Doc Dave

MPhys Notes

Mathematical Methods for Physicists

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Contents

Chapter 1

Review of Linear Vector Spaces

For a more complete description of vector spaces, refer to my Mathematical Fundamentals of Quantum Mechanics notes.

1.1 Linear Independence and Basis Vectors

Any vector $\mathbf{x}$ in a **vector space** can be written in terms of n **linearly independent** unit vectors, $\{\mathbf{e}_i\}$, which form a **basis**:

$$\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{e}_i.$$

Definition 1.1: Vector Space

A vector space is a collection of objects that can be added or "scaled".

Example 1.1

The space $\mathbb{C}^2$ of complex 2D spinors $\chi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ is a vector space.

Definition 1.2: Linear Independence

A set of vectors $\{\mathbf{a}, \mathbf{b}, \ldots, \mathbf{u}\}$ are said to be linearly independent if

$$\lambda\mathbf{a} + \mu\mathbf{b} + \ldots + \sigma\mathbf{u} = 0$$

has no solutions except $\lambda = \mu = \ldots = \sigma = 0$, i.e. all vectors are orthogonal. A space is said to be n-dimensional if there is a maximum number, n, of linearly independent vectors.

1.1.1 The Scalar Product

The scalar product is a binary operation in which a pair of vectors operate to give a scalar, i.e. $(\mathbf{a}, \mathbf{b}) = \langle a|b\rangle = \mathbf{a} \cdot \mathbf{b}$. This satisfies laws of commutativity and distributivity, i.e.

$$\begin{aligned}(\mathbf{a}, \mathbf{b}) &= (\mathbf{b}, \mathbf{a})^* \\ (\mathbf{a}, \lambda\mathbf{b} + \mu\mathbf{c}) &= \lambda(\mathbf{a}, \mathbf{b}) + \mu(\mathbf{a}, \mathbf{c}) \\ (\mathbf{a}, \mathbf{a}) &\geq 0,\end{aligned}$$

where the last condition is the squared norm of vector, i.e. $\|\mathbf{a}\| \equiv (\mathbf{a}, \mathbf{a})^{\frac{1}{2}} \geq 0$.

1.1.2 Orthogonality

Vectors are said to be linearly independent if their scalar product is zero, i.e. $(\mathbf{a}, \mathbf{b}) = 0$ and so $\mathbf{a}$ and $\mathbf{b}$ are orthogonal. These scalar products satisfy the Cauchy-Schwarz inequality;

$$|(\mathbf{a}, \mathbf{b})| \leq \|\mathbf{a}\| \, \|\mathbf{b}\| \, ,$$

and vector norms satisfy the triangle inequality;

$$\|\mathbf{a} + \mathbf{b}\| \leq \|\mathbf{a}\| + \|\mathbf{b}\| \, .$$

If a set of vectors $\{\mathbf{e}_i\}$ forms an orthogonal basis then

$$(\mathbf{e}_i, \mathbf{e}_j) = 0 \quad \forall i \neq j.$$

It is easy to find components x_i of vector $\mathbf{x} = \sum_i x_i \mathbf{e}_i$ if the basis vectors $\{\mathbf{e}_i\}$ are orthogonal, i.e. $(\mathbf{e}_i, \mathbf{e}_j) = \delta_{ij}$;

$$\begin{aligned}(\mathbf{e}_i, \mathbf{x}) &= \sum_j x_j (\mathbf{e}_i, \mathbf{e}_j) \\ &= x_i (\mathbf{e}_i, \mathbf{e}_i) \\ &= x_i.\end{aligned}$$

1.2 Function Spaces

Definition 1.3: Function Space

A function space is a space for which the elements are functions. The dimensionality of a function space may be infinite, e.g. periodic functions $f(x) = f(x + 2n\pi)$ with $(f, f) = \int_0^{2\pi} |f|^2 \, \mathrm{d}x < \infty$.

For a vector space of complex functions one may choose the basis functions to be $\mathbf{e}_n = \boldsymbol{\phi}_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx} : n \in \mathbb{Z}$, i.e. $\mathbf{f}(x) = \sum_{n=-\infty}^{\infty} f_n \boldsymbol{\phi}_n(x)$. Therefore the components of the functions are given by

$$\begin{aligned}\mathbf{f}(x) &= (\boldsymbol{\phi}_n(x), \mathbf{f}(x')) \\ &= \int_0^{2\pi} \boldsymbol{\phi}_n^*(x) \mathbf{f}(x') \, \mathrm{d}x' \\ &= \int_0^{2\pi} \boldsymbol{\phi}_n^*(x) \sum_{n=-\infty}^{\infty} f_n \boldsymbol{\phi}_n(x') \, \mathrm{d}x' \\ &= \int_0^{2\pi} \left(\sum_{n=-\infty}^{\infty} \boldsymbol{\phi}_n^*(x) \boldsymbol{\phi}_n(x') \right) f_n \, \mathrm{d}x'.\end{aligned}$$

The scalar product of these periodic basis functions is given by a Dirac delta function;

$$\sum_{n=-\infty}^{\infty} \boldsymbol{\phi}_n^*(x)\boldsymbol{\phi}_n(x') = \big(\boldsymbol{\phi}_n(x), \boldsymbol{\phi}_n(x')\big) = \delta(x - x' + 2n\pi).$$

A Hilbert space is a vector space in which all functions of vectors have finite norms.

1.2.1 Completeness Relations

The **completeness relation** states that
The sum over these periodic basis functions is given by a Dirac delta function;

$$\sum_{n=-\infty}^{\infty} \boldsymbol{\phi}_n^*(x)\boldsymbol{\phi}_n(x') = \delta(x - x' + 2n\pi).$$

Example 1.2: Calculate the integral $\int_{-\infty}^{\infty} f(x)\delta(x^2 - c^2t^2)\,\mathrm{d}x$

To calculate this, one must first establish the zeros of the delta function's argument, a_i, and use them to calculate the value of the delta using the relation

$$\delta(g(x)) = \sum_i \frac{\delta(x - a_i)}{|g'(a_i)|}.$$

The argument of the delta is $x^2 - c^2t^2$, hence the zeros are at $x = \pm ct$. The function of the argument, g, is then $g(x) = x^2$, hence its derivative is $g'(x) = 2x$ and so at the zeros $g'(\pm ct) = 2c|t|$. The delta is thus given by $\delta(g(x)) = \sum_i \frac{\delta(x^2 - c^2t^2)}{2c|t|}$ and therefore the integral is

$$\frac{1}{2c|t|}\int_{-\infty}^{\infty} f(x)\delta(x^2 - c^2t^2)\,\mathrm{d}x = \frac{1}{2c|t|}\big(f(ct) + f(-ct)\big).$$

Chapter 2

Eigenvectors and Eigenvalues

2.1 Review of Linear Operators

A linear operator L acts upon vectors $\mathbf{a}, \mathbf{b}, \ldots$ to give new vectors $L\mathbf{a}, L\mathbf{b}, \ldots$ such that

$$L(\lambda\mathbf{a} + \mu\mathbf{b}) = \lambda L\mathbf{a} + \mu L\mathbf{b}.$$

Example 2.1: Linear Operators

- Matrix multiplication

$$L\mathbf{x} = \begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} \mathbf{x}$$

- Differentiation

$$Lf(x) = \frac{\mathrm{d}f(x)}{\mathrm{d}x}$$

- Integration

$$(Lf)(x) = \int_0^x f(x')\,\mathrm{d}x'$$

2.1.1 Mapping, Domains and Codomains

If a linear operator **maps** vector $\mathbf{f}$ onto another vector $\mathbf{g}$, i.e. $L\mathbf{f} = \mathbf{g}$ or $L : \mathbf{f} \to \mathbf{g}$, then the vector spaces of $\mathbf{f}$ (the **domain**) and $\mathbf{g}$ (the **codomain**) may be different.

Definition 2.1: Domain and Codomain

The **domain** of a function is the set of argument values for which it is defined. The **codomain** of a function is the set of values that the function is allowed to take, however the **image** is the set of outputs that the function *can* take.

Example 2.2

The domain of cosine is the set of all real numbers as it can take any real argument. The "output" of cosine is always real, hence its codomain is the set of all real numbers, however the values that this output can take are within the interval $[-1, 1]$, which is its image.

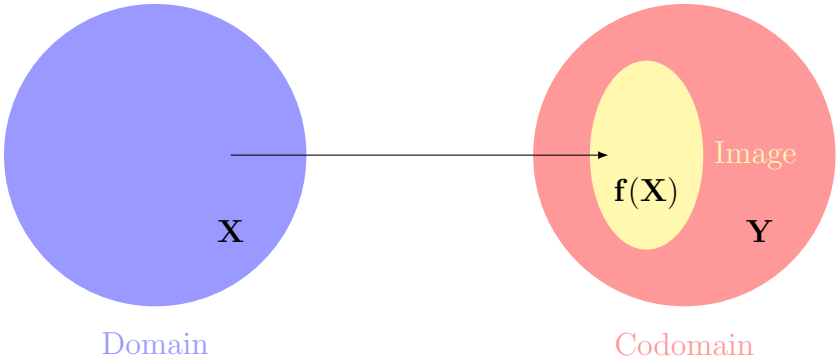

Figure 2.1: Function f acts upon members of the domain X, mapping it to codomain Y. The yellow ellipse is the image of the function.

Example 2.3

The matrix $L = \begin{pmatrix} 3 & 2 & 1 \\ 6 & 4 & 2 \end{pmatrix}$ maps from domain $\mathbb{R}^3$ to codomain $\mathbb{R}^2$.

The range is the one-dimensional subset of vectors $\lambda \begin{pmatrix} 1 \\ 2 \end{pmatrix}; \lambda \in \mathbb{R}$.

Taking a three-dimensional position vector $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$, the vector $\mathbf{u} = L\mathbf{x}$ is then given by $\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = (3x_1 + 2x_2 + x_3) \begin{pmatrix} 1 \\ 2 \end{pmatrix}$.

2.2 Adjoint and Hermitian Operators

The adjoint operator † produces the Hermitian conjugate of the initial operator. The Hermitian conjugate of an operator in matrix form is the transposed complex conjugate, i.e. for a matrix m the Hermitian conjugate is

$$m^\dagger_{ij} = m^*_{ji}.$$

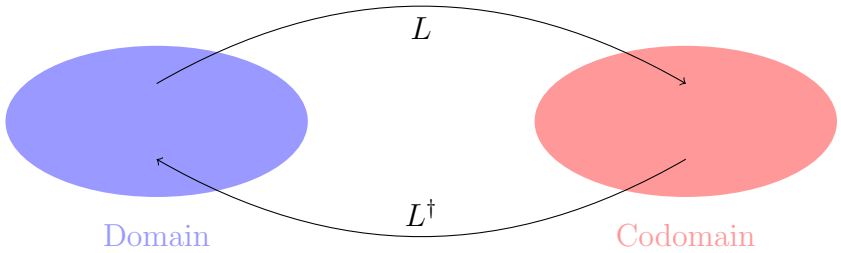

Figure 2.2: Directionality of linear operator L and its Hermitian conjugate.

