacques Charles François Sturm (1803–1855) and Joseph Liouville (1809–1882).

3.5.1 Self-Adjoint Differential Operators

Consider the differential operator

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + \sigma(x), \tag{3.1}$$

where $\rho(x)$ and $\sigma(x)$ are defined on $x \in [a, b]$ and we require that $\rho(x) > 0$ on $x \in [a, b]$. Such an operator is said to be in *self-adjoint form*.

Furthermore, consider the inner product

$$\begin{aligned}
\langle u|\mathcal{L}v\rangle &= \int_a^b u^*(x)\mathcal{L}v(x)\,\mathrm{d}x \\
&= -\int_a^b u^*(x)\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho(x)\frac{\mathrm{d}v}{\mathrm{d}x}\right)\,\mathrm{d}x + \int_a^b u^*(x)\sigma(x)v(x)\,\mathrm{d}x \\
&= -\left[u^*(x)\rho(x)v'(x)\right]_a^b + \int_a^b u^{*\prime}(x)\rho(x)v'(x)\,\mathrm{d}x + \int_a^b u^*(x)\sigma(x)v(x)\,\mathrm{d}x \\
&= \left[-u^*\rho v' + u^{*\prime}\rho v\right]_a^b - \int_a^b v(x)\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho(x)\frac{\mathrm{d}u^*}{\mathrm{d}x}\right)\,\mathrm{d}x + \int_a^b u^*(x)\sigma(x)v(x)\,\mathrm{d}x \\
&= \int_a^b v(x)\mathcal{L}u^*(x)\,\mathrm{d}x + \left[\rho(u^{*\prime}v - u^*v')\right]_a^b \\
&= \langle v|\mathcal{L}u\rangle^* + \left[\rho(u^{*\prime}v - u^*v')\right]_a^b.
\end{aligned}$$

Therefore, if the boundary term

$$\left[\rho(u^{*\prime}v - u^*v')\right]_a^b = 0, \tag{3.2}$$

then $\langle u|\mathcal{L}v\rangle = \langle v|\mathcal{L}u\rangle^*$ and $\mathcal{L}$ is said to be *self-adjoint* and is analogous to a Hermitian matrix.

Any second order linear differential operator can be put into self-adjoint form. Consider the most general operator

$$\widetilde{\mathcal{L}} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(a(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) - b(x)\frac{\mathrm{d}}{\mathrm{d}x} + c(x), \tag{3.3}$$

where we require $a(x) \neq 0$ for $x \in [a, b]$. If $\mathcal{L}$ is multiplied by a function $w(x) > 0$,

$$\begin{aligned}
w\widetilde{\mathcal{L}} &= -w\frac{\mathrm{d}}{\mathrm{d}x}\left(a\frac{\mathrm{d}}{\mathrm{d}x}\right) - bw\frac{\mathrm{d}}{\mathrm{d}x} + cw \\
&= -\frac{\mathrm{d}}{\mathrm{d}x}\left(aw\frac{\mathrm{d}}{\mathrm{d}x}\right) + \left(aw' - bw\right)\frac{\mathrm{d}}{\mathrm{d}x} + cw,
\end{aligned}$$

which is in self-adjoint form (with $\rho = aw$ and $\sigma = cw$) if we choose $w(x)$ such that

$$\begin{aligned}
aw' &= bw \\
\Rightarrow \quad w(x) &= \exp\int_\alpha^x \frac{b(x')}{a(x')}\,\mathrm{d}x',
\end{aligned}$$

where we have chosen $w(\alpha) = 1$.

Self-adjoint, or Hermitian, operators take a very special role in the theory of Quantum Mechanics. According to the Copenhagen Interpretation, any physical quantum mechanical *observable*, such as position, energy, momentum, is an eigenvalue of a corresponding self-adjoint operator. The fact that self-adjoint operators have a discrete eigenspectrum $\{\lambda_n\}$ is the way in which quantisation is built in to quantum mechanics since observables can only take these discrete values[4].

3.5.2 Eigenfunctions and Eigenvalues

Consider the inhomogeneous equation

$$\widetilde{\mathcal{L}}y = \lambda y,$$

where $\widetilde{\mathcal{L}}$ is a general second order linear differential operator as given in Eqn. (3.3). As shown above, we may define a self-adjoint operator $\mathcal{L} = w\widetilde{\mathcal{L}}$ by means of a suitable weight function $w(x)$:

$$\mathcal{L}y = \lambda w y. \tag{3.4}$$

In general, the solutions to Eqn. (3.4) form a discrete, yet infinite, set with eigenvlaues $\{\lambda_n\}$ and eigenfunctions $\{y_n(x)\}$ for $n \in \{1, 2, 3, \ldots, \infty\}$. Analogously to the the eigenvalues and eigenvectors of Hermitian matrices, the eigenvalues of a self-adjoint operator are real and the eigenfunctions corresponding to distinct eigenvalues are orthogonal. The proof is as follows (note that the weight function is implicit in the definition of the inner product):

$$\begin{aligned} \widetilde{\mathcal{L}}y_i &= \lambda_i y_i \\ \left\langle y_j | \widetilde{\mathcal{L}} y_i \right\rangle &= \lambda_i \langle y_j | y_i \rangle \\ \left\langle y_j | \widetilde{\mathcal{L}} y_i \right\rangle^* &= \lambda_i^* \langle y_j | y_i \rangle^* \\ \left\langle y_i | \widetilde{\mathcal{L}} y_j \right\rangle &= \lambda_i^* \langle y_i | y_j \rangle \end{aligned} \qquad \begin{aligned} \widetilde{\mathcal{L}}y_j &= \lambda_j y_j \\ \left\langle y_i | \widetilde{\mathcal{L}} y_j \right\rangle &= \lambda_j \langle y_i | y_j \rangle \end{aligned}$$

Comparing the final expression in each of the columns above we find

$$(\lambda_i^* - \lambda_j) \langle y_i | y_j \rangle = 0.$$

1. For $i = j$ we have
$$(\lambda_i^* - \lambda_i)||y_i||^2 = 0,$$
so, if we have non-trivial eigenfunctions, then $\lambda_i^* = \lambda_i$, i.e., the eigenvalues are real.

2. For $i \neq j$ we have,
$$(\lambda_i - \lambda_j) \langle y_i | y_j \rangle = 0,$$
so, if we are considering distinct eigenvalues, then $\langle y_i | y_j \rangle = 0$, i.e., the eigenfunctions are orthogonal.

[4] For more details see, eg, P. A. M. Dirac, *The Principles of Quantum Mechanics*.

3.5.3 Eigenfunction Expansions

If $\{y_n\}$ is a complete set of orthonormal eigenfunctions of a self-adjoint operator, then any function with the same boundary conditions can be expressed as an eigenfunction expansion:

$$f(x) = \sum_{n=1}^{\infty} a_n y_n(x). \tag{3.5}$$

The coefficients a_n can be found by orthogonality of the eigenfunctions:

$$\begin{aligned}\langle y_m|f\rangle &= \sum_{n=1}^{\infty} a_n \langle y_m|y_n\rangle \\ &= \sum_{n=1}^{\infty} a_n \delta_{mn} \\ &= a_m.\end{aligned}$$

Substituting into the expansion we find

$$\begin{aligned}f(x) &= \sum_{n=1}^{\infty} \langle y_n|f\rangle\, y_n(x) \\ &= \sum_{n=1}^{\infty} \left[\int_a^b w(x')y_n^*(x')f(x')\,\mathrm{d}x'\right] y_n(x) \\ &= \int_a^b \mathrm{d}x' f(x') \left[w(x')\sum_{n=1}^{\infty} y_n(x)y_n^*(x')\right],\end{aligned}$$

which gives us the *completeness relation*

$$w(x')\sum_{n=1}^{\infty} y_n(x)y_n^*(x') = \delta(x-x'), \tag{3.6}$$

which defines what we mean by a *complete* set of functions.

In practice, particularly in numerical methods, the infinite sum in Eqn. (3.5) must be approximated by a finite sum

$$f(x) \approx \sum_{n=1}^{N} a_n y_n(x).$$

Defining the error to be

$$\varepsilon_N \equiv \left|\left| f(x) - \sum_{n=1}^{N} a_n y_n(x) \right|\right|^2 = ||f(x)||^2 - \sum_{n=1}^{N} \left[a_n^* \langle y_n|f\rangle + a_n \langle f|y_n\rangle\right] + \sum_{n=1}^{N} |a_n|^2$$

we see that the error is minimised when

$$\frac{\delta\varepsilon_N}{\delta a_n^*} = 0 \quad \Rightarrow \quad a_n - \langle y_n|f\rangle = 0 \quad \Rightarrow \quad a_n = \langle y_n|f\rangle\,,$$

and the value of the error at this point is

$$\varepsilon_N = ||f||^2 - \sum_{n=1}^{N} |a_n|^2 .$$

Using the fact that $\varepsilon_N \geq 0$, we obtain *Bessel's inequality*:

$$||f||^2 \geq \sum_{n=1}^{N} |a_n|^2 , \tag{3.7}$$

which, in the limit $N \to \infty$, becomes an equality and gives *Parseval's theorem*

$$||f||^2 = \sum_{n=1}^{\infty} |a_n|^2 . \tag{3.8}$$

3.5.4 Eigenfunction Expansion of Green Function

If $\{y_n\}$ are a set of orthonormal eigenfunctions of $\mathcal{L}$ with corresponding eigenvalues $\{\lambda_n\}$, then the Green function for $\mathcal{L}$ is given by

$$G(x, x') = \sum_{n=1}^{\infty} \frac{y_n(x) y_n^*(x')}{\lambda_n}. \tag{3.9}$$

$G(x, x')$ satisfies the appropriate boundary conditions, because $y_n(x)$ does, and it satisfies the defining property of a Green function:

$$\begin{aligned}
\mathcal{L}[G(x, x')] &= \sum_{n=1}^{\infty} \frac{\mathcal{L}[y_n(x)] y_n^*(x')}{\lambda_n} \\
&= \sum_{n=1}^{\infty} w(x) y_n(x) y_n^*(x') \\
&= \frac{w(x)}{w(x')} \left[w(x') \sum_{n=1}^{\infty} y_n(x) y_n^*(x') \right] \\
&= \delta(x - x'),
\end{aligned}$$

where we have used the completeness relation of Eqn. (3.6).

When $\lambda_n = 0$, for any n, then the Green function does not exist, which is another way of phrasing what we discovered earlier: if a solution to the homogeneous problem $\mathcal{L}y = 0$ exists that satisfies both boundary conditions, then the inhomogeneous problem $\mathcal{L}y = f$ has no solution; $\lambda_n = 0$ implies that y_n is exactly such a solution to the homogeneous problem.

3.5.5 Eigenfunction Expansions for Solving ODEs

As an example, consider the differential equation

$$\mathcal{L}y(x) - \nu y(x) = f(x),$$

subject to some boundary conditions, and where $\mathcal{L}$ is a self-adjoint operator with weight function $w(x) = 1$, eigenvalues λ_n, and corresponding eigenfunctions $\{y_n\}$, subject to the same boundary conditions.

We may expand both the solution $y(x)$ and the inhomogeneous term $f(x)$ in terms of the complete set of eigenfunctions of $\mathcal{L}$:

$$y(x) = \sum_{n=1}^{\infty} a_n y_n(x), \qquad f(x) = \sum_{n=1}^{\infty} f_n y_n(x),$$

where the coeeficients $\{a_n\}$ and $\{f_n\}$ are to be determined. Substituting into the original equation, we find

$$\sum_{n=1}^{\infty} a_n \left[\mathcal{L}y_n(x) - \nu y_n(x)\right] = \sum_{n=1}^{\infty} f_n y_n(x)$$
$$\sum_{n=1}^{\infty} a_n \left[\lambda_n - \nu\right] y_n(x) = \sum_{n=1}^{\infty} f_n y_n(x).$$

Orthogonality of the eigenfunctions implies that

$$a_n = \frac{f_n}{\lambda - \nu},$$

so that the solution is given by

$$y(x) = \sum_{n=1}^{\infty} \frac{f_n}{\lambda_n - \nu} y_n(x),$$

where, from the expansion for $f(x)$, $f_n = \langle y_n | f \rangle$.

Substituting f_n into $y(x)$ we find

$$\begin{aligned} y(x) &= \sum_{n=1}^{\infty} \frac{\langle y_n | f \rangle}{\lambda_n - \nu} y_n(x) \\ &= \int_a^b \sum_{n=1}^{\infty} \frac{y_n(x) y_n^*(x')}{\lambda_n - \nu} f(x')\, \mathrm{d}x' \\ &= \int_a^b G(x, x') f(x')\, \mathrm{d}x', \end{aligned}$$

hence we may identify the Green function of the problem as

$$G(x, x') = \sum_{n=1}^{\infty} \frac{y_n(x) y_n^*(x')}{\lambda_n - \nu}.$$

Note that if $\nu = \lambda_n$, for any n, then there is no solution: taking the inner product with y_n of the differential equation with $\nu = \lambda_n$

$$\begin{aligned}\langle y_n|\mathcal{L}y - \lambda_n y\rangle &= \langle y_n|f\rangle \\ \langle y_n|\mathcal{L}y\rangle - \lambda_n \langle y_n|y\rangle &= \langle y_n|f\rangle \\ \langle y|\mathcal{L}y_n\rangle^* - \lambda_n \langle y_n|y\rangle &= \langle y_n|f\rangle \\ \lambda_n \langle y|y_n\rangle^* - \lambda_n \langle y_n|y\rangle &= \langle y_n|f\rangle \\ 0 = \langle y_n|f\rangle &= f_n.\end{aligned}$$

3.6 Legendre Polynomials

Legendre's equation[5]

$$(1-x^2)y'' - 2xy' + l(l+1)y = 0, \tag{3.10}$$

arises is a number of contexts in science, for example in the solution of Laplace's equation in spherical co-ordinates. Eqn. (3.10) may be put easily into the form of a self-adjoint eigenvalue problem with $\rho(x) = (1-x^2)$, $\sigma(x) = 0$, $w(x) = 1$ and $\lambda = l(l+1)$,

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)\frac{\mathrm{d}y}{\mathrm{d}x}\right] = l(l+1)y(x). \tag{3.11}$$

If the boundary conditions are chosen such that $y(x)$ is finite at $x = \pm 1$, then $\rho(x)y(x) = 0$ at $x = \pm 1$, so Eqn. (3.2) is satisfied and $\mathcal{L}$ is self-adjoint on the interval $x \in [-1, 1]$. It may be shown that this condition can be met only when $l \in \{0, 1, 2, ...\}$[6]. The resulting eigenfunctions are known as Legendre polynomials and are usually denoted $P_l(x)$. Since they are the eigenfunctions of a self-adjoint operator, it follows that polymonials associated with different values of l must be orthogonal on the interval $x \in [-1, 1]$

$$\langle P_m|P_n\rangle = \int_{-1}^{1} P_m(x)P_n(x)\,\mathrm{d}x = \frac{2}{2m+1}\delta_{mn}. \tag{3.12}$$

For $m \neq n$, we may prove this directly. $P_m(x)$ satisfies Eqn. (3.11), so if we multiply by $P_n(x)$ and integrate we obtain

$$\int_{-1}^{1} P_n\left[(1-x^2)P_m'\right]'\,\mathrm{d}x + \int_{-1}^{1} P_n m(m+1)P_m\,\mathrm{d}x = 0.$$

Integrating once by parts the first term on the left-hand side we obtain

$$-\int_{-1}^{1} P_n'(1-x^2)P_m'\,\mathrm{d}x + \int_{-1}^{1} P_n m(m+1)P_m\,\mathrm{d}x = 0.$$

Repeating the same analysis but with m and n switched around we find

$$-\int_{-1}^{1} P_m'(1-x^2)P_n'\,\mathrm{d}x + \int_{-1}^{1} P_m n(n+1)P_n\,\mathrm{d}x = 0,$$

[5] Named after French mathematician Adrien-Marie Legendre (1752–1833).

[6] One may show this by obtaining the series solution to the Legendre equation.

which, when subtracted from the equation previous to it gives

$$[n(n+1) - m(m+1)] \int_{-1}^{1} P_n P_m \, \mathrm{d}x = 0,$$

which, for $m \neq n$, gives the orthogonality relation of Eqn. (3.12)[7].

The first few Legendre polynomials are given by

$$\begin{aligned} P_0(x) &= 1, & P_1(x) &= x, \\ P_2(x) &= \tfrac{1}{2}(3x^2 - 1), & P_3(x) &= \tfrac{1}{2}(5x^3 - 3x), \end{aligned}$$

and in general

$$P_l(x) = \frac{1}{2^l l!} \frac{\mathrm{d}^l}{\mathrm{d}x^l}(x^2 - 1)^l.$$

3.7 Spherical Harmonics

Laplace's equation in spherical co-ordinates is given by

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial f}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 f}{\partial \phi^2} = 0.$$

If we take $f(r, \theta, \phi) = r^l \Theta(\theta)\Phi(\phi)$ as an ansatz[8], where $l \in \{0, 1, 2, ...\}$, Laplace's equation becomes

$$\begin{aligned} & l(l+1)\Theta(\theta)\Phi(\phi) + \frac{\Phi(\phi)}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta \frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \frac{\Theta(\theta)}{\sin^2\theta}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2} = 0 \\ \Rightarrow \quad & \sin^2\theta l(l+1) + \frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \frac{1}{\Phi(\phi)}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2} = 0. \end{aligned}$$

The first two terms on the left-hand side above are purely functions of θ, while the remaining term is purely a function of ϕ. For non-trivial solutions, therefore, both these terms must be equal to the same constant, i.e.,

$$\begin{aligned} & \frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \sin^2\theta l(l+1) = m^2, \\ & \frac{1}{\Phi(\phi)}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2} = -m^2, \end{aligned}$$

for some constant m. Since $f(r, \theta, \phi) = f(r, \theta, \phi + 2\pi)$ must be periodic, it can be seen from the second equation that $m \in \mathbb{Z}$ and

$$\Phi(\phi) = c\mathrm{e}^{im\phi}.$$

[7] For $m = n$ see, e.g., Riley, Hobson & Bence.

[8] This is the technique of *separation of variables*, where we have "guessed" the right answer for the radial part of f(r) to save time!

Substituting $u = \cos\theta$ into the first equation, after some algebra we find that

$$(1-u^2)\frac{\mathrm{d}^2\Theta}{\mathrm{d}u^2} - 2u\frac{\mathrm{d}\Theta}{\mathrm{d}u} + l(l+1)\Theta(u) = \frac{m^2}{1-u^2}\Theta(\theta)$$
$$\Rightarrow \quad -\left[(1-u^2)\Theta'\right]' = \left[l(l+1) - \frac{m^2}{1-u^2}\right]\Theta, \tag{3.13}$$

which is called the associated Legendre equation. It has non-singular solutions when l is an integer and $0 \leq m \leq l$. These solutions are called the *associated Legendre polynomials* $P_l^m(u)$. From Eqn. (3.13), it can be seen that $P_l^{-m}(u)$ must be proportional to $P_l^m(u)$. A common convention for the constant of proportionality is

$$P_l^{-m}(u) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(u). \tag{3.14}$$

When $m = 0$, the associated Legendre polynomials reduce to the Legendre polynomials, i.e., $P_l^0(u) = P_l(u)$. Eqn. (3.13) is in self-adjoint form with $\rho = (1-u^2)$, $\sigma = \frac{m^2}{(1-u^2)}$, $\lambda = l(l+1)$ and $w = 1$. Over the interval $x \in [-1, 1]$, the associated Legendre polymonials form an orthogonal basis set for different values of l:

$$\int_{-1}^{1} P_l^m(u) P_{l'}^m(u)\,\mathrm{d}u = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'}.$$

Furthermore, since we could also have defined the Sturm-Liouville problem with $\sigma = -l(l+1)$, $\lambda = -m^2$ and $w = \frac{1}{1-u^2}$, a second orthogonality condition must be also obeyed for different values of m:

$$\int_{-1}^{1} \frac{P_l^m(u) P_l^{m'}(u)}{1-u^2}\,\mathrm{d}u = \frac{(l+m)!}{m(l-m)!}\delta_{mm'}, \quad m \neq m' \neq 0.$$

The first few associated polynomials (for $m \neq 0$) are

$$P_1^1(u) = (1-u^2)^{1/2}, \quad P_2^1(u) = 3u(1-u^2)^{1/2},$$
$$p_2^2(u) = 3(1-u^2), \quad P_3^1(u) = \tfrac{3}{2}(5u^2-1)(1-u^2)^{1/2}.$$