More generally, where $\mathbf{a} \in \text{domain}(m)$ and $\mathbf{b} \in \text{codomain}(m)$ then

$$(\mathbf{a}, m^\dagger \mathbf{b}) = (m\mathbf{a}, \mathbf{b}) = (\mathbf{b}, m\mathbf{a})^*.$$

The scalar product of two vectors $\mathbf{v}$ and $\mathbf{w}$ may therefore be written

$$(\mathbf{v}, \mathbf{w}) = \mathbf{v}^\dagger \mathbf{w}.$$

The self-adjoint operator is an operator that it equal to its own adjoint, i.e. it satisfies $L = L^\dagger$, such that the domain and codomain coincide.

2.3 Eigenvectors and Eigenvalues

The eigenvalue problem can be summarised in a simple equation:

$$L\mathbf{a} = \lambda \mathbf{a} \qquad \mathbf{a} \neq 0,$$

where λ is an eigenvalue and $\mathbf{a}$ is an eigenvector. For a Hermitian operator the eigenvalues are real and the eigenvectors corresponding to eigenvalues are orthogonal.

Theorem 2.1: Hermitian operators have real eigenvalues

The eigenvalue equation for an operator and its adjoint are given by

$$\begin{aligned}(\mathbf{a}, L\mathbf{a}) &= \lambda(\mathbf{a}, \mathbf{a}) \\ (L^\dagger \mathbf{a}, \mathbf{a}) &= \lambda^*(\mathbf{a}, \mathbf{a}).\end{aligned}$$

For a Hermitian operator $L = L^\dagger$, then

$$\begin{aligned}(L^\dagger \mathbf{a}, \mathbf{a}) &= (\mathbf{a}, L\mathbf{a}) \\ \longrightarrow 0 &= (\mathbf{a}, L\mathbf{a}) - (L^\dagger \mathbf{a}, \mathbf{a}) \\ &= (\lambda - \lambda^*)(\mathbf{a}, \mathbf{a}),\end{aligned}$$

therefore $\lambda = \lambda^*$ and hence is real.

Theorem 2.2: Hermitian operators have orthogonal eigenvectors

Consider two eigenvectors $\mathbf{a}$ and $\mathbf{b}$ that satisfy the eigenvalue equation:

$$L\mathbf{a} = \lambda\mathbf{a}$$
$$L\mathbf{b} = \mu\mathbf{b}.$$

By Hermiticity $(\mathbf{b}, L\mathbf{a}) = (L\mathbf{b}, \mathbf{a})$ and so

$$\begin{aligned}(\mathbf{b}, L\mathbf{a}) &= \lambda(\mathbf{b}, \mathbf{a}) \\ (L\mathbf{b}, \mathbf{a}) &= \mu(\mathbf{b}, \mathbf{a}) \\ \longrightarrow (\lambda - \mu)(\mathbf{b}, \mathbf{a}) &= 0,\end{aligned}$$

the scalar product is therefore zero, and hence the eigenvectors are orthogonal.

2.4 Weight Functions

For function spaces the generalised eigenvalue equation is

$$Lf = \lambda\rho f,$$

where ρ is a weighting function which is real and non-negative. Reality of eigenvalues and orthogonality of eigenvectors still hold in this more generalised form.

Theorem 2.3

Consider solution to the eigenvalue equation

$$Lf_1 = \lambda_1\rho f_1 \quad \rightarrow (f_2, Lf_1) = \lambda_1(f_2, \rho f_1).$$

If the operator L is Hermitian then

$$(f_1, Lf_2) = (f_2, Lf_1)^* = \lambda_2(f_1, \rho f_2)$$

and so the difference of these two equations is

$$0 = (\lambda_1 - \lambda_2^*)(f_2, \rho f_1).$$

This draws two conclusions:

- If $f_1 = f_2$ then $(f_2, \rho f_1) \neq 0$ and so eigenvalues are real, i.e.

$$\lambda_1 = \lambda_2^* \qquad \forall \lambda_{1,2}.$$

- If $\lambda_1 \neq \lambda_2$ then $(f_2, \rho f_1) = 0$ and so f_1 and f_2 are orthogonal eigenvectors with a weight function ρ, i.e.

$$(\mathbf{u}, \mathbf{v})_\rho = \int \rho(x) u^*(x) v(x)\, \mathrm{d}x = 0.$$

2.5 Sturm-Liouville Theory

There is a very important class of equations with weighting functions, known as Sturm-Liouville equations. These are second-order ODEs of the form

$$L = -\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\tfrac{\mathrm{d}}{\mathrm{d}x}\right) + q(x),$$

which can be applied to the eigenvalue equation

$$Ly(x) = \lambda \rho(x) y(x),$$

where $p, q, \rho \in \mathbb{R}$ and $p, q, \rho \geq 0$ over an interval $[a, b]$. Explicitly this equation becomes

$$-\tfrac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\tfrac{\mathrm{d}y}{\mathrm{d}x}\right) + q(x)y(x) - \lambda\rho(x)y(x) = 0 \,\text{or}$$
$$-p(x)\tfrac{\mathrm{d}^2y}{\mathrm{d}x^2} - \tfrac{\mathrm{d}p}{\mathrm{d}x}\tfrac{\mathrm{d}y}{\mathrm{d}x} + q(x)y(x) - \lambda\rho(x)y(x) = 0.$$

Example 2.4

Consider a quantum particle in a one-dimensional box (or a vibrating string), whose equation of motion is given by

$$-\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} = E\Psi, \qquad x \in [0, L]$$

hence $p(x) = 1$; $q(x) = 0$; $\rho(x) = 1$; $\lambda = E$.

Alternatively, if the particle is defined on a disc, i.e. $r \in [0, a]$, then the equation becomes

$$-\nabla^2 \Psi = E\Psi,$$

which in cylindrical coordinates is

$$-\frac{\partial^2 \Psi}{\partial r^2} - \frac{1}{r}\frac{\partial \Psi}{\partial r} - \frac{1}{r^2}\frac{\partial^2 \Psi}{\partial \phi^2} = E\Psi.$$

Assuming the wavefunction takes the form $\Psi(r, \phi) = f(r)e^{im\phi}$ this then becomes

$$-\frac{\mathrm{d}^2 f}{\mathrm{d}r^2} - \frac{1}{r}\frac{\mathrm{d}f}{\mathrm{d}r} + \frac{m^2}{r^2} f = Ef.$$

Multiplying all terms by r and rearranging to obtain the form of a Sturm-Liouville equation, one gets

$$-\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}}{\mathrm{d}r} f\right) + \frac{m^2}{r} f = Erf$$

and hence $p(r) = r$; $q(r) = \frac{m^2}{r}$; $\rho(r) = r$; $\lambda = E$.

It is possible to an equation into the form of a Sturm-Liouville equation. Consider a more generalised form:

$$y'' + \alpha y' + \beta y + \lambda \tau y = 0.$$

Multiplying both sides by a so-called "integrating factor", $-p(x)$;

$$\underbrace{-p(x)y'' - p(x)\alpha y'}_{\stackrel{!}{=} -\frac{\mathrm{d}}{\mathrm{d}x}(py') = -py'' - p'y'} - p(x)\beta y - \lambda \underbrace{p(x)\tau}_{=\rho} y = 0.$$

One therefore gets that $\frac{\mathrm{d}p}{\mathrm{d}x} = \alpha p$, resulting in $p(x) = Ae^{\int^x \alpha(x')\,\mathrm{d}x'}$, where $A = e^c$ is the constant of integration. This is real and positive if $A > 0$, i.e. $c > -\infty$, with other solutions being trivial, i.e. $p(x) = 0$. As $\rho \geq 0$ by definition and $p \geq 0$ then one get $\tau \geq 0$. The parameters for the Sturm-Liouville form are then $p(x) = Ae^{\int^x \alpha(x')\,\mathrm{d}x'}$; $q(x) = -\beta p(x)$; $\rho(x) = \tau p(x)$.

Example 2.5

Reconsider the particle defined on a disc from Example 2.4:

$$-\frac{\mathrm{d}^2 f}{\mathrm{d}r^2} - \frac{1}{r}\frac{\mathrm{d}f}{\mathrm{d}r} + \frac{m^2}{r^2} f = Ef.$$

One gets $\alpha = \frac{1}{r}$ and so the integrating factor is

$$\begin{aligned} p &= e^{\int^r \alpha(r')\,\mathrm{d}r'} \\ &= e^{\ln(r)+c} \\ &= Ar, \end{aligned}$$

as before.

For any two real functions $u(x)$ and $v(x)$ defined over the interval $x \in [a, b]$ the Sturm-Liouville operator may also be defined over the interval $[a, b]$.

Theorem 2.4: Defined interval of Sturm-Liouville operator

The difference of the Sturm-Liouville operator acting on the functions is given by

$$\begin{aligned} v(Lu) - (Lv)u &= -v(x)\tfrac{\mathrm{d}}{\mathrm{d}x}\left(p\tfrac{\mathrm{d}u}{\mathrm{d}x}\right) + vqu + \tfrac{\mathrm{d}}{\mathrm{d}x}\left(p\tfrac{\mathrm{d}v}{\mathrm{d}x}\right)u - vqu \\ &= \tfrac{\mathrm{d}}{\mathrm{d}x}\left(-vp\tfrac{\mathrm{d}u}{\mathrm{d}x} + up\tfrac{\mathrm{d}v}{\mathrm{d}x}\right). \end{aligned}$$

Integrating this over the interval for which the functions are defined then gives

$$\begin{aligned} \int_a^b v(Lu) - (Lv)u\,\mathrm{d}x &= \left[-vp\tfrac{\mathrm{d}u}{\mathrm{d}x} + up\tfrac{\mathrm{d}v}{\mathrm{d}x}\right]_a^b \\ \Rightarrow (v, Lu) - (u, Lv) &= \left[p\left(u\tfrac{\mathrm{d}v}{\mathrm{d}x} - v\tfrac{\mathrm{d}u}{\mathrm{d}x}\right)\right]_a^b, \end{aligned}$$

and so L is defined over the interval $[a, b]$.