Returning now to Laplace's equation, we denote the angular part of $f(r, \theta, \phi)$ by

$$Y_l^m(\theta,\phi) \equiv \Theta(\theta)\Phi(\phi) = (-1)^m \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta)\mathrm{e}^{im\phi},$$

where $Y_l^m(\theta,\phi)$ is known as a *spherical harmonic*. Using Eqn. (3.13), it can be shown that spherical harmonics satisfy

$$\nabla^2 Y_l^m(\theta,\phi) = -l(l+1)Y_l^m(\theta,\phi)$$

on the unit sphere $r = 1$. Using Eqn. (3.14) we find that

$$Y_l^{-m}(\theta,\phi) = (-1)^m Y_l^{m*}(\theta,\phi).$$

Since the spherical harmonics are the eigenfunctions of the self-adjoint operator ∇^2, they form a complete, orthogonal set on the unit sphere

$$\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} Y_{l'}^{m'*} Y_l^m \mathrm{d}\Omega = \delta_{ll'}\delta_{mm'},$$

where $\mathrm{d}\Omega = \sin\theta \mathrm{d}\theta \mathrm{d}\phi$. The first few spherical harmonics are listed below

$$\begin{aligned} Y_0^0 &= \tfrac{1}{\sqrt{4\pi}}, & Y_1^0 &= \sqrt{\tfrac{3}{4\pi}}\cos\theta, \\ Y_1^{\pm 1} &= \mp\sqrt{\tfrac{3}{8\pi}}\sin\theta \mathrm{e}^{\pm i\phi}, & Y_2^0 &= \sqrt{\tfrac{5}{16\pi}}(3\cos^2\theta - 1), \\ Y_2^{\pm 1} &= \mp\sqrt{\tfrac{15}{8\pi}}\sin\theta\cos\theta \mathrm{e}^{\pm i\phi}, & Y_2^{\pm 2} &= \sqrt{\tfrac{15}{32\pi}}\sin^2\theta \mathrm{e}^{\pm 2i\phi}. \end{aligned}$$

Completeness implies that any (reasonable) angular function may be expanded in terms of the set of spherical harmonics:

$$f(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} a_{lm} Y_l^m(\theta,\phi),$$

where the coefficients $\{a_{lm}\}$ may be found using orthogonality:

$$a_{lm} = \int Y_l^{m*}(\theta,\phi) f(\theta,\phi)\,\mathrm{d}\Omega.$$

One final relation that we should mention is the *spherical harmonic addition theorem*: for two arbitrary directions in space defined by the angles (in spherical polar co-ordinates) (θ,ϕ) and (θ',ϕ'), separated by an angle ψ

$$P_l(\cos\psi) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_l^m(\theta,\phi) Y_l^{m*}(\theta',\phi').$$

This result is very useful, for example, in scattering theory.

Chapter 4

Integral Transforms

4.1 Learning Outcomes

To be able to represent periodic functions in terms of a Fourier series of sine and cosine functions. The case of discontinuous functions. Parseval's theorem for Fourier series and its relation to power spectra. To understand the relationship between Fourier series and Fourier transforms. To know the definition and fundamental properties of the Fourier transform. The Parseval and convolution theorems for Fourier transforms. Application of Fourier methods to diffraction and differential equations. Laplace transforms: definition, properties, examples; their application to solving differential equations; inverse transform by inspection; convolution theorem.

4.2 Further Reading

1. Riley, Hobson & Bence, *Mathematical Methods for Physics and Engineering, 3rd Ed.*, Chapter 12: Fourier Series; Chapter 13: Integral Transforms.
2. Arfken & Weber, *Mathematical Methods for Physicists, 4th Ed.*, Chapter 14: Fourier Series; Chapter 15: Integral Transforms.
3. Boas, *Mathematical Methods in the Physical Sciences, 2nd Ed.*, Chapter 7: Fourier Series; Chapter 15: Integral Transforms.

4.3 Introduction

As we saw in the previous chapter, the eigenfunctions $\{y_n(x)\}$ of a self-adjoint operator form a complete, orthogonal set of basis functions for the Hilbert space which they span and can therefore be used to expand any (reasonable) function $f(x)$ in that space

$$f(x) = \sum_n a_n y_n(x).$$

In this chapter we focus first on one particular set of eigenfunctions that form the *Fourier*[1] basis. If we consider the properties of expansions in this basis on a periodic interval, the expansion is known as a *Fourier series*[2]. For an infinite interval, it is known as a *Fourier transforms*, which is an example of an *integral transform*. Towards the end of this chapter we will look at another example of an integral transform, namely the *Laplace transform*.

The methods we will cover in this chapter have an important place in science and engineering, with applications in signal processing and electronics, solving dierential equations, image processing and image enhancement, diraction and interferometry, and much more besides.

4.4 Fourier Series*

4.4.1 The Fourier Basis*

Consider the set of functions $s_n(x) = \sin(\frac{n\pi x}{L})$, $n \in \{1, 2, ...\}$ and $c_n(x) = \cos(\frac{n\pi x}{L})$, $n \in \{0, 1, ...\}$. They have a common period of $2L$, e.g., $s_n(x + 2L) = s_n(x)$ and, as they are the eigenfunctions of the Sturm-Liouville problem

$$\mathcal{L}y(x) = -\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = \Big(\frac{n\pi}{L}\Big)^2 y(x),$$

subject to periodic boundary conditions $y(x + 2L) = y(x)$, they form a mutually orthogonal set over any interval of length $2L$:

$$\begin{aligned} &\langle s_m | s_n \rangle = \langle c_m | c_n \rangle = L\delta_{mn} \quad m, n \neq 0 \\ &\langle c_0 | c_0 \rangle = 2L \\ &\langle c_m | s_n \rangle = 0 \quad \forall\ m, n \end{aligned} \tag{4.1}$$

We may also prove these orthogonality relations directly. For example, consider the symmetric interval $[-L, L]$,

$$\begin{aligned} \langle s_m | s_n \rangle &= \int_{-L}^{L} \sin\big(\tfrac{m\pi x}{L}\big) \sin\big(\tfrac{n\pi x}{L}\big)\, \mathrm{d}x \\ &= \frac{1}{2} \int_{-L}^{L} \Big[\cos\big(\tfrac{(m-n)\pi x}{L}\big) - \cos\big(\tfrac{(m+n)\pi x}{L}\big)\Big]\, \mathrm{d}x \\ &= \frac{1}{2} \left[\frac{L}{\pi(m-n)} \sin\big(\tfrac{(m-n)\pi x}{L}\big) - \frac{L}{\pi(m+n)} \sin\big(\tfrac{(m+n)\pi x}{L}\big)\right]_{-L}^{L} \qquad m \neq n \\ &= 0 \qquad \text{since } \sin p\pi = 0 \text{ for any integer } p \end{aligned}$$

[1] Jean Baptiste Joseph Fourier (1768–1830), French mathematician and physicist. Fourier also discovered the greenhouse effect.

[2] This part should be mainly revision and is included only for completeness.

And for the case of $m = n$, we have

$$\begin{aligned}\langle s_n | s_n \rangle &= \int_{-L}^{L} \sin^2(\tfrac{n\pi x}{L})\, \mathrm{d}x \\ &= \frac{1}{2}\int_{-L}^{L} \left[1 - \cos(\tfrac{2n\pi x}{L})\right] \mathrm{d}x \\ &= \frac{1}{2}\left[x - \frac{L}{2n\pi}\sin(\tfrac{2n\pi x}{L})\right]_{-L}^{L} \\ &= \frac{1}{2}\cdot 2L = L.\end{aligned}$$

A similar analyis may be done for the remaining conditions[3].

The set of functions comprising $s_n(x)$, $n \in \{1, 2, ...\}$, and $c_n(x)$, $n \in \{0, 1, ...\}$, form what is known as the Fourier basis, an orthogonal basis for the Hilbert space of functions that are periodic (in this case with period $2L$).

This means that, in the same way that any vector may be expressed as a linear combination of basis vectors, any periodic function $f(x) = f(x + 2L)$ may be represented as a linear combination of sines and cosines with the same periodicity,

$$f(x) = \sum_{n=0}^{\infty} a_n \cos(\tfrac{n\pi x}{L}) + \sum_{n=1}^{\infty} b_n \sin(\tfrac{n\pi x}{L}). \tag{4.2}$$

The expression above is known as a Fourier series, and Fourier analysis is all about finding the expansion coefficients $\{a_n\}$ and $\{b_n\}$.

As an example, consider a triangular wave $f(t)$, periodic on the interval $t \in [0, T]$

$$f(t) = \begin{cases} 4t/T & t \in [0, T/4] \\ 2(1 - 2t/T) & t \in [T/4, 3T/4] \\ 4(t/T - 1) & t \in [3T/4, T] \end{cases}$$

Its Fourier series is given by[4]

$$f(t) = \sum_{n=1}^{\infty} \frac{8\cdot(-1)^{n+1}}{(2n-1)^2\pi^2} \sin(\tfrac{2(2n-1)\pi t}{T}). \tag{4.3}$$

The first few terms are

$$f(t) = \frac{8}{\pi^2}\left(\sin(\tfrac{2\pi t}{T}) - \frac{1}{9}\sin(\tfrac{6\pi t}{T}) + \frac{1}{25}\sin(\tfrac{10\pi t}{T}) - \frac{1}{49}\sin(\tfrac{14\pi t}{T}) + ...\right).$$

Figure 4.1 shows that by including more and more terms in the Fourier series, successively better approximations to $f(t)$ are obtained. The coefficients of the expansion in Eqn. 4.3 are known as the *Fourier coefficients* and can be found by orthogonality.

[3] Similar orthogonality relations exist for the complex Fourier basis functions $e^{in\pi x/L}$, $n \in \{-\infty, \ldots, \infty\}$.

[4] We shall see in due course how to calculate Fourier series explicitly.