2.6 Hermitian Sturm-Liouville Operators

If L is Hermitian then $(v, Lu) = (u, Lv)$ and so two conclusions can be reached:

$$\int_a^b v(Lu) - (Lv)u \, \mathrm{d}x = 0 \quad \text{or}$$
$$\left[p\left(u\frac{\mathrm{d}v}{\mathrm{d}x} - v\frac{\mathrm{d}u}{\mathrm{d}x} \right) \right]_a^b = 0,$$

the second of which can be written explicitly as

$$\left[p\left(u\frac{\mathrm{d}v}{\mathrm{d}x} - v\frac{\mathrm{d}u}{\mathrm{d}x} \right) \right]_a^b = p(b)u(b)v'(b) - p(b)u'(b)v(b) - p(a)u(a)v'(a) + p(a)u'(a)v(a).$$

This can be written in terms of the Wronskian, $w(x) = \begin{vmatrix} u(x) & v(x) \\ u'(x) & v'(x) \end{vmatrix}$;

$$\left[p\left(u\frac{\mathrm{d}v}{\mathrm{d}x} - v\frac{\mathrm{d}u}{\mathrm{d}x} \right) \right]_a^b = p(b)w(b) - p(a)w(a).$$

Self-adjointness is a property of the operator *and* the boundary conditions applied to the function; in general boundary conditions are $p(a) = p(b) = 0$. If this is not the case then the operator is still Hermitian but the boundaries are said to be **separated**.

Since, by definition, Sturm-Liouville equations are second-order, there are two independent solutions. One solution, $u(x)$, has already been found for a given eigenvalue λ. Consider both solutions y_1 and y_2:

$$Ly_1 = \lambda\rho y_1$$
$$Ly_2 = \lambda\rho y_2,$$

one then gets

$$y_2 Ly_1 = \lambda\rho y_1 y_2$$
$$y_1 Ly_2 = \lambda\rho y_1 y_2.$$

The difference of these then becomes

$$\begin{aligned}
0 &= y_2 L y_1 - y_1 L y_2 \\
&= -y_2 \tfrac{\mathrm{d}}{\mathrm{d}x}\left(p\tfrac{\mathrm{d}y_1}{\mathrm{d}x}\right) - \tfrac{\mathrm{d}y_2}{\mathrm{d}x} p \tfrac{\mathrm{d}y_1}{\mathrm{d}x} + y_1 \tfrac{\mathrm{d}}{\mathrm{d}x}\left(p\tfrac{\mathrm{d}y_2}{\mathrm{d}x}\right) + \tfrac{\mathrm{d}y_2}{\mathrm{d}x} p \tfrac{\mathrm{d}y_1}{\mathrm{d}x} \\
&= \tfrac{\mathrm{d}}{\mathrm{d}x}\left(-y_2 p \tfrac{\mathrm{d}y_1}{\mathrm{d}x} + y_1 p \tfrac{\mathrm{d}y_2}{\mathrm{d}x}\right) \\
&= \tfrac{\mathrm{d}}{\mathrm{d}x}\left(pw\right) \\
\therefore pw &= c,
\end{aligned}$$

where c is constant over the interval for which the Sturm-Liouville operator is defined $x \in [a, b]$. Separate boundary conditions may be equivalent to $c = 0$, in which case $pw = 0$ for $x = a, b$. In this instance if $p \neq 0$ then the Wronskian is equal to zero, i.e. $y_1 y_2' - y_2 y_1' = 0 \Rightarrow y_1 = y_2 e^d$, where d is some constant of integration. The second solution is therefore a scaled first solution, hence is not independent. However, if the boundary conditions are not $c = 0$ then

$$\begin{aligned}
pw = p(y_1 y_2' - y_2 y_1') &= c \\
\rightarrow \underbrace{\frac{1}{y_1} y_2' - \frac{y_1'}{y_1^2} y_2}_{=\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{y_2}{y_1}\right)} &= \frac{c}{p y_1^2}
\end{aligned}$$

$$\Rightarrow y_2 = y_1 \int^x \frac{c}{p(x') y_1^2(x')} \, \mathrm{d}x.$$

Thus if the second solution y_2 exists it can be constructed, though there is no guarantee it will satisfy boundary conditions. This second solution may diverge if $p(a) = 0$ or $p(b) = 0$ and be indivisible as a solution, i.e. $p(x) = 0$ for singular points (automatic boundaries).

For Sturm-Liouville operators with separated ($p(a, b) \neq 0$) boundary conditions:

- Eigenvalues are real and non-degenerate.
- There exists a lowest eignvalue λ_0 in an unbounded space, i.e.

$$\lambda_0 < \lambda_1 < \lambda_2 < \ldots ; \lim_{n \to \infty} \lambda_n \to \infty.$$

- The number of nodes in the n$^{\text{th}}$ eigenvector is exactly n.
- The eigenfunctions $(u_m, u_n; m \neq n)$ are orthogonal such that

$$(u_m, u_n)_\rho = \int_a^b u_m^* u_n \, \mathrm{d}x = 0.$$

- The eigenfunctions $u_1(x), u_2(x), \ldots, u_n(x)$ form a complete basis set of functions over the interval $[a, b]$ suitable for the boundary conditions.

2.7 Spherical Harmonics and Legendre's Equations

An example of a series solution is the usage of Legendre polynomials. A use for such is by considering a potential f around a point charge placed at $z = 1$ along the z-axis, as shown in Figure 2.3.

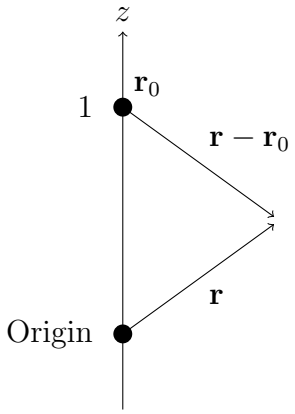

Figure 2.3: Potential at a field point with coordinates $\mathbf{r}$ due to a point charge placed at $\mathbf{r}_0$ with $z = 1$.

Setting $\frac{q}{4\pi\epsilon_0}$, the potential is given by

$$\begin{aligned} f &= \frac{q}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}-\mathbf{r}_0|} = \frac{1}{|\mathbf{r}-\mathbf{r}_0|} \\ &= \frac{1}{\left(r_0^2+r^2-2rr_0\cos(\theta)\right)^{\frac{1}{2}}} \\ &= \frac{1}{\left(1+r^2-2r\cos(\theta)\right)^{\frac{1}{2}}}. \qquad (\mathbf{r}_0 = 1) \end{aligned}$$

For small $\mathbf{r}$, f can be expanded in powers of r thus becoming a **generating function**, i.e.

$$f(r,u) = \sum_{n=0}^{\infty} r^n P_n(u), \qquad (u = \cos(\theta))$$

where $P_n(u)$ are Legendre polynomials. For very small r, $\cos(\theta) \approx 1$, and so

$$\begin{aligned} f(r,1) &= \sum_{n=0}^{\infty} r^n P_n(1) \\ f(r,1) = \frac{1}{(1+r^2-2r)^{\frac{1}{2}}} &= \frac{1}{1-r} \\ &= 1 + r + r^2 + \ldots \\ \Rightarrow P_n(1) &= 1. \end{aligned}$$

f satisfies the Laplace equation except at $\mathbf{r} = \mathbf{r}_0$, i.e.

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

Note that this is independent of azimuthal angle ϕ as $\cos(\theta) \sim 1$, so $\theta \sim 0$. Furthermore, each term $r^n P_n(\cos(\theta))$ is a solution because ∇^2 just reduces the power of r by 2, i.e.

$$\begin{aligned} \frac{\partial^2 r^n}{\partial r^2} + \frac{2}{r}\frac{\partial r^n}{\partial r} &= n(n-1)r^{n-2} + 2nr^{n-2} \\ &= n(n+1)r^{n-2}. \end{aligned}$$

Attention may now be paid to the $\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial f}{\partial\theta}\right)$ term. From the chain rule $\frac{\partial}{\partial\theta} = \frac{\partial u}{\partial\theta}\frac{\partial}{\partial u}$, where $u = \cos(\theta)$ and so $\frac{\partial u}{\partial\theta} = -\sin(\theta)$, thus the overall term

becomes

$$\frac{-\sin(\theta)}{\sin(\theta)}\frac{\partial}{\partial u}\left(-\sin^2(\theta)\frac{\partial P_n}{\partial u}\right)=\frac{\partial}{\partial u}\left(\left(1-u^2\right)\frac{\partial P_n}{\partial u}\right).$$

Combining all of the above then gives Legendre's equation:

$$-\frac{\mathrm{d}}{\mathrm{d}u}\left(\underbrace{\left(1-u^2\right)}_{=p(u)}\frac{\mathrm{d}P_n}{\mathrm{d}u}\right)=\underbrace{n(n+1)}_{=\lambda}P_n. \qquad (\rho=1)$$

There is regular singular points at $u=\pm 1$ which give $1-u^2=0$. By orthogonality of Legendre polynomials

$$\underbrace{\int_{-1}^{1}P_n(u)P_m(u)\,\mathrm{d}u}_{=(P_n,P_m)}=k_m\delta_{mn},$$

where k_m are a family of values for the integral. At constant k_m the inner product of a function with itself is given by

$$\begin{aligned}
(f,f)&=\int_{-1}^{1}\frac{1}{1-2ru+r^2}\,\mathrm{d}u\\
&=-\frac{1}{2r}\left[\ln\left(1-2ru+r^2\right)\right]_{-1}^{1}\\
&=-\frac{1}{2r}\left[\ln\left(1-2r+r^2\right)-\ln\left(1+2r+r^2\right)\right]\\
&=-\frac{1}{r}\left(\ln(1-r)-\ln(1+r)\right)\\
&=-\frac{1}{r}\left(\left(-r-\frac{r^2}{2}-\frac{r^3}{3}-\frac{r^4}{4}-\dots\right)-\left(r-\frac{r^2}{2}+\frac{r^3}{3}-\frac{r^4}{4}+\dots\right)\right)\\
&=2+\frac{2}{3}r^2+\frac{2}{5}r^4+\dots\\
&=\sum_{n=0}^{\infty}\frac{2}{2n+1}r^{2n}.
\end{aligned}$$

In terms of Legendre polynomials the inner product of f with itself is also given by

$$\begin{aligned}(f,f) &= \int_{-1}^{1} \sum_{n=0}^{\infty} r^n P_n(u) \sum_{m=0}^{\infty} r^m P_m(u)\,\mathrm{d}u \\ &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} r^{m+n} \underbrace{\int_{-1}^{1} P_n P_m\,\mathrm{d}u}_{=k_m\delta_{mn}} \\ &= \sum_{n=0}^{\infty} r^{2n} k_n.\end{aligned}$$

The inner product of a Legendre polynomial with itself it hence

$$(P_n, P_n) = k_n = \frac{2}{2n+1}.$$

Returning to the example of potential due to a point charge;

$$\begin{aligned}f(r,u) &= (1-2ru+r^2)^{-\frac{1}{2}} \\ &= 1 + \left(-\frac{1}{2}\right)(-2ru) + \mathcal{O}(r^2) \\ &= \underbrace{1}_{=P_0(u)} + \underbrace{ru}_{=P_1(u)} + \mathcal{O}(r^2).\end{aligned}$$

In order to obtain a recurrence relation between P_n's, take the derivative of the generating function:

$$\begin{aligned}
f(r,u) &= (1-2ru+r^2)^{-\frac{1}{2}} \\
&= \frac{1}{r}\frac{1}{\left(\frac{1}{r^2}-\frac{2}{r}u+1\right)^{\frac{1}{2}}} \\
&= \frac{1}{r}f\left(\frac{1}{r},u\right) \\
&= \frac{1}{r}\sum_{n=0}^{\infty}\frac{1}{r^n}P_n(u) \\
&= \sum_{n=0}^{\infty}\frac{1}{r^{n+1}}P_n(u) \\
\frac{\partial f}{\partial r} &= (k-r)\left(1-2ru+r^2\right)^{-\frac{3}{2}} \\
&= \sum_{n=0}^{\infty} nr^{n-1}P_n(u),
\end{aligned}$$

then multiply both sides by $1-2ru+r^2$:

$$(k-r)\sum_{n=0}^{\infty} r^n P_n(u) = (1-2ru+r^2)\sum_{n=0}^{\infty} nr^{n-1}P_n(u).$$

Equating coefficients of r^m gives

$$\begin{aligned}
uP_m - P_{m-1} &= (m+1)P_{m+1} + (m-1)P_{m-1} - 2umP_m \\
\Rightarrow (m+1)P_{m+1} &= (2m+1)uP_m - mP_{m-1}.
\end{aligned}$$

Taking, for examplem $m=1$:

$$\begin{aligned}
2P_2 &= 3u\cdot u - 1 \\
\Rightarrow P_2(u) &= \frac{3u^2-1}{2}.
\end{aligned}$$

Example 2.6: Find the potential $\psi(r, u = \cos(\theta))$ of a ring of uniform charge for $r > a$

Expanding ψ as $\psi(r,u) = \sum_{n=0}^{\infty} c_n \frac{a^n}{r^{n+1}} P_n(u)$ (and preventing singularities by ignoring $n = 0$), one can calculate the coefficients c_n by setting $u = 1$, i.e. calculating the on-axis potential ($\theta = 0$):

$$\begin{aligned}
\psi(r,1) &= \sum_{n=1}^{\infty} c_n \frac{a_n}{r^{n+1}} && (P_n(1) = 1) \\
&= \frac{q}{4\pi\epsilon_0} \frac{1}{(a^2 + r^2)^{\frac{1}{2}}} \\
&= \frac{q}{4\pi\epsilon_0 r} \left(1 + \frac{a^2}{r^2}\right)^{-\frac{1}{2}} \\
&= \frac{q}{4\pi\epsilon_0 r} \left(1 + \frac{\left(-\frac{1}{2}\right)}{1!} \left(\frac{a^2}{r^2}\right) + \frac{\left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right)}{2!} \left(\frac{a^2}{r^2}\right)^2 + \ldots\right).
\end{aligned}$$

The non-vanishing coefficients have $n = 2m$, i.e.

$$c_{2m} = \frac{q}{4\pi\epsilon_0} \left(-\frac{1}{2}\right)^m \frac{1}{m!} (2m+1)!!,$$

where $(2m+1)!! = 1 \times 3 \times 5 \times \ldots \times (2m-1) \times (2m+1)$.

Example 2.7: Conducting cone

Consider the tip of a conducting cone just touching a zero-potential plane. The solution to this is a solution to the Laplace equation with boundary conditions $V(r,0)=0$ and $V(r,\cos(\alpha))=V_0$. As the boundary conditions do not depend on r one can trial a solution of $V=\phi(u)$, i.e. solving Laplace equation of the form

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}u}\left(\left(1-u^2\right)\frac{\mathrm{d}\phi}{\mathrm{d}u}\right)&=0\\
\left(1-u^2\right)\frac{\mathrm{d}\phi}{\mathrm{d}u}&=A\\
\rightarrow\phi(u)&=\int\frac{A}{1-u^2}\,\mathrm{d}u\\
&=\underbrace{A\,\mathrm{arctanh}(u)}_{\substack{\text{second solution of}\\ \text{Legendre polynomial}}}+BP_0(u)\\
&=\underbrace{\frac{A}{2}\ln\left(\frac{1+u}{1-u}\right)}_{\substack{\text{second solution diverges}\\ \text{at } u=\pm1\text{, i.e. the regular}\\ \text{singular points of Legendre}}}+B. \qquad (P_0(u)=1)
\end{aligned}$$

The solution is only required for $0\leq u\leq\cos(\alpha)$, thus one can fix the constants A and B from the boundary conditions:

$$\begin{aligned}
\phi(0)&=0\\
&=A\,\mathrm{arctanh}(0)+B\\
\Rightarrow B&=0
\end{aligned}
\qquad
\begin{aligned}
\phi(\cos(\alpha))&=V_0\\
&=A\,\mathrm{arctanh}(\cos(\alpha))\\
\Rightarrow\phi&=V_0\frac{\mathrm{arctanh}(\cos(\theta))}{\mathrm{arctanh}(\cos(\alpha))}.
\end{aligned}$$

2.8 The Quantum Oscillator and Hermite's Equation

2.9 Orthogonal Polynomials

Chapter 3

Green's Functions

3.1 General Properties

Green's functions are used extensively in numerous areas of physics, including electrodynamics, scattering kinematics and quantum mechanics.

Definition 3.1: Green's Function

Green's functions are used to solve equations of the form

$$Lu(x) = f(x),$$

where L is a linear differential operator[a], the function $u(x)$ satisfies boundary conditions at $x = \{a, b\}$ and $f(x)$ is a *source* term. The function u can always be written in the form

$$u(x) = \int_a^b G(x, x')f(x')\,\mathrm{d}x',$$

where the Green's function $G(x, x')$ is given by the **defining equation**

$$LG(x, x') = \delta(x - x').$$

The Green's function works by solving the differential equation for a singular source point - equivalent to a Dirac delta function - which is then integrated over in order to encompass the entire source.

[a] L acts only upon the argument of the function, i.e. x but not x'

Theorem 3.1: The function u of the linear differential equation $Lu(x) = f(x)$ can always be written in the form $u(x) = \int_a^b G(x, x')f(x')\,\mathrm{d}x'$

In terms of a Dirac delta function, a general function $f(x) : x \in [a, b]$ may be written

$$f(x) = \int_a^b \delta(x - y)f(y)\,\mathrm{d}y.$$

By the definition of the Green's function this can be rewritten as

$$\begin{aligned} f(x) &= \int_a^b LG(x, y)f(y)\,\mathrm{d}y \\ &= L\int_a^b G(x, y)f(y)\,\mathrm{d}y. \end{aligned}$$

Green's functions are defined for equations of the form $Lu(x) = f(x)$, thus by equating the source terms $f(x)$ one can see that the solution can always be written in the form

$$u(x) = \int_a^b G(x, y)f(y)\,\mathrm{d}y.$$

Example 3.1: Electrostatics

Gauss' law for electrostatics is given by

$$\boldsymbol{\nabla} \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}.$$

By relating the electric potential to the electric field as $\mathbf{E} = -\boldsymbol{\nabla}\Phi$, Poisson's equation for the potential is given by

$$\nabla^2\Phi = -\frac{\rho}{\epsilon_0},$$

with the boundary condition that it falls off with distance from the source, i.e. $\lim_{x\to\infty} \Phi(x) = 0$. The Green's function (setting $\epsilon_0 = 1$) is therefore given by the solution to

$$\nabla^2 G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}'),$$

known as the **fundamental solution**;

$$G(\mathbf{x}, \mathbf{x}') = -\frac{1}{4\pi|\mathbf{x} - \mathbf{x}'|}.$$

Using the initial notation, i.e. $u(x) = \int G(\mathbf{x}, \mathbf{x}')f(\mathbf{x}')\,\mathrm{d}\mathbf{x}'$, one gets $u(x) = \Phi(\mathbf{x}); G(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi}\frac{1}{|\mathbf{x}-\mathbf{x}'|}; f(\mathbf{x}') = \rho(\mathbf{x}')$, and so the potential is

$$\Phi(\mathbf{x}) = \frac{1}{4\pi}\int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}\,\mathrm{d}^3\mathbf{x}'.$$

Theorem 3.2: Fundamental solution

Consider the Laplace equation for a Green's function, i.e.

$$\nabla^2 G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}').$$

Integrating this over volume resolves the delta function, thus

$$\iiint \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} G(\mathbf{x}, \mathbf{x}')r^2 \sin(\theta)\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi = 1,$$

where $r = |\mathbf{x} - \mathbf{x}'|$. By the divergence theorem, one gets $\boldsymbol{\nabla} G$ as

$$\boldsymbol{\nabla} G = \frac{1}{4\pi r^2}.$$

Taking a path integral of this cancels the gradient operator, thus

$$G(\mathbf{x}, \mathbf{x}') = -\frac{1}{4\pi r} = -\frac{1}{4\pi|\mathbf{x} - \mathbf{x}'|}.$$

3.2 Construction of Green's Functions

There are three main methods of constructing Green's functions: decomposing the Green's function into eigenfunctions, decomposing the functions u and f as eigenstates, and using continuity for boundary-oriented problems.

3.2.1 The Eigenfunction Method

The eigenvalue equation for linear Hermitian operators with normalised eigenfunctions $u_k(x)$ is written

$$Lu_k(x) = \lambda_k u_k(x),$$

where λ_k is real. Assuming the Green's function can be decomposed into these eigenfunctions, i.e. $G(x,y) = \sum_k c_k(y)u_k(x)$ and using the defining equation $LG(x,y) = \delta(x-y)$, then

$$\begin{aligned}\delta(x-y) &= \sum_k c_k(y) L u_k(x) \\ &= \sum_k c_k(y)\lambda_k u_k(x).\end{aligned}$$

This can be projected onto another eigenfunction $u_\ell(x)$ to give to coefficients

$$\begin{aligned}\big(u_\ell(x), \delta(x-y)\big) &= \int u_\ell^*(x)\delta(x-y)\,\mathrm{d}x \\ &= u_\ell^*(y);\end{aligned} \qquad \begin{aligned}\big(u_\ell(x), \delta(x-y)\big) &= \sum_k c_k(y)\lambda_k(u_\ell(x), u_k(x)) \\ &= \sum_k c_k(y)\lambda_k\delta_{k\ell} \\ &= c_\ell(y)\lambda_\ell\end{aligned}$$

$$\Rightarrow c_\ell(y) = \frac{u_\ell^*(y)}{\lambda_\ell}.$$

The decomposed Green's function in terms of eigenfunctions - sometimes known as the **bilinear expansion** - is hence

$$G(x,y;\lambda) = \sum_k c_k(y)u_k(x) = \sum_k \frac{u_k^*(y)u_k(x)}{\lambda_k}.$$

From the $\frac{1}{\lambda_n}$ relation it can be seen that **zero-mode** terms ($\lambda_n = 0$) diverges and hence has no unique solution. Furthermore, from this summation form one can see that for a Hermitian operator the Green's function is also Hermitian:

$$G(x,y) = \sum_\ell \frac{u_\ell(x)u_\ell^*(y)}{\lambda_\ell} = \left(\sum_\ell \frac{u_\ell^*(x)u_\ell(y)}{\lambda_\ell}\right)^* = \big(G(y,x)\big)^*.$$