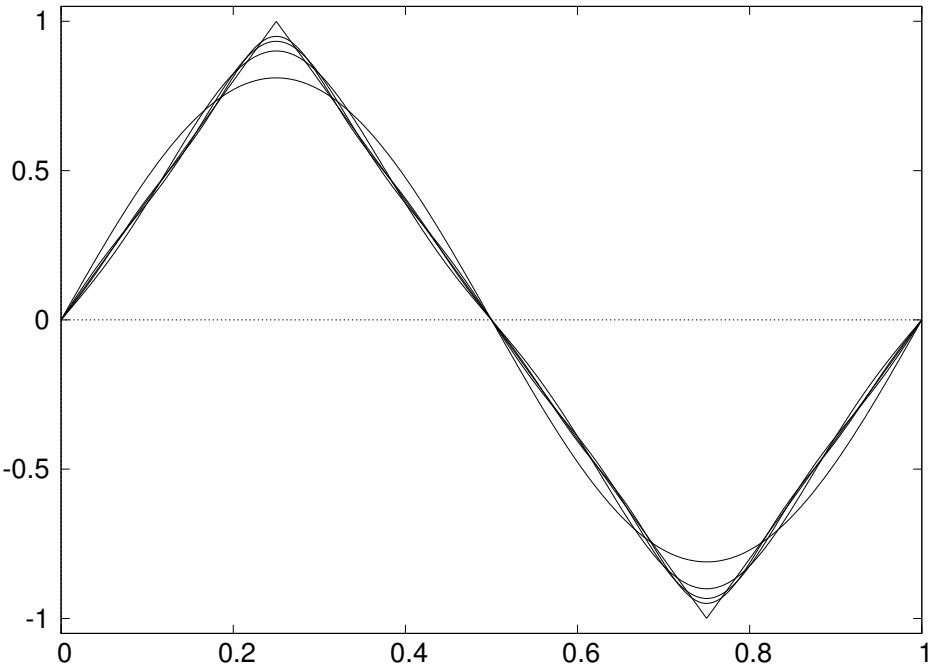

Figure 4.1: Triangular wave $f(t)$ (with $T = 1$) along with its Fourier series representations consisting of 1, 2, 3, and 4 terms.

4.4.2 Fourier Coefficients*

First, let us reexpress the Fourier series of Eqn. (4.2) as

$$f(x) = a_0 + \sum_{n=1}^{\infty} a_n \cos(\tfrac{n\pi x}{L}) + \sum_{n=1}^{\infty} b_n \sin(\tfrac{n\pi x}{L}). \tag{4.4}$$

We may use the orthogonality relations of Eqn. (4.1) to find the coefficients $\{a_n\}$ and $\{b_n\}$:

$$\begin{aligned} \langle f|s_m\rangle &= Lb_m \\ \langle f|c_m\rangle &= La_m \quad m \neq 0 \\ \langle f|c_0\rangle &= 2La_0 \end{aligned} \tag{4.5}$$

4.4.3 Symmetry*

A great deal of effort can be saved in calculating the integrals of Eqn. (4.5) if one considers the symmetry of $f(x)$ in advance. Note that $\cos(x) = \cos(-x)$ is an even function, while $\sin(x) = -\sin(-x)$ is an odd function. Then it follows that

- if $f(x)$ is odd, i.e., $f(x) = -f(-x)$, then $a_n = 0 \ \forall \ n$ and only sine terms are present in the Fourier series,

- and if $f(x)$ is even, i.e., $f(x) = f(-x)$, then $b_n = 0 \; \forall \; n$ and only cosine terms are present in the Fourier series.

4.4.4 Discontinuous Functions*

Consider the periodic sawtooth function given by

$$f(x) = x, \quad x \in [-1, 1], \quad f(x) = f(x + 2).$$

This function is odd, therefore $a_n = 0$ for all n. Calculating the remaining coefficients we find the Fourier series to be

$$f(x) = \sum_{n=1}^{\infty} \frac{2}{n\pi}(-1)^{n+1} \sin(n\pi x). \tag{4.6}$$

Writing out the first few terms explicitly:

$$f(x) = \frac{2}{\pi}\left[\sin(\pi x) - \frac{1}{2}\sin(2\pi x) + \frac{1}{3}\sin(3\pi x) - \frac{1}{4}\sin(4\pi x) + ...\right]$$

Figure 4.2 shows $f(x)$ and Fourier series approximations to $f(x)$ with successively more terms. This example highlights an interesting feature: why does the Fourier series for the sawtooth funtion

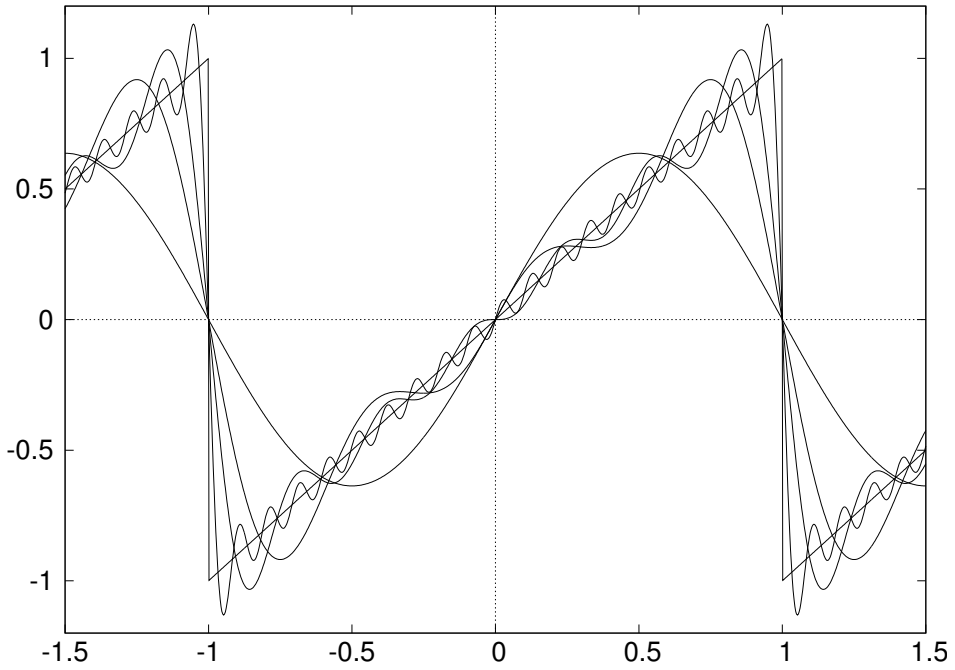

Figure 4.2: Sawtooth function $f(x)$ along with its Fourier series representations consisting of 1, 3, 6, and 20 terms.

converge more slowly than that for the triangular wave and what is going on with the apparent overshoot of the Fourier series for the sawtooth function at $x = \pm 1$?

The sawtooth function $f(x)$ is discontinuous at $x = \pm 1$. Notice how the value of the Fourier series at these points takes the arithmetic mean value of $f(x)$ on either side of the discontinuity. This is a general result: if $x = x_0$ is a point of discontinuity of $f(x)$, then the value of the Fourier series $F(x)$ at $x = x_0$ is

$$F(x_0) = \tfrac{1}{2}\left[f(x_0+) + f(x_0-)\right]$$

Compare the Fourier series for the triangular wave (Eqn. 4.3 and Fig. 4.1) and the sawtooth function (Eqn. 4.6 and Fig. 4.2). What is noticeable is that for the former, the Fourier coefficients decrease as n^{-2}, while for the latter they decrease more slowly as n^{-1}. In other words, the Fourier series for the sawtooth function converges more slowly as the importance of successive terms does not decrease as fast. The difference is due to the fact that the sawtooth function is discontinuous, while the triangular wave is continuous and has a discontinuous first derivative. In general if $f^{(k-1)}(x)$ is continuous, but $f^{(k)}(x)$ is not, then the Fourier coefficients will decrease as $n^{-(k+1)}$.

Take a closer look at Fig. 4.2. Let us denote the Fourier series truncated at the N^{th} term by $F_N(x)$:

$$F_N(x) = \sum_{n=0}^{N} a_n \cos(k_n x) + \sum_{n=1}^{N} \sin(k_n x).$$

What is clear is that as more terms of the Fourier series are included, a better representation of the function $f(x)$ is achieved in the sense that for a given value of x

$$||F_N(x) - f(x)|| \to 0 \quad \text{as } n \to \infty.$$

However, if we zoom in on the discontinuity in Fig. 4.2, as shown in Fig. 4.3, we see that there is a significant overshoot of $F_N(x)$. Furthermore, as we add more terms to the series, although the position of the overshoot moves further towards the discontinuity, its magnitude remains finite. This is called the *Gibbs phenomenon* and it means that there is always an error in representing a discontinuous function[5]. By adding in more terms the size of the region over which there is an overshoot may be decreased, but the overshoot will always remain.

4.4.5 Parseval's Theorem and Bessel's Inequality*

Eqns. (3.7) and (3.8) apply to Fourier series and may be easily derived using the orthogonality relations.

$$||f||^2 \geq a_0^2 + \frac{1}{2}\sum_{n=1}^{N}\left[|a_n|^2 + |b_n|^2\right], \tag{4.7}$$

$$||f||^2 = a_0^2 + \frac{1}{2}\sum_{n=1}^{\infty}\left[|a_n|^2 + |b_n|^2\right]. \tag{4.8}$$

In order to understand the physical meaning of Parseval's theorem, consider the n^{th} harmonic in the Fourier series of $f(x)$ is

$$h_n(x) = a_n \cos(\tfrac{n\pi x}{L}) + b_n \sin(\tfrac{n\pi x}{L}).$$

[5]This phenomenon is not unique to Fourier series and is true of other basis function expansions.

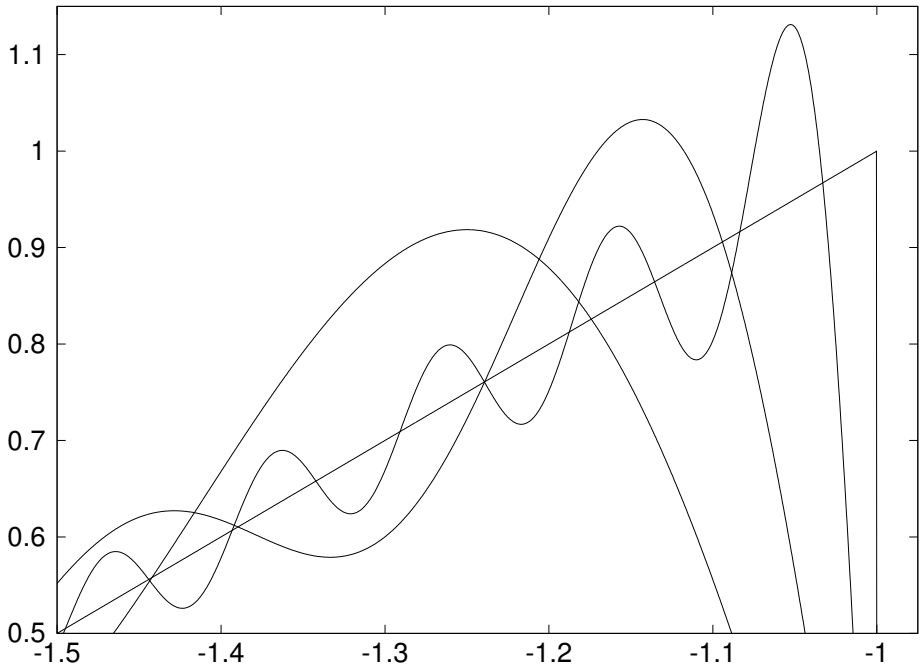

Figure 4.3: Sawtooth function $f(x)$ along with its Fourier series representations consisting of 3, 6, and 20 terms.

Using a suitable trigonometric identity, this may be expressed as

$$h_n(x) = \gamma_n \sin(\tfrac{n\pi x}{L} + \varphi_n),$$

where $\gamma_n = \sqrt{a_n^2 + b_n^2}$ and $\tan(\varphi_n) = \dfrac{a_n}{b_n}$. Comparing with Parseval's theorem, Eqn. 4.8, it can be seen that each harmonic in the Fourier series contributes independently to the mean square value of $f(x)$. In many applications in physics, for example where $f(x)$ represents a time-varying current in an electrical circuit, or an electromagnetic wave, the power density (energy per unit length transmitted per unit time) is proportional to the mean square value of $f(x)$, given by Eqn. 4.8, and the set of coefficients $a_0^2, \{\frac{1}{2}\gamma_n^2\}$ is known as the *power spectrum* of $f(x)$.

4.5 Fourier Transforms

An entirely equivalent representation to sines and cosines is provided by a basis of complex exponential functions (also known as *plane-waves*)

$$e^{\pm ik_n x} = \cos(k_n x) \pm i \sin(k_n x).$$

Substituting into Eqn. (4.2) this Euler[6] relation into the expression for $f(x)$ gives

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{ik_n x}$$

[6]Leonhard Paul Euler (1707–1783), Swiss mathematician and physicist who made many pioneering contributions.

where the (complex) coefficient c_n is related to a_n and b_n.

Consider the function to have periodicity of L, i.e., $f(x) = f(x + L)$. Then we require $k_n L = 2n\pi \Rightarrow k_n = \frac{2n\pi}{L}$. I.e., we have a sum of plane waves that have *wavevectors*[7] k_n separated by $\Delta k = \dfrac{2\pi}{L}$. Hence

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \mathrm{e}^{ik_n x} \, \frac{L\Delta k}{2\pi}$$

If we now let $L \to \infty$[8], the spacing of wavevectors (and hence frequencies) approaches zero $\Delta k \to 0$, and the discrete set of k_n becomes a continuous variable k, and the infinite sum becomes an integral over k:

$$f(x) \overset{L\to\infty, \Delta k \to 0}{\longrightarrow} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) \mathrm{e}^{ikx} \, \mathrm{d}k$$

where we have defined $\tilde{f}(k) \equiv \lim\limits_{\Delta k \to 0} \dfrac{c_n L}{\sqrt{2\pi}}$. This is the definition of the *Fourier transform*, which may be thought of as the generalisation of Fourier series to the case of non-periodic functions.

4.5.1 Definition and Notation

Given $f(x)$ such that $\int_{-\infty}^{\infty} |f(x)| \, \mathrm{d}x < \infty$, its Fourier transform $\tilde{f}(k)$ is defined as

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \, \mathrm{e}^{-ikx} \, \mathrm{d}x. \tag{4.9}$$

The *inverse Fourier transform* is defined as

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) \, \mathrm{e}^{ikx} \, \mathrm{d}k. \tag{4.10}$$

A varied set of notation is used to represent Fourier transforms, the most common of which are given below.

$$\tilde{f} \equiv \hat{f} \equiv F \equiv \mathfrak{F}[f] \equiv \mathrm{FT}[f] \qquad \text{and} \qquad f \equiv \mathfrak{F}^{-1}[\tilde{f}] \equiv \mathrm{FT}^{-1}[\tilde{f}]$$

For the Fourier transform of a function $f(x)$ to be well-defined a number of conditions must be fulfilled:

- $f(x)$ is piecewise continuous
- $f(x)$ is differentiable
- $f(x)$ is absolutely integrable: $\int_{-\infty}^{\infty} |f(x)| \, \mathrm{d}x < \infty$

[7] The wavevector k is related to the wavelength L and frequency f by $k = \dfrac{2\pi}{L} = \dfrac{2\pi f}{c}$, where c is the wave speed.

[8] In other words, the function $f(x)$ is no longer periodic on any finite interval.

Fourier transforms are defined such that if one starts with $f(x)$ and performs a forward transform followed by an inverse transform on the result, then one ends up with $f(x)$ again,

$$f(x) \xrightarrow{\mathfrak{F}} \tilde{f}(k) \xrightarrow{\mathfrak{F}^{-1}} f(x)$$

which provides a definition of the *Dirac delta-function*.

4.5.2 Dirac Delta-Function

Taking Eqn. 4.10 as our starting point and substituting $\tilde{f}(k)$ from Eqn. 4.9 into it we find

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k)\, \mathrm{e}^{ikx}\, \mathrm{d}k \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x')\, \mathrm{e}^{-ikx'}\, \mathrm{d}x' \right] \mathrm{e}^{ikx}\, \mathrm{d}k \\ &= \int_{-\infty}^{\infty} f(x') \underbrace{\left[\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x-x')}\, dk \right]}_{\delta(x-x')} dx' \\ \Rightarrow \quad f(x) &= \int_{-\infty}^{\infty} f(x')\, \delta(x-x')\, \mathrm{d}x' \end{aligned} \tag{4.11}$$

where we have defined the Dirac delta-function

$$\delta(x-x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x-x')}\, dk. \tag{4.12}$$

4.5.3 Properties of the Fourier Transform

Usually $f(x) = f^*(x)$ is a real function, and we shall assume this to be the case. $\tilde{f}(k)$ is, however, in general complex,

$$\tilde{f}^*(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f^*(x) \left(\mathrm{e}^{-ikx} \right)^*\, \mathrm{d}x = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, \mathrm{e}^{ikx}\, \mathrm{d}x \neq \tilde{f}(k).$$

If $f(x)$ has definite symmetry, then $\tilde{f}(k)$ may be either purely real or purely imaginary,

- If $f(x) = f(-x)$ is an even function $\Rightarrow$ $\tilde{f}^*(k) = \tilde{f}(k)$ is purely real.
- If $f(x) = -f(-x)$ is an odd function $\Rightarrow$ $\tilde{f}^*(k) = -\tilde{f}(k)$ is purely imaginary.

Further useful properties include[9]

[9] Proofs are left as an exercise.

- Differentiation.
$$\mathfrak{F}\left[f^{(n)}(x)\right] = (ik)^n \tilde{f}(k)$$
In particular
  - $\mathfrak{F}\left[\dfrac{\mathrm{d}f}{\mathrm{d}x}\right] = ik\tilde{f}(k)$
  - $\mathfrak{F}\left[\dfrac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right] = -k^2\tilde{f}(k)$
- Multiplication by x.
$$\mathfrak{F}[xf(x)] = i\frac{\mathrm{d}\tilde{f}(k)}{\mathrm{d}k}$$
- Rigid shift of co-ordinate.
$$\mathfrak{F}[f(x-a)] = \mathrm{e}^{-ika}\tilde{f}(k)$$

4.5.4 Examples of Fourier Transforms

1. Square wave
$$f(x) = \begin{cases} 1 & x \in [0,1] \\ -1 & x \in [-1,0] \\ 0 & |x| > 1 \end{cases}$$
$$\begin{aligned} \tilde{f}(k) &= \frac{1}{\sqrt{2\pi}}\left[-\int_{-1}^{0}\mathrm{e}^{-ikx}\,\mathrm{d}x + \int_{0}^{1}\mathrm{e}^{-ikx}\,\mathrm{d}x\right] \\ &= \frac{1}{\sqrt{2\pi}}\left\{-\left[\frac{-1}{ik}\mathrm{e}^{-ikx}\right]_{x=-1}^{0} + \left[\frac{-1}{ik}\mathrm{e}^{-ikx}\right]_{x=0}^{1}\right\} \\ &= \frac{1}{\sqrt{2\pi}}\frac{2}{ik}(1-\cos k) = \frac{1}{\sqrt{2\pi}}\cdot\frac{4}{ik}\sin^2\left(\tfrac{k}{2}\right) \end{aligned}$$
Note that since $f(x)$ is odd, $\tilde{f}(k)$ is imaginary.

2. *Top-hat* function
$$f(x) = \begin{cases} 1 & |x| < a \\ 0 & |x| \geq a \end{cases}$$
$$\begin{aligned} \tilde{f}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-a}^{a}\mathrm{e}^{-ikx}\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}}\left[-\frac{1}{ik}\mathrm{e}^{-ikx}\right]_{x=-a}^{a} \\ &= \sqrt{\frac{2}{\pi}}\frac{\sin(ka)}{k} \end{aligned}$$
Note that since $f(x)$ is even, $\tilde{f}(k)$ is real.

4.5.5 Bandwidth Theorem

The last example is a good demonstration of the *bandwidth theorem* or *uncertainty principle*: if a function $f(x)$ has a spread Δx in x-space of, then its spread Δk in k-space will be such that

$$\Delta x \sim \frac{1}{\Delta k}$$

The mathematics here is analogous to that behind the Heisenberg Uncertainty Principle in Quantum Mechanics, which states that for a quantum mechanical particle, such as an electron, its position x and momentum p cannot be both known simultaneously to arbitrary accuracy.

$$\Delta x \geq \frac{h}{\Delta p}$$

where h is Planck's constant. Another implication is for, eg, laser pulses: the shorter the pulse in time t, the larger the spread $\Delta\omega$ of frequencies of harmonics that constitute it (see example on question sheet).