3.2.2 The Eigenstate Method

Decomposing the two functions $u(x)$ and $f(x)$ of the differential equation $f(x) = Lu(x)$ into the same eigenfunctions;

$$u(x) = \sum_n c_n u_n(x) \quad \text{and} \quad f(x) = \sum_n d_n u_n(x),$$

the equation then becomes

$$\begin{aligned}\sum_n d_n u_n(x) &= \sum_n c_n L u_n(x) \\ &= \sum_n c_n \lambda_n u_n(x).\end{aligned}$$

Projecting this onto another eigenfunction $u_m(x)$

$$\begin{aligned}\sum_n d_n \left(u_m, u_n\right) &= \sum_n d_n \delta_{mn} & \sum_n c_n \lambda_n \left(u_m, u_n\right) &= \sum_n c_n \lambda_n \delta_{mn} \\ &= d_m; & &= c_m \lambda_m \\ &\Rightarrow (u_m, f) = d_m = c_m \lambda_m.\end{aligned}$$

For the zero-mode eigenvalue $\lambda_n = \lambda_0 = 0$, then

$$(u_0, f) = d_0 = c_0 \lambda_0 = 0,$$

hence the zero-mode solution $u_0(x)$ and source $f(x)$ functions are orthogonal. This leads to the coefficient c_0 being indeterminate and hence a family of solutions is required for a full solution. The solution is then given by

$$\begin{aligned}u(x) &= \sum_n c_n u_n(x) \\ &= c_0 u_0(x) + \sum_{n=1}^{\infty} \frac{d_n}{\lambda_n} u_n(x) \\ &= c_0 u_0(x) + \sum_{n=1}^{\infty} \frac{1}{\lambda_n} f(x) \\ &= c_0 u_0(x) + \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \int \delta(x - x') f(x') \, \mathrm{d}x' \\ &= c_0 u_0(x) + \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \int u_n(x) u_n^*(x') f(x') \, \mathrm{d}x',\end{aligned}$$

however the Green's function is given by $G(x,x') = \sum_{n\neq 0} \frac{u_n(x)u_n^*(x')}{\lambda_n}$, thus

$$u_n(x) = c_0 u_0(x) + \int G(x,x') f(x')\,\mathrm{d}x'.$$

Example 3.2: Driven vibrating string I

Consider a driven vibrating string with fixed end points whose driving force F is given by

$$F = F(x)e^{-i\omega t}.$$

The forces on the string are then related by

$$\underbrace{\rho\frac{\partial^2 u}{\partial t^2}}_{\text{Density}} = \underbrace{T\frac{\partial^2 u}{\partial x^2}}_{\text{Tension}} - \underbrace{\beta\frac{\partial u}{\partial t}}_{\text{Friction}} - \underbrace{F(x)e^{-i\omega t}}_{\text{Driving}},$$

where u is the displacement of point x along the string from equilibrium. Assuming that friction in the system is negligible then one can seek a solution of the form

$$u(t,x) = y(x)e^{-i\omega t}.$$

Substituting this into the force equation then gives

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + \frac{\rho\omega^2}{T}y = \frac{F(x)}{T}.$$

Defining $k^2 \equiv \frac{\rho\omega^2}{T}$ and $f(x) \equiv \frac{F(x)}{T}$ then the equation takes on the form

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + k^2 y = f(x).$$

To solve this, one uses the Green's function to solve a similar form:

$$\frac{\partial^2 G(x,y)}{\partial x^2} + k^2 G(x,y) = \delta(x-y).$$

Expanding $f(x) \to \lambda_n y$ and rearranging to $\dfrac{\mathrm{d}^2 y}{\mathrm{d}x^2} = \left(\lambda_n - k^2\right) y$ and defining $k_n^2 \equiv k^2 - \lambda_n^2$, then the problem is similar to a simple harmonic

oscillator, i.e. $y'' = -k_n^2 y$, whose boundary conditions allow only $y = \sqrt{\frac{2}{L}}\sin(k_n x)$, where $k_n = \frac{n\pi}{L}$. The Green's function is then

$$G(x,y) = \sum_n \frac{u_n(x)u_n^*(y)}{\lambda_n} = \frac{2}{L}\sum_n \frac{\sin(k_n x)\sin(k_n y)}{k^2 - k_n^2},$$

and so the solution is

$$u_n(x) = \int_0^L G(x,y)f(y)\,\mathrm{d}y = \sum_n d_n \frac{u_n(x)}{\lambda_n} = \sum_n d_n \sqrt{\frac{2}{L}}\frac{\sin(k_n x)}{k^2 - k_n^2},$$

where $d_n = \sqrt{\frac{2}{L}}\int_0^L f(y)\sin(k_n y)\,\mathrm{d}y$.

3.2.3 The Continuity Method

The continuity method can be used to find the Green's function of ODEs of any order, e.g. a second order ODE given by

$$\underbrace{\left[\alpha(x)\frac{\partial^2}{\partial x^2} + \beta(x)\frac{\partial}{\partial x} + \gamma(x)\right]}_{=L} G(x,x') = \delta(x - x').$$

The method to solve this is as follows:

1. Separately solve for regions $x < x'$ and $x > x'$, where the equation reduces to
$$LG(x,x') = 0$$
plus boundary conditions.

2. Integrate about $x = x'$ and use the continuity of $G(x,x')$ to generalise the solution, i.e. using that $\lim_{\epsilon\to 0}\left[G(x,x')\right]_{x'-\epsilon}^{x'+\epsilon} = 0$ then
$$\lim_{\epsilon\to 0}\left[\frac{\partial}{\partial x}G(x,x')\right]_{x'-\epsilon}^{x'+\epsilon} = \frac{1}{\alpha(x)}.$$

Example 3.3: Driven vibrating string II

Reconsidering Example 3.2, whose equation of motion was

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2\right) u(x) = f(x).$$

This matches the form for Green's function:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2\right) G(x, x') = \delta(x, x'),$$

with boundary conditions $G(x, x') = 0$ for $x = \{0, L\}$, i.e.

$x < x'$	$x > x'$
$G(x, x') = A(x') \sin(kx)$	$G(x, x') = N(x') \sin(k(L - x))$
$(G \to 0 \text{ at } x = 0)$	$(G \to 0 \text{ at } x = L)$

$G(x, x')$ is required to be continuous, i.e. the string does not break, at $x = x'$ and that $\partial_x G(x, x')$ is discontinuous (has a step) at $x = x'$, i.e. a point force induces a "kink" in the string). To find the discontinuity, integrate the Green's equation about x';

$$\int_{x'-\epsilon}^{x'+\epsilon} \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2\right) G(x, x')\,\mathrm{d}x = \int_{x'-\epsilon}^{x'+\epsilon} \delta(x - x')\,\mathrm{d}x$$

$$\left[\frac{\partial}{\partial x} G(x, x')\right]_{x'-\epsilon}^{x'+\epsilon} + \underbrace{\int_{x'-\epsilon}^{x'+\epsilon} k^2 G(x, x')\,\mathrm{d}x}_{= k^2 G 2\epsilon, \text{ in the limit } \epsilon \to 0 \text{ this tends to zero}} = 1$$

$$\therefore \left[\frac{\partial G}{\partial x}\right]_{x'-\epsilon}^{x'+\epsilon} = 1$$

$$\Rightarrow -kB\cos(k(L - x')) - kA\cos(kx') = 1.$$

In summary then, from continuity

$$A\sin(kx') = B\sin(k(L - x'))$$

and from discontinuity

$$-kA\cos(kx') - kB\cos(k(L - x')) = 1.$$

Rearranging the continuity equation for B and substituting into the discontinuity equation gives

$$\begin{aligned}1 &= -kA\cos(kx') - k\left[A\frac{\sin(kx')}{\sin(k(L-x'))}\right]\cos(k(L-x')) \\ &= -kA\left[\cos(kx') + \frac{\cos(k(L-x'))}{\sin(k(L-x'))}\sin(kx')\right] \\ &= -\frac{kA}{\sin(k(L-x'))}\left[\cos(kx')\sin(k(L-x')) + \sin(kx')\cos(k(L-x'))\right].\end{aligned}$$

Using the trigonometric identity $\sin(A+B) = \sin(A)\cos(B) + \sin(B)\cos(A)$ and recalling $-\frac{kA}{\sin(k(L-x))}\sin(kL) = 1$, then

$$\begin{aligned}A &= -\frac{\sin(k(L-x))}{k\sin(kL)}; \\ B &= -\frac{\sin(kx)}{k\sin(kL)}.\end{aligned}$$

The Green's function is finally given by

$$G(x,x') = \begin{cases} -\frac{\sin(kx)\sin(k(L-x'))}{k\sin(kL)} & x < x' \\ -\frac{\sin(k(L-x))\sin(kx')}{k\sin(kL)} & x > x'. \end{cases}$$

One should note the symmetry under exchange of x and x'.

3.3 Quantum Scattering in the Time-Independent Approach

Consider a wavefunction of the form

$$\Psi(t,\mathbf{r}) = \Phi(\mathbf{r})e^{-i\omega t},$$

which satisfies the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Phi(\mathbf{r}) + V(\mathbf{r})\Phi(\mathbf{r}) = E\Phi(\mathbf{r}).$$

For positive energies one can introduce a wavenumber k such that the energy is given by $E = \frac{\hbar^2 k^2}{2m}$, thus Schrödinger's equation becomes

$$\left(\nabla^2 + k^2\right)\Phi(\mathbf{r}) = \frac{2m}{\hbar^2}V(\mathbf{r})\Phi(\mathbf{r}) \equiv \rho(\mathbf{r}).$$

In order to solve this the boundary conditions must first be determined. Consider a beam of quantum particles for which $\lim_{r\to\infty} rV(\mathbf{r}) = 0$ and outside the range of interaction the beam is a plane wave, i.e. $\Phi(\mathbf{r}) = e^{ikz}$. The radial Laplacian operator for spherical coordinates is given by $\nabla^2 = -\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}\right)$. The spherical wave eigenfunctions are then of the form $\frac{1}{r}e^{\pm ikr}$, thus the *outgoing* spherical waves are of the form $f(\theta,\phi)\frac{e^{ikr}}{r}$, written $\chi(\mathbf{r})$. For the asymptotic boundary condition ($r \to \infty$) the radial wavefunction is then $\Phi(\mathbf{r}) \to e^{ikz} + \chi(\mathbf{r})$. The Schrödinger equation thus becomes

$$\left(\nabla^2 + k^2\right)\chi(\mathbf{r}) = \rho(\mathbf{r}),$$

which is subject to $\lim_{r\to\infty}\chi(\mathbf{r}) = f(\theta,\phi)\frac{e^{ikr}}{r}$. In order to solve this, one first solves the Green's function equation

$$\left(\nabla^2 + k^2\right)G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}').$$

In general, if the operator is translationally invariant then the Green's function can be taken to be a convolution operator, that is to say $G(x,s) = G(x-s)$. Therefore the Green's function of the Schrödinger equation becomes $G(\mathbf{r},\mathbf{r}') = G(|\mathbf{r}-\mathbf{r}'|)$, thus

$$\left(\nabla^2 + k^2\right)G(\mathbf{r}) = \delta(\mathbf{r}).$$

From the fundamental Green's solution it is already known that

$$\nabla^2\left(\frac{1}{r}\right) = -4\pi\delta(\mathbf{r}),$$

which is the asymptotic limit of the Green's function as $r \to 0$. However, the limit $r \to \infty$ leads to the boundary

$$\left(\nabla^2 + k^2\right) \frac{e^{\pm ikr}}{r} = 0 \qquad r \neq 0$$
$$\Rightarrow G_\pm(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \frac{e^{\pm ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}.$$

It is more natural to use the outgoing Green's function, G_+, thus

$$\begin{aligned} u_n(x) &= c_0 u_0(x) + \int G_+(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}' \\ \to \Phi(\mathbf{r}) &= e^{ikz} + \int G_+(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}' \\ &= e^{ikz} + \frac{2m}{\hbar^2} \int G_+(\mathbf{r}, \mathbf{r}')V(\mathbf{r}')\Phi(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}', \end{aligned}$$

which is known as the **Lippmann-Schwinger** equation.