4.6 Diffraction Through an Aperture

An application of Fourier transforms is in determining diffraction patterns resulting from light incident on an aperture. (The analysis is the same for diffraction of X-rays through crystals.) It can be shown (though we do not have time to do so here) that the intensity $I(k)$ of light observed in the diffraction pattern is just the square of the Fourier transform of the aperture function $h(x)$:

$$I(k) = |\mathfrak{F}[h(x)]|^2 ,$$

where, refering to Fig. 4.4, $k = \frac{2\pi \sin\theta}{\lambda}$, where λ is the wavelength of the incident light and θ is the angle to the observation point on the screen. For small values of θ we have $\sin\theta \approx \tan\theta = X/D$, hence $k \approx \frac{2\pi X}{\lambda D}$, i.e., k is proportional to the displacement of the observation point on the screen.

Consider diffraction through a single slit of width a as an example. The aperture function is given by a top-hat

$$h(x) = \begin{cases} 1 & x \in [-\frac{a}{2}, \frac{a}{2}] \\ 0 & \text{otherwise} \end{cases}$$

i.e., $h = 1$ corresponds to transparent parts of the aperture, and $h = 0$ to opaque parts. As we showed before, the fourier transform of a top-hat function is given by a sinc function:

$$\tilde{h}(k) = \sqrt{\frac{2}{\pi}} \frac{\sin(ka/2)}{k} = \frac{a\,\mathrm{sinc}(ka/2)}{\sqrt{2\pi}}.$$

Hence the intensity is given by

$$I(k) = \frac{a^2\,\mathrm{sinc}^2(ka/2)}{2\pi}.$$

The aperture function and intensity are plotted in Figs. 4.5 and 4.6.

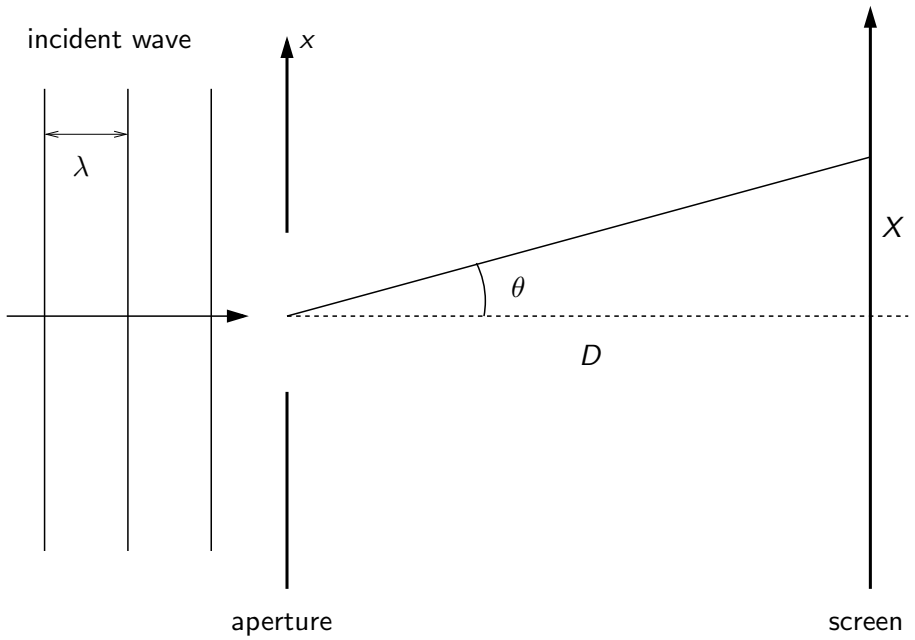

Figure 4.4: Geometry for Fraunhofer diffraction.

4.6.1 Parseval's Theorem for Fourier Transforms

Parseval's theorem for Fourier transforms states that

$$\int_{-\infty}^{\infty} |f(x)|^2 \, \mathrm{d}x = \int_{-\infty}^{\infty} |\tilde{f}(k)|^2 \, \mathrm{d}k \tag{4.13}$$

Proof:

$$\begin{aligned}
\int_{-\infty}^{\infty} |f(x)|^2 \, \mathrm{d}x &= \int_{-\infty}^{\infty} f(x) f^*(x) \, \mathrm{d}x \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \tilde{f}(k) \mathrm{e}^{ikx} \, \mathrm{d}k \right] \cdot \left[\int_{-\infty}^{\infty} \tilde{f}^*(k') \mathrm{e}^{-ik'x} \, \mathrm{d}k' \right] \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{f}(k) \tilde{f}^*(k') \underbrace{\left[\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{i(k-k')x} \, \mathrm{d}x \right]}_{\delta(k-k')} \mathrm{d}k \mathrm{d}k' \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{f}(k) \tilde{f}^*(k') \, \delta(k-k') \, \mathrm{d}k \mathrm{d}k' \\
&= \int_{-\infty}^{\infty} \tilde{f}(k) \tilde{f}^*(k) \, \mathrm{d}k = \int_{-\infty}^{\infty} |\tilde{f}(k)|^2 \, \mathrm{d}k.
\end{aligned}$$

The above proof may be easily generalised for two different functions $f(x)$ and $g(x)$:

$$\int_{-\infty}^{\infty} f(x) g^*(x) \, \mathrm{d}x = \int_{-\infty}^{\infty} \tilde{f}(k) \tilde{g}^*(k) \, \mathrm{d}k \tag{4.14}$$

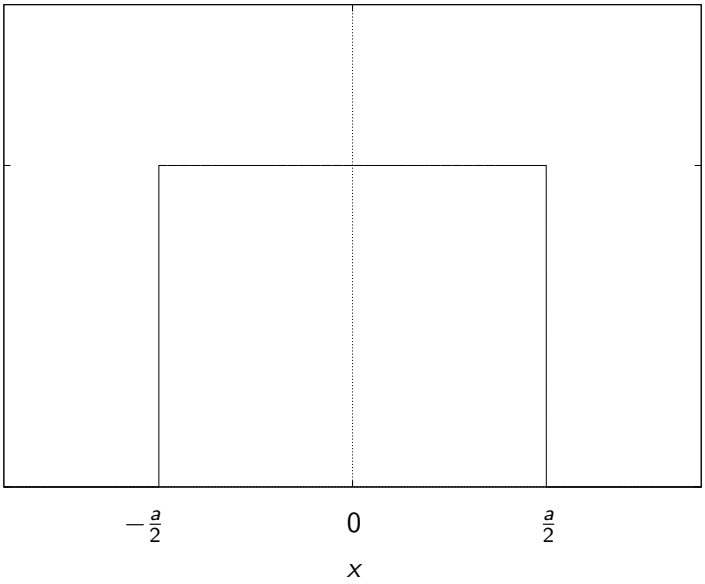

Figure 4.5: Aperture function for single slit of width a.

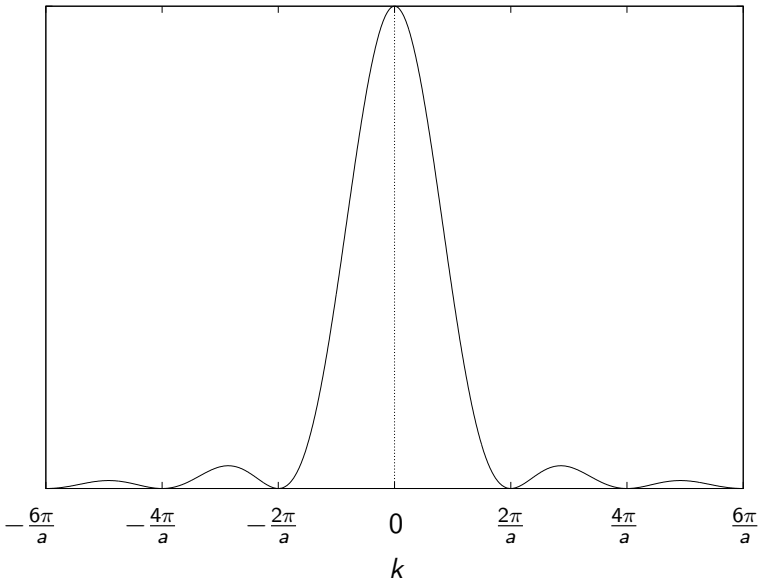

Figure 4.6: Diffraction pattern for single slit of width a: $I(k) = \frac{a^2}{2\pi}\text{sinc}^2(ka/2)$.

4.6.2 Convolution Theorem for Fourier Transforms

The *convolution* of two functions $f(x)$ and $g(x)$ is defined as

$$f * g \equiv \int_{y=-\infty}^{\infty} f(y)g(x-y)\,\mathrm{d}y, \tag{4.15}$$

from which it is easy to show that $f * g = g * f$: in the above equation, let $\xi = x - y \Rightarrow y = x - \xi,\ \mathrm{d}y = -\mathrm{d}\xi$

$$\begin{aligned} f * g &= \int_{\xi=\infty}^{-\infty} f(x-\xi)g(\xi)\,(-\mathrm{d}\xi) \\ &= \int_{-\infty}^{\infty} g(\xi)f(x-\xi)\,\mathrm{d}\xi \\ \Rightarrow \qquad f * g &= g * f \end{aligned}$$

The *convolution theorem* may be stated in two, equivalent forms. Given two functions f and g,

1. the Fourier transform of their convolution is directly proportional to the product of their Fourier transforms:
$$\mathfrak{F}[f * g] = \sqrt{2\pi}\,\tilde{f}\tilde{g} \tag{4.16}$$
2. the Fourier transform of their product is directly proportional to the convolution of their Fourier transforms:
$$\mathfrak{F}[fg] = \frac{1}{\sqrt{2\pi}}\tilde{f} * \tilde{g} \tag{4.17}$$

The proofs are very similar, so we shall treat one here and the other is left as an exercise in the examples sheet.

Proof:

$$\begin{aligned} \mathfrak{F}[f * g] &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}[f * g](x)\mathrm{e}^{-ikx}\,\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} f(y)g(x-y)\,\mathrm{d}y\right]\mathrm{e}^{-ikx}\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty} f(y)\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(x-y)\mathrm{e}^{-ikx}\,\mathrm{d}x\right]\mathrm{d}y \qquad \text{(interchanging order of integration)} \\ &= \int_{-\infty}^{\infty} f(y)\mathrm{e}^{-iky}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(x-y)\mathrm{e}^{-ik(x-y)}\,\mathrm{d}x\right]\mathrm{d}y \qquad (\times \text{ by } \mathrm{e}^{-iky}\mathrm{e}^{iky} = 1) \\ &= \int_{-\infty}^{\infty} f(y)\mathrm{e}^{-iky}\underbrace{\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(\xi)\mathrm{e}^{-ik\xi}\,\mathrm{d}\xi\right]}_{\tilde{g}(k)}\mathrm{d}y \qquad \text{(substituting } \xi = x-y) \\ &= \underbrace{\left[\int_{-\infty}^{\infty} f(y)\mathrm{e}^{-iky}\,\mathrm{d}y\right]}_{\sqrt{2\pi}\tilde{f}(k)}\tilde{g}(k) = \sqrt{2\pi}\,\tilde{f}(k)\tilde{g}(k). \end{aligned}$$

Among many other things, the convolution theorem may be used to calculate diffraction patterns of light incident on complicated apertures. In the next section, we will consider the case of Young's double slit experiment.

4.6.3 Double Slit Diffraction

Earlier it was discussed how, in a Fraunhofer diffraction experiment, the amplitude of the signal at the detection screen is given by the fourier transform of the aperture function $h(x)$. The intensity $I(k)$ that is observed is then just the square of this amplitude:

$$I(k) = \left|\tilde{h}(k)\right|^2,$$

where, with reference to Fig. 4.4, $k = \frac{2\pi \sin\theta}{\lambda}$, where λ is the wavelength of the incident wave and θ is the angle of observation. For small values of θ we have $\sin\theta \approx \tan\theta = X/D$, hence $k \approx \frac{2\pi X}{\lambda D}$, i.e., k is proportional to the displacement of the observation point on the screen.

We saw earlier that for a single slit of width a, the aperture function of which is described by a top-hat function, the intensity observed is given by

$$I(k) = \frac{a^2}{2\pi}\text{sinc}^2(ka/2).$$

The aperture function and intensity are plotted in Figs. 4.5 and 4.6.

The aperture function for a double slit is shown in Fig. 4.7. Here the slit separation is d and the slit width is a. We could go ahead and evaluate the Fourier transform of the aperture function $h(x)$ for the double slit, but there is a more clever approach which uses the convolution theorem. We note that $h(x)$ is actually the convolution of a double Dirac-delta function (with separation d) with a top-hat function of width a, as shown in Fig. 4.8

$$h(x) = f * g(x).$$

The intensity at the screen is given by

$$I(k) = \left|\tilde{h}(k)\right|^2 = |\mathfrak{F}[f * g]|^2$$

and, from the convolution theorem we know that

$$\mathfrak{F}[f * g] = \sqrt{2\pi}\mathfrak{F}[f]\mathfrak{F}[g].$$

Hence, we can obtain the intensity from the Fourier transforms of $f(x)$ and $g(x)$. $g(x)$ is a top-hat, and as we've seen before, it is easy to show that

$$\mathfrak{F}[g] = \frac{a}{\sqrt{2\pi}}\text{sinc}(ka/2).$$

For the double Dirac-delta function, we see that

$$f(x) = \delta(x - d/2) + \delta(x + d/2),$$

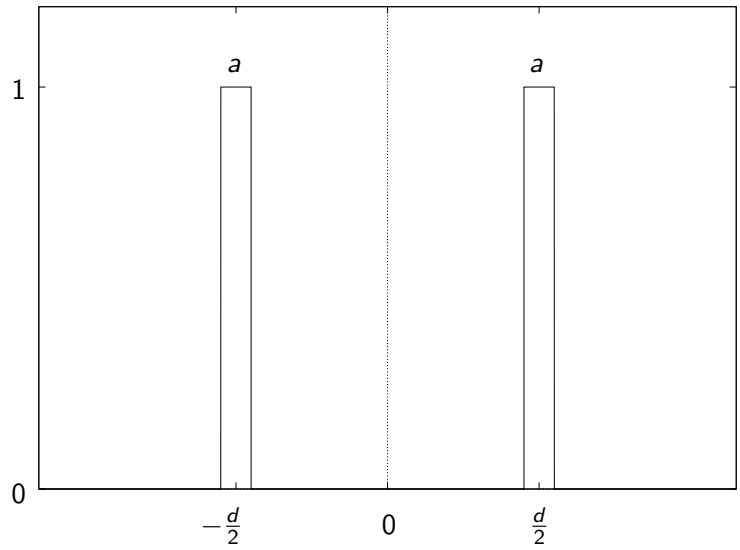

Figure 4.7: Aperture function for double slit: slit width a, separation d.

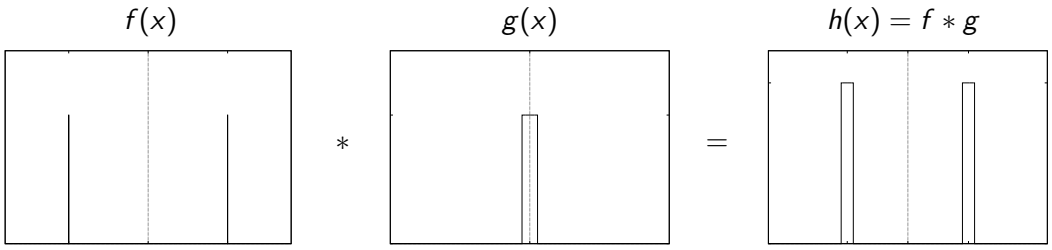

Figure 4.8: Convolution theorem for double slit.

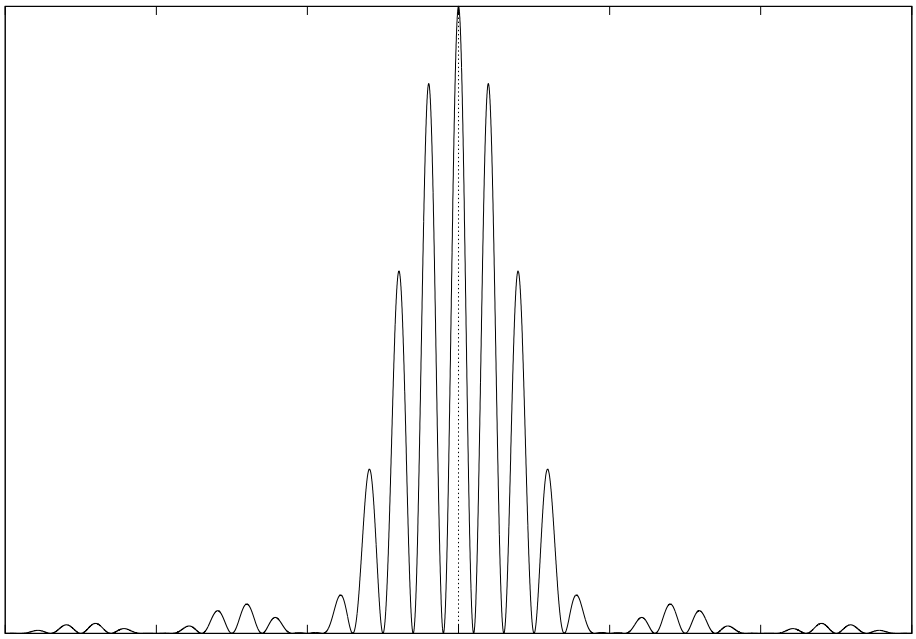

Figure 4.9: Diffraction pattern for double slit.

hence

$$\begin{aligned}\mathfrak{F}[f] &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}[\delta(x-d/2)+\delta(x+d/2)]\,\mathrm{e}^{-ikx}\,\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}}\left[\mathrm{e}^{-ikd/2}+\mathrm{e}^{ikd/2}\right] \\ &= \sqrt{\frac{2}{\pi}}\cos(kd/2).\end{aligned}$$

Putting it all together we see that the intensity on the screen is given by

$$I(k) = \frac{2a^2}{\pi}\mathrm{sinc}^2(ka/2)\cos^2(kd/2)$$

which is plotted in Fig. 4.9.

What is seen is the broad envelope function which comes from the $\mathrm{sinc}(ka/2)$ factor, and the denser interference fringes that come from the $\cos(kd/2)$ factor. Note that $d > a$, which is why the frequency of the fringes is higher than that of the envelope function (a manifestation of the bandwidth theorem that was discussed earlier).

4.6.4 Differential Equations

One important use of Fourier transforms is in solving differential equations. A Fourier transform may be used to transform a differential equation into an algebraic equation since

$$\mathfrak{F}\left[\frac{\partial^n f}{\partial x^n}\right] = (ik)^n \mathfrak{F}[f].$$

Example: Heat Diffusion Equation

Consider an infinite, one-dimensional bar which has an initial temperature distribution given by $\theta(x, t = 0) = \delta(x)$. This is clearly a somewhat unphysical situation, but it's not such a bad approximation to having a situation in which a lot of heat is initially concentrated at the mid-point of the rod.

The flow of heat is determined by the diffusion equation

$$D\frac{\partial^2 \theta}{\partial x^2} = \frac{\partial \theta}{\partial t},$$

which is second-order in x and first-order in t. D is the diffusion coefficient. The boundary conditions on this problem are that $\theta(\pm\infty, t) = 0$.

Consider what happens if we Fourier transform both sides of this equation with respect to the variable x:

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} D\frac{\partial^2 \theta}{\partial x^2} e^{-ikx}\, dx &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \frac{\partial \theta}{\partial t} e^{-ikx}\, dx \\
D\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \frac{\partial^2 \theta}{\partial x^2} e^{-ikx}\, dx &= \frac{\partial}{\partial t}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \theta(x,t) e^{-ikx}\, dx\right] \\
D\mathfrak{F}\left[\frac{\partial^2 \theta(x,t)}{\partial x^2}\right] &= \frac{\partial}{\partial t}\mathfrak{F}[\theta(x,t)] \\
-Dk^2\tilde{\theta}(k,t) &= \frac{\partial \tilde{\theta}(k,t)}{\partial t}.
\end{aligned}$$

So the differential equation in x is replaced by an algebraic equation in k. We still have a differential equation in t which is first-order, and also easy to solve:

$$\tilde{\theta}(k,t) = A(k)e^{-Dk^2 t},$$

where $A(k) = \tilde{\theta}(k, t = 0)$, a constant of integration, is just the Fourier transform of the initial condition $\theta(x, t = 0) = \delta(x)$, which we can calculate:

$$A(k) = \tilde{\theta}(k, t = 0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \delta(x) e^{-ikx}\, dx = \frac{1}{\sqrt{2\pi}}.$$

Hence,

$$\tilde{\theta}(k,t) = \frac{1}{\sqrt{2\pi}} e^{-Dk^2 t}.$$

So, we have Fourier transformed the original differential equation from "x-space" to "k-space", solved it in k-space, and applied the initial condition in k-space. All that remains to be done is to inverse Fourier transform $\tilde{\theta}(k,t)$ back in order to obtain the solution in x-space.