3.4 Perturbation Theory

It is possible to expand mathematical problems in orders of a small parameter, known as a **perturbation** expansion.

Definition 3.2: Perturbation theory

Some mathematical problems cannot be solved analytically (exactly), however

One of the ways of solving the problem of weak potentials is by iteration, i.e. replacing each $\Phi(\mathbf{r})$ with a corresponding integral for the Lippmann-Schwinger equation, known as a **Born expansion**;

$$\begin{aligned} \Phi(\mathbf{r}) = e^{ikz} &+ \frac{2m}{\hbar^2} \int G_+(\mathbf{r}, \mathbf{r}')V(\mathbf{r}') \underbrace{e^{ikz'}}_{=\Phi(\mathbf{r}')}\,\mathrm{d}^3\mathbf{r}' \\ &+ \left(\frac{2m}{\hbar^2}\right)^2 \iint G_+(\mathbf{r}, \mathbf{r}')V(\mathbf{r}')G_+(\mathbf{r}', \mathbf{r}'')V(\mathbf{r}'') \underbrace{e^{ikz''}}_{=\Phi(\mathbf{r}'')}\,\mathrm{d}^3\mathbf{r}'\,\mathrm{d}^3\mathbf{r}'' \\ &+ \ldots. \end{aligned}$$

For weak potentials, one usually truncates this at the first line and substitutes for the Green's function - known as the **Born approximation** - giving

$$\Phi(\mathbf{r}) = e^{ikz} - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(\mathbf{r}')e^{ikz}\,\mathrm{d}^3\mathbf{r}'.$$

Therefore within the Born approximation $\Phi(\mathbf{r}) \to e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$ with $f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int V(\mathbf{r}')e^{i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{r}}\,\mathrm{d}^3\mathbf{r}'$ - this is a good approximation for, say, electron scattering.

3.4.1 Diffusion

One can now consider particles diffusing in a medium and being injected by an external source. Where the number of particles at a position $\mathbf{r}$ at a given time t is given by $n(t,\mathbf{r})$, the flux of the particles $\mathbf{J}$ should be given by

$$\mathbf{J} = -D\boldsymbol{\nabla}n + \underbrace{\alpha n\left(\nabla^2 n\right) + \ldots}_{\text{Ignore}}.$$

In the absence of the a source, the continuity equation is then

$$\frac{\partial n}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{J} = \frac{\partial n}{\partial t} - D\nabla^2 n = 0,$$

however, when a source $S(t,\mathbf{r})$ is introduced this becomes

$$\frac{\partial n}{\partial t} - D\nabla^2 n = S(t,\mathbf{r}).$$

Drawing similarities to the Green's equation, in this scenario $u_n(\mathbf{r}) = n$, $f(\mathbf{r}) = S(t,\mathbf{r})$ and $L_{t,\mathbf{r}} = \frac{\partial}{\partial t} - D\nabla^2$, thus the Green's equation becomes

$$\frac{\partial G}{\partial t} - D\nabla^2 G = \delta(t-t')\delta(\mathbf{r}-\mathbf{r}').$$

Homogeneity in t and $\mathbf{r}$ means that $G(\mathbf{r}-\mathbf{r}', t-t')$ will satisfy

$$\frac{\partial G}{\partial t} - D\nabla^2 G = \delta(t)\delta(\mathbf{r}).$$

Using the Fourier representation in k-space;

$$\begin{aligned} G(t,\mathbf{r}) &= \int e^{i\mathbf{k}\cdot\mathbf{r}} G_k(t) \left(\frac{1}{2\pi}\right)^3 \mathrm{d}^3k \\ &= \int e^{i\mathbf{k}\cdot\mathbf{r}} \left(\frac{\partial G}{\partial t} - D\nabla^2 G\right) \frac{\mathrm{d}^3k}{(2\pi)^3}; \\ \delta(t) &= \int \delta(t) e^{i\mathbf{k}\cdot\mathbf{r}} \left(\frac{1}{2\pi}\right)^3 \mathrm{d}^3k. \end{aligned}$$

The Green's diffusion equation in the Fourier-representation is hence

$$\frac{\partial G_k}{\partial t} + Dk^2 G_k = \delta(t).$$

Applying the continuity method, the above is a homogeneous equation for which

$$\frac{\partial G_k}{\partial t} + Dk^2 G_k = 0, \qquad t \neq 0$$

thus $G_k \propto e^{-Dk^2 t}$ and so

$$G_k = \begin{cases} Ae^{-Dk^2 t} & t > 0 \\ Be^{-Dk^2 t} & t < 0. \end{cases}$$

However, for $t < 0$ the Green's function diverges as $t \to -\infty$, thus $B = 0$ - this could also be argued from continuity. Integrating about the point of continuity gives

$$\begin{aligned} &\int_{-\epsilon}^{\epsilon} \frac{\partial G}{\partial t} + Dk^2 G \,\mathrm{d}t = 1 \\ &= [G]_{-\epsilon}^{\epsilon} + 2\epsilon Dk^2 G. \end{aligned}$$

Taking the limit of $\epsilon \to 0$ about the point of continuity this then becomes

$$\begin{aligned} \lim_{\epsilon\to 0} [G]_{-\epsilon}^{\epsilon} + 2\epsilon Dk^2 G &= \big[G_+(0) - G_-(0)\big] + 0 \\ &= A - B \\ \Rightarrow A &= 1. \end{aligned}$$

Therefore the Green's function for diffusion is

$$G_k = \begin{cases} e^{-Dk^2 t} & t > 0 \\ 0 & t < 0. \end{cases}$$

Reverting back to x-space, this becomes

$$\begin{aligned} G(t,\mathbf{r}) &= \int G_k(t) e^{i\mathbf{k}\cdot\mathbf{r}} \frac{\mathrm{d}k^3}{(2\pi)^3} \\ &= \left(\frac{1}{2\pi}\right)^3 \iiint e^{-D\left(k_x^2+k_y^2+k_z^2\right)t+i\left(k_x x+k_y y+k_z z\right)} \,\mathrm{d}k_x \,\mathrm{d}k_y \,\mathrm{d}k_z \\ &= \left[\frac{1}{2\pi}\sqrt{\frac{\pi}{Dt}} e^{-\frac{x^2}{4Dt}}\right]\left[\frac{1}{2\pi}\sqrt{\frac{\pi}{Dt}} e^{-\frac{y^2}{4Dt}}\right]\left[\frac{1}{2\pi}\sqrt{\frac{\pi}{Dt}} e^{-\frac{z^2}{4Dt}}\right] \\ &= \left[\frac{1}{2\pi}\sqrt{\frac{\pi}{Dt}}\right]^3 e^{-\frac{x^2+y^2+z^2}{4Dt}} \\ &= \left(\frac{1}{4\pi Dt}\right)^{\frac{3}{2}} e^{-\frac{r^2}{4Dt}}, \qquad\qquad t>0 \end{aligned}$$

that is to say that for a small amount of time the diffusion pattern is a thin Gaussian in which a particle is localised near $r = 0$, whereas following a longer amount of time the spread increases but remains Gaussian in shape, as shown in Figure 3.1.

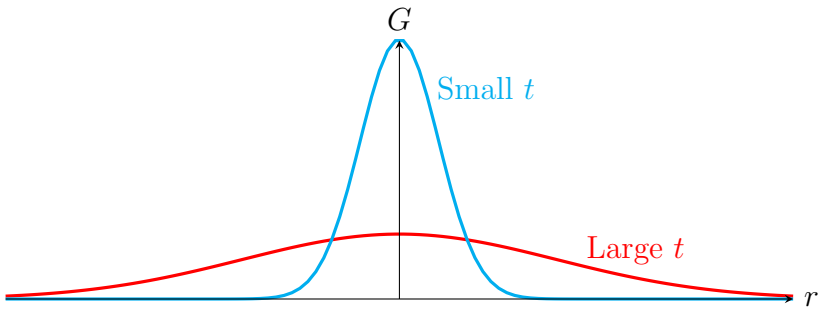

Figure 3.1: Diffusion distributions for different time periods.