In practice, this is typically the most difficult part of the process (there's no such thing as a free lunch!), but for the example we have chosen, it turns out to be not too bad because, through completing the square and changing the variable of integration, we are able to reduce the problem to a Gaussian integral of known value[10]:

$$\begin{aligned}
\theta(x,t) &= \mathfrak{F}^{-1}[\tilde{\theta}(k,t)] \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-Dk^2t}\mathrm{e}^{ikx}\,\mathrm{d}k \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-Dt\left[(k-ix/2Dt)^2\right]-x^2/4Dt}\,\mathrm{d}k \qquad \text{combining exponents and completing the square} \\
&= \frac{1}{2\pi}\mathrm{e}^{-x^2/4Dt}\int_{-\infty}^{\infty} \mathrm{e}^{-Dtq^2}\,\mathrm{d}q \qquad \text{changing variable to } q = k - ix/2Dt \Rightarrow \mathrm{d}q = \mathrm{d}k \\
&= \frac{1}{2\pi}\sqrt{\frac{\pi}{Dt}}\mathrm{e}^{-x^2/4Dt} \qquad \text{using the standard result for a Gaussian integral}
\end{aligned}$$

Hence the final result[11]

$$\theta(x,t) = \frac{1}{2\sqrt{\pi Dt}}\mathrm{e}^{-x^2/4Dt}.$$

Fig. 4.10 shows the temperature distribution for different times t. Is the behaviour as you would expect?

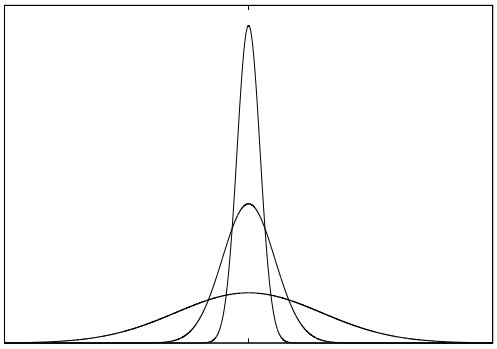

Figure 4.10: $\theta(x,t)$ for three different values of t.

[10] $\int_{-\infty}^{\infty} \mathrm{e}^{-\alpha x^2}\,\mathrm{d}x = \sqrt{\pi/\alpha}$.

[11] The observant will have noticed that, in the fourth line of the derivation above, I should also have changed the limits on the integral to $q = \pm\infty - ix/2Dt$, thus taking the contour of the integral off the real-q axis. It turns out that I'm allowed to shift the contour back to the real-axis since the integrand has no singularities anywhere. This is the subject of fields of mathematics known as *complex analysis* and *contour integration*, which have many uses in physics and engineering, and which you will meet later in the course.

4.7 Laplace Transforms

A question arises as to what to do if a function $f(x)$ does not tend to zero as $x \to \pm\infty$ or if $f(x)$ does not exist for $x < x_0$, in which cases the Fourier transform of $f(x)$ is not well-defined. Indeed, often we are interested in following the evolution of a function $f(t)$ given an initial condition at $t = 0$. The Laplace transform may be used for this purpose and is defined as

$$\mathcal{L}[f(t)] \equiv \hat{f}(s) = \int_0^\infty e^{-st} f(t) \mathrm{d}t, \tag{4.18}$$

where $s = \sigma + i\omega$ is in general a complex variable and $\sigma > 0$ is required for convergence of the integral.

4.7.1 Properties

- Linearity: $\mathcal{L}[af_1(t) + bf_2(t)] = a\mathcal{L}[f_1(t)] + b\mathcal{L}[f_2(t)]$
- $\mathcal{L}\left[\frac{\partial f}{\partial t}\right] = s\hat{f}(s) - f(0)$
- More generally, $\mathcal{L}[f^{(n)}(t)] = s^n\hat{f}(s) - s^{n-1}f(0) - \ldots - f^{(n-1)}(0)$
- $\mathcal{L}[t^n f(t)] = (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}s^n}\hat{f}(s)$

4.7.2 Examples

- $\mathcal{L}[1] = \frac{1}{s}$
- $\mathcal{L}[e^{-at}] = \frac{1}{s+a}$
- $\mathcal{L}[\cos\omega t] = \frac{s}{s^2+\omega^2}$
- $\mathcal{L}[\sin\omega t] = \frac{\omega}{s^2+\omega^2}$
- $\mathcal{L}[t^n] = \frac{n!}{s^{n+1}}$
- $\mathcal{L}[te^{-at}] = \frac{1}{(s+a)^2}$
- $\mathcal{L}[f(at)] = \frac{1}{|a|}\hat{f}(s/a)$
- $\mathcal{L}[e^{at}f(t)] = \hat{f}(s-a)$
- $\mathcal{L}\left[\int_0^t f(t')\mathrm{d}t'\right] = \frac{1}{s}\hat{f}(s)$

Proofs of the above will be given in the lectures.

4.7.3 Solving Differential Equations

As can be seen from the examples above, Laplace transforms convert differentials and integrals in the t-domain to algebraic forms in the s-domain. As a result, they are of use in solving differential equations.

Example

$$\ddot{f} + 5\dot{f} + 6f = 1; \qquad f(0) = \dot{f}(0) = 0.$$

Applying a Laplace transform to the entire equation we find,

$$\begin{aligned} \mathcal{L}[\ddot{f} + 5\dot{f} + 6f] &= \mathcal{L}[1] \\ s^2\hat{f} - sf(0) - \dot{f}(0) + 5[s\hat{f} - f(0)] + 6\hat{f} &= \frac{1}{s} \\ (s^2 + 5s + 6)\hat{f} &= \frac{1}{s}. \end{aligned}$$

On rearrangement, we obtain

$$\hat{f} = \frac{1}{s(s+2)(s+3)} \equiv \frac{A}{s} + \frac{B}{s+2} + \frac{C}{s+3},$$

where, using partial fractions, we can show that $A = \frac{1}{6}$, $B = -\frac{1}{2}$ and $C = \frac{1}{3}$. The inverse transform can now be done by inspection, using the results derived earlier, to give

$$f(t) = \frac{1}{6} - \frac{1}{2}e^{-2t} + \frac{1}{3}e^{-3t}.$$

4.7.4 Convolution Theorem for Laplace Transforms

As we saw earlier, a convolution of two functions $f_1(t)$ and $f_2(t)$ is defined as

$$f_1 * f_2 = \int_{-\infty}^{\infty} f_1(t')f_2(t-t')\mathrm{d}t'.$$

If f_1 and f_2 vanish for $t < 0$, then

$$f_1 * f_2 = \int_{0}^{t} f_1(t')f_2(t-t')\mathrm{d}t'.$$

Defining $g(t) \equiv f_1 * f_2$, the convolution theorem for Laplace transforms states that

$$\hat{g}(s) = \hat{f}_1(s)\hat{f}_2(s).$$

The proof is as follows:

$$\begin{aligned} \hat{g}(s) &= \int_0^{\infty} \mathrm{d}t\, e^{-st} \left[\int_0^t f_1(t')f_2(t-t')\mathrm{d}t' \right] \\ &= \int_0^{\infty} \mathrm{d}t \int_0^t \mathrm{d}t'\, f_1(t')f_2(t-t')e^{-st} \end{aligned}$$

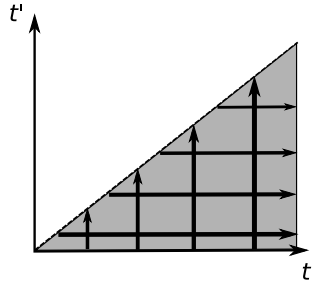

Figure 4.11: Integration area for proof of convolution theorem for Laplace transforms.

The integrals over t and t' cover the area in the t-t' plane shown in Fig. 4.11. As can be seen, therefore, the integrals can equivalently be written

$$\hat{g}(s) = \int_0^\infty \mathrm{d}t' \left[\int_{t'}^\infty \mathrm{d}t \, f_2(t-t') e^{-st} \right] f_1(t')$$

Substituting $t'' = t - t'$ in the term in square brackets gives

$$\begin{aligned}
\hat{g}(s) &= \int_0^\infty \mathrm{d}t' \left[\int_0^\infty \mathrm{d}t'' f_2(t'') e^{-s(t''+t')} \right] f_1(t') \\
\hat{g}(s) &= \int_0^\infty \mathrm{d}t' \left[\int_0^\infty \mathrm{d}t'' f_2(t'') e^{-st''} \right] e^{-st'} f_1(t') \\
&= \hat{f}_2(s) \int_0^\infty \mathrm{d}t' e^{-st'} f_1(t') \\
&= \hat{f}_2(s) \hat{f}_1(s),
\end{aligned}$$

as required.

Example: Evaluate the integral $J = \int_0^1 y^n (1-y)^m \mathrm{d}y$.

Consider

$$g(t) \equiv t^n * t^m = \int_0^t \tau^n (t-\tau)^m \mathrm{d}\tau. \tag{4.19}$$

Substituting $\tau = st$ and $\mathrm{d}\tau = t\mathrm{d}s$ gives

$$\begin{aligned}
g(t) &= \int_0^1 s^n t^n (t-ts)^m t \mathrm{d}s \\
&= t^{n+m+1} \int_0^1 s^n (1-s)^m \mathrm{d}s \\
&= t^{n+m+1} J.
\end{aligned}$$

Taking the Laplace transform of this result gives

$$\hat{g}(s) = \frac{(n+m+1)!}{s^{n+m+2}} J,$$

while using the convolution theorem on Eqn. 4.19 gives

$$\hat{g}(s) = \mathcal{L}[t^n]\mathcal{L}[t^m] = \frac{n!m!}{s^{n+m+2}}.$$

Then, on equating the last two expressions we have derived for $\hat{g}(s)$, we obtain the final result

$$J = \frac{n!m!}{(n+m+1)!}.$$