3.5 Travelling Waves

3.6 Example: Electromagnetism

In previous modules the reader should have met the Lorenz gauge, $\frac{1}{c^2}\frac{\partial \phi}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{A} = 0$, resulting in the wave equations for a vector potential $\mathbf{A}$ and a scalar potential Φ, i.e.

$$\begin{aligned} \Box \Phi(\mathbf{r}, t) &= \frac{\rho(\mathbf{r}, t)}{\epsilon_0} \\ \Box \mathbf{A}(\mathbf{r}, t) &= \mu_0 \mathbf{j}(\mathbf{r}, t), \end{aligned}$$

where $\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$ is the d'Alembert operator. The aim of using Green's functions in electromagnetism is to consider what happens for an arbitrary source, thus one must study what happens for the d'Alembert of G:

$$\Box G(\mathbf{r}, t; \mathbf{r}', t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t').$$

The solution to this is subject to two physical constraints:

1. The potentials fall off with distance from source

$$\lim_{r \to \infty} G(\mathbf{r}, t; \mathbf{r}', t') = 0$$

2. Causality is preserved

$$G(\mathbf{r}, t; \mathbf{r}', t') = 0. \qquad t < t'$$

For Galilean invariance one takes the Green's function as only a function of *differences* in quantities, i.e.

$$G(\mathbf{r}, t; \mathbf{r}', t') \equiv G(\mathbf{r} - \mathbf{r}', t - t').$$

In order to obtain a function form of G, take $|\mathbf{r}'| = t' = 0$, thus

$$\Box G = \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 \right) G(\mathbf{r}, t) = \delta(\mathbf{r})\delta(t).$$

Solving this is equivalent to solving for the scalar potential by

$$\Phi(\mathbf{r}, t) = \iint G(\mathbf{r} - \mathbf{r}', t - t') \frac{\rho(\mathbf{r}', t')}{\epsilon_0} \, \mathrm{d}^3\mathbf{r}' \, \mathrm{d}t'.$$

3.6.1 The Fourier Transform Method

The Fourier transforms of the temporal delta function and a Green's function are given by

$$\begin{aligned}\delta(t) &= \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} \\ G(\mathbf{r}, t) &= \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} G_\omega(\mathbf{r}),\end{aligned}$$

where G_ω is the Green's function in ω space. The Fourier representation of the wave equation of the Green's function is thus

$$\begin{aligned}\Box G = \int \frac{\mathrm{d}\omega}{2\pi} \left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right) e^{-i\omega t} G_\omega(\mathbf{r}) \qquad &= \delta(\mathbf{r})\delta(t) \\ = \int \frac{\mathrm{d}\omega}{2\pi} \left(- \underbrace{\frac{\omega^2}{c^2}}_{=k^2} - \nabla^2 \right) e^{-i\omega t} G_\omega(\mathbf{r}) \qquad &= \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} \delta(\mathbf{r})\end{aligned}$$

$$\Rightarrow -\left(\nabla^2 + k^2\right) G_\omega(\mathbf{r}) = \delta(\mathbf{r}),$$

where $\nabla^2 + k^2$ is known as the *Helmholtz operator*. As expected, this solves to

$$G_\omega(\mathbf{r}) = \frac{e^{ikr}}{4\pi r} = \frac{e^{i\frac{\omega}{c}r}}{4\pi r}.$$

3.6.2 Retarded Green's Functions

Solving for the original Green's function by inverse Fourier transforming, then

$$\begin{aligned} G(\mathbf{r},t) &= \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} G_\omega(\mathbf{r}) \\ &= \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} \frac{e^{i\frac{\omega}{c}r}}{4\pi r} \\ &= \frac{1}{4\pi r} \underbrace{\int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega\left(t-\frac{r}{c}\right)}}_{\substack{\text{Fourier representation} \\ \text{of } \delta\left(t-\frac{r}{c}\right) \equiv \delta(t_{\mathrm{ret}})}} \\ &= \frac{\delta(t_{\mathrm{ret}})}{4\pi r}, \end{aligned}$$

which is called the *retarded* Green's function. One should note that when $t < 0$ the delta function can never be non-zero and so G falls to zero, thus preserving causality. This result came in the choice of outgoing waves as a solution to the scattering problem.

3.6.3 Retarded Potentials

Using the retarded Green's function the retarded scalar potential for a charge distribution is thus

$$\begin{aligned} \Phi(\mathbf{r},t) &= \Phi_0(\mathbf{r},t) + \int \mathrm{d}^3\mathbf{r}' \int \mathrm{d}t' \, \frac{\delta\left(t - t' - \left|\frac{\mathbf{r}-\mathbf{r}'}{c}\right|\right)}{4\pi|\mathbf{r}-\mathbf{r}'|} \frac{\rho(\mathbf{r},\mathbf{r}')}{\epsilon_0} \\ &= \Phi_0(\mathbf{r},t) + \frac{1}{4\pi\epsilon_0} \int \mathrm{d}^3\mathbf{r}' \, \frac{\rho\left(t' - \left|\frac{\mathbf{r}-\mathbf{r}'}{c}\right|, \mathbf{r}'\right)}{|\mathbf{r}-\mathbf{r}'|}, \end{aligned}$$

where c is the speed at which a signal must be emitted from $\mathbf{r}'$ in order to be received by an observer at $\mathbf{r}$ at a time t.

An alternative method of solving this by Fourier transforms is to transform

both temporal and spatial coordinates, i.e.

$$\delta(t)\delta(\mathbf{r}) = \int \frac{\mathrm{d}\omega}{2\pi} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$
$$G(t,\mathbf{r}) = \int \frac{\mathrm{d}\omega}{2\pi} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \tilde{G}(\omega,\mathbf{k})$$
$$\tilde{G}(\omega,\mathbf{k}) = \int \mathrm{d}t \int \mathrm{d}^3\mathbf{r}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} G(t,\mathbf{r}).$$

The wave equation for the Green's function is therefore

$$\Box G = \delta(t)\delta(\mathbf{r})$$
$$= \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right) G(t,\mathbf{r}) = \int \frac{\mathrm{d}\omega}{2\pi} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$

$$= \int \frac{\mathrm{d}\omega}{2\pi} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \left(-\frac{\omega^2}{c^2} + k^2\right) \tilde{G}(\omega,\mathbf{k}).$$

Comparing the integrands, the transformed Green's function is then

$$\tilde{G}(\omega,\mathbf{k}) \left(-\frac{\omega^2}{c^2} + k^2\right) = 1$$
$$\Rightarrow \tilde{G} = -\frac{c^2}{\omega^2 - c^2k^2}.$$

Taking the inverse Fourier transform, the original Green's function is thus

$$G(t,\mathbf{r}) = -c^2 \int \frac{\mathrm{d}\omega}{2\pi} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}}{\omega^2 - c^2k^2}.$$

Chapter 4

Integral Equations

4.1 Classification

An integral equation is one for which an unknown function appears under an integral sign, i.e. an equation of the form

$$\Theta f(x) = g(x) + \lambda \int_a^b K(x,y) f(y)\,\mathrm{d}y,$$

where Θ can be equal to 1 or 0, $g(x)$ is usually a given function, λ is a constant - possibly taking part as an eigenvalue - K is the **kernel** and $f(y)$ is the function to be found. It is usual to make a distinction between the following cases:

1 If $g = 0$ the equation is **homogeneous**

2 If $K(x,y) > 0$ for $y > x$ $(b \to \infty)$, it is the **Volterra equation**

3 a. If $\Theta = 0$ it is a **Fredholm equation of the first kind**

b. If $\Theta = 1$ it is a **Fredholm equation of the second kind**.

These cases are not mutually exclusive, i.e. a Volterra equation can also be regarded as a Fredholm equation with $b = \infty$ and having a special kind of kernel.

A number of integral equations are equivalent to differential equations, i.e.

- $Lg = f(x) \Leftrightarrow g(x) = \int_a^b G(x,y) f(y)\,\mathrm{d}y$
  - Fredholm equation of the first kind ($\Theta = 0$).
- $Lg = \lambda g \Leftrightarrow g(x) = \lambda \int_a^b G(x,y) g(y)\,\mathrm{d}y$
  - Homogeneous ($g(x) = 0$) Fredholm equation of the second kind ($\Theta = 1$).
- $\frac{\mathrm{d}P}{\mathrm{d}t} = -\alpha(t)P(t) \Leftrightarrow P(t) = \underbrace{P(0)}_{=1} - \int_0^t \alpha(t')P(t')\,\mathrm{d}t'$;

  $\alpha \geq 0$, $P(t=0) = 1$
  - This is a Volterra equation.
- Solution to quantum mechanical scattering (Lippmann-Schwinger):

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{2m}{\hbar^2} \int G_+(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\Psi(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}'$$

The latter three of these examples demonstrate cases in which integral equations are preferable to differential equations.

4.1.1 First Kind

4.1.2 Second Kind

4.2 Fredholm and Volterra Equations

4.3 Simple Cases

There are also numerous integral equations which are *not* equivalent to differential equations. For example, consider an astrophysicist taking a photograph of a galaxy cluster or a globular cluster of stars, then wanting to deduce the three-dimensional distribution of the stars from the two-dimensional photograph. The 2D photo has a distribution $\sigma(R)$ (where $R = \sqrt{x^2 + y^2}$), as shown in Figure 4.1, which is essentially the 3D distribution projected onto the x-y plane. The number of stars in an area $\delta x\,\delta y$ is thus $\sigma(R)\,\delta x\,\delta y$,

where the 2D density function is given by the 3D density function $\rho(t)$ (where $t = \sqrt{R^2 + z^2}$) integrated over its third dimension, i.e.

$$\sigma(R) = \int_{-\infty}^{\infty} \rho \, \mathrm{d}z.$$

This integral can be split into two integrals, i.e. $\int_{-\infty}^{\infty} \to \int_{-\infty}^{0} + \int_{0}^{\infty}$, and since the distribution is independent of direction these separated integrals must be equal, thus $\int_{-\infty}^{\infty} \to 2\int_{0}^{\infty}$. The distribution is now of the integral equation form ($\Theta f(x) = g(x) + \lambda \int_a^b K(x,y) f(y) \, \mathrm{d}y$):

$$\begin{aligned}
\sigma(R) &= 2\int_0^{\infty} \rho(t) \, \mathrm{d}z \\
&= 2\int_R^{\infty} \rho(t) \frac{\mathrm{d}z}{\mathrm{d}t} \, \mathrm{d}t \\
&= 2\int_R^{\infty} \frac{t\rho(t)}{\sqrt{t^2 - R^2}} \, \mathrm{d}t.
\end{aligned}$$

The independent variable R now appears as one of the limits of the integral, thus it is a Volterra equation, i.e. $f(t) = \int_a^t K(t,s) x(s) \, \mathrm{d}s$.
Considering instead low pressure gas flowing through a narrow tube, such that the mean free path is much greater than the width of the tube so that the rate of flow is only limited by the collisions between the molecules and walls. When a particle hits the tube wall it sticks and is reemitted, then leaving in a random direction at which point it may then be reabsorbed and remitted in another collision. The tube is of length L and aligned along the x-axis, as shown in Figure 4.2, where particles start from $x < 0$ at rate $s(t)$. Eventually each particle will leave the tube. Over a small length Δx the rate of arrival is given by $s(x)\Delta x$, and that of reemission is taken to be $V(x)\Delta x$. For equilibrium the input-output must be in a steady state, $S(x)\Delta x$, plus the additional rate of arrival from other portions of the tube's surface, i.e. satisfies

$$V(x)\Delta x = S(x)\Delta x + \int_0^L \left(P\left(|x - x'|\right) \Delta x \right) V(x') \, \mathrm{d}x'.$$

This is therefore a Fredholm equation of the second kind, i.e.

$$\phi(t) = f(t) + \lambda \int_a^b K(t,s)\phi(s) \, \mathrm{d}s.$$

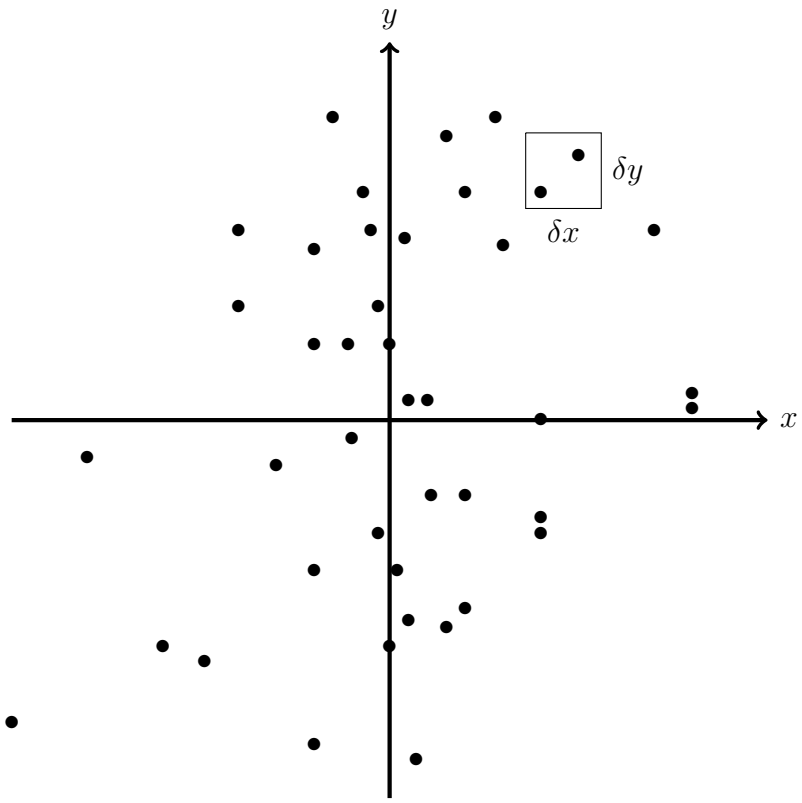

Figure 4.1: Representation of 2D photograph of galaxy or globular cluster of stars.

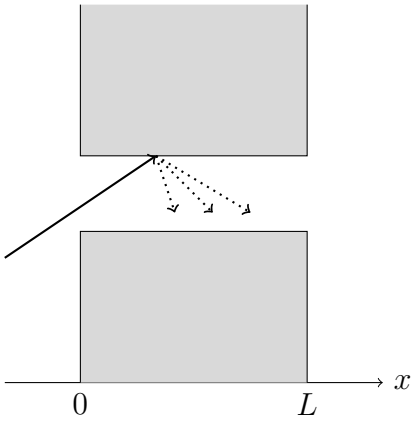

Figure 4.2: Schematic of a low pressure gas tavelling through a thin tube.

The possibility of analytically solving an integral equation depends on its form. It is useful to find how a function behaves as a parameter gets very large or very small. Methods for solving integral equations include (but are not limited to)

1. Degenerate (separable) kernels

2. Displacement (or convolution) kernels; limits of integration $[-\infty, \infty]$

3. Displacement kernel, limits of integration $[0, x]$

4. Reduction to a differential equation

4.3.1 Degenerate Kernels

Definition 4.1: Degenerate Kernel

A kernel is said to **degenerate** or **separable** if it can be written in the form

$$K(x, y) = \sum_{i=1}^{N} \phi_i(x)\psi_i(y),$$

where N is finite and the functions ϕ_i and ψ_i are linearly independent but not necessarily orthogonal or normalised to unity.

The integral equation corresponding to a degenerate kernel can always be reduced to a set of linear algebraic equations.

Theorem 4.1

$$
\begin{aligned}
f(x) &= g(x) + \int_a^b K(x,y) f(y)\,\mathrm{d}y \\
&= g(x) + \int_a^b \sum_{j=1}^{N} \phi_j(x)\psi_j(y) f(y)\,\mathrm{d}y \\
&= g(x) + \sum_{j=1}^{N} \phi_j(x) \underbrace{\int_a^b \psi_j(y) f(y)\,\mathrm{d}y}_{\text{Definition of dot product}} \\
&= g(x) + \sum_{j=1}^{N} \phi_j(x) \cdot (\psi_j, f) \\
\therefore (\psi_i, f) &= (\psi_i, g) + \sum_{j=1}^{N} (\psi_i, \phi_j)(\psi_j, f) \\
\Rightarrow f_i &= g_i + \sum_{j=1}^{N} K_{ij} f_j \text{ or} \\
\mathbf{f} &= \mathbf{g} + K\mathbf{f},
\end{aligned}
$$

where K is the kernel matrix.

Example 4.1

Consider the integral equation

$$f(x) = x + \int_0^1 (1 + xy) f(y)\,\mathrm{d}y.$$

The parenthesised term is separable as it can be written in the form

$f(x) = A + Bx$, thus the equation is of the form

$$\begin{aligned} A + Bx &= x + \int_0^1 (1 + xy)\,(A + By)\,\mathrm{d}y \\ &= x + \int_0^1 \left(A + Axy + By + Bxy^2\right)\,\mathrm{d}y \\ &= x + \left[Ay + \frac{1}{2}Axy^2 + \frac{1}{2}By^2 + \frac{1}{3}Bxy^3\right]_0^1 \\ &= x + A + \frac{1}{2}Ax + \frac{1}{2}B + \frac{1}{3}Bx. \end{aligned}$$

Equating coefficients of x^0 and x^1 gives

$$\begin{aligned} x^0\text{:} \quad & A = A + \tfrac{1}{2}B && \to B = 0 \\ x^1\text{:} \quad & B = 1 + \tfrac{1}{2}A + \tfrac{1}{3}B && \to A = -2 \\ & \Rightarrow f(x) = -2. \end{aligned}$$

Example 4.2

Consider the eigenvalue problem

$$f(x) = \lambda \int_0^{2\pi} \cos(x - y) f(y)\,\mathrm{d}y,$$

the kernel of which is thus $K(x, y) = \cos(x - y)$. This is separable as

$$K(x, y) = \cos(x - y) = \cos(x)\cos(y) - \sin(x)\sin(y).$$

By inspection, $f(x) = A\cos(x) + B\sin(x)$, hence

$$\begin{aligned}
A\cos(x) + B\sin(x) &= \lambda \int_0^{2\pi} \big(\cos(x)\cos(y) - \sin(x)\sin(y)\big)\big(A\cos(y) + B\sin(y)\big)\,\mathrm{d}y \\
&= \lambda \left[A\cos(x) \int_0^{2\pi} \cos^2(y)\,\mathrm{d}y - A\sin(x) \int_0^{2\pi} \sin(y)\cos(y)\,\mathrm{d}y - B\cos \right. \\
&= \lambda \left(A\cos(x) \left[\frac{1}{2}\big(y + \sin(y)\cos(y)\big) \right]_0^{2\pi} - A\sin(x)\cdot 0 - B\cos(x)\cdot 0 \right. \\
&= \lambda \big(A\pi\cos(x) + B\pi\sin(x)\big) \\
\Rightarrow A\cos(x) + B\sin(x) &= \lambda\pi\big(A\cos(x) + B\sin(x)\big).
\end{aligned}$$

If $\lambda \neq \frac{1}{\pi}$ then the only other solution is $A = B = 0$, all other solutions must have $\lambda = \frac{1}{\pi}$.

4.3.2 Displacement Kernels

Equations Soluble by Fourier Transforms

A kernel of the form $K(x-y)$ is said to be a **displacement** or **convolution** kernel. If the limits are $[-\infty, \infty]$ then the equation may be solved by a Fourier transform. The Fredholm equation of the second kind utilises a convolution kernel, i.e.

$$f(x) = g(x) + \lambda \int_{-\infty}^{\infty} K(x-y) f(y)\,\mathrm{d}y.$$

The syntax of Fourier transform used in this document is given by

$$\begin{aligned}
\tilde{f}(q) &= \int_{-\infty}^{\infty} f(x) e^{-iqx}\,\mathrm{d}x \\
f(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(q) e^{iqx}\,\mathrm{d}q.
\end{aligned}$$

Taking the Fourier transform of the Fredholm equation then gives

$$\begin{aligned}\mathcal{F}\left(f(x)\right) &= \mathcal{F}\left(g(x) + \lambda \int_{-\infty}^{\infty} K(x-y) f(y)\,\mathrm{d}y\right) \\ \rightarrow \tilde{f}(q) &= \tilde{g}(q) + \lambda \tilde{K}(q), \tilde{f}(q) \\ \Rightarrow \tilde{f}(q) &= \frac{\tilde{g}(q)}{1 - \lambda \tilde{K}(q)}.\end{aligned}$$

This solution is unique provided $1 - \lambda \tilde{K}(q) \neq 0$. In order to obtain $f(x)$ this solution must be inverted.

Example 4.3

$$\begin{aligned} g(x) = K(x) &= e^{-\alpha|x|} \qquad \alpha > 0 \\ \Rightarrow \tilde{g}(k) = \tilde{K}(k) &= \int_{-\infty}^{\infty} e^{-\alpha|x|} e^{-ikx}\,\mathrm{d}x \\ &= \int_{0}^{\infty} e^{-(\alpha+ik)|x|}\,\mathrm{d}x + \int_{-\infty}^{0} e^{-(ik-\alpha)|x|}\,\mathrm{d}x \\ &= \frac{1}{\alpha + ik} + \frac{1}{\alpha - ik} \\ &= \frac{2\alpha}{\alpha^2 + k^2}.\end{aligned}$$

The transformed solution $\tilde{f}(k)$ is then

$$\begin{aligned}\tilde{f}(k) &= \frac{\left(\frac{2\alpha}{\alpha^2+k^2}\right)}{1 - \lambda\left(\frac{2\alpha}{\alpha^2+k^2}\right)} \\ &= \frac{2\alpha}{\alpha^2 - 2\lambda\alpha + k^2}.\end{aligned}$$

The denominator is non-zero and is solution is unique if $\alpha^2 - 2\lambda\alpha > 0$, which requires $\lambda < \frac{\alpha}{2}$. Writing this as $\beta^2 \equiv \alpha^2 - 2\lambda\alpha$, inverse Fourier transforming the previous solution gives the final solution by

$$\begin{aligned}\tilde{f}(k) = \frac{2\alpha}{\beta^2 + k^2} &= \frac{\alpha}{\beta}\left(\frac{2\beta}{\beta^2 + k^2}\right) = \frac{\alpha}{\beta}\mathcal{F}\left(e^{-\beta|x|}\right) \\ \Rightarrow f(x) &= \frac{\alpha}{\beta} e^{-\beta|x|}.\end{aligned}$$

Equations Soluble by Laplace Transforms

If the kernel is of displacement form ($K(x-y)$) and the limits of integration are $[0, x]$, as in the Volterra equation, then the integral has the form of convolution that appears in Laplace transform theory. The Laplace transform $\hat{f}(s)$ is defined by

$$\hat{f}(s) = \int_0^\infty f(x)e^{-sx}\,\mathrm{d}x.$$

Theorem 4.2: Convolution theorem of Laplace transforms

Taking the convolution of a displacement kernel $K(x-y)$ with some function of the integrand parameter $f(y)$, the Laplace transform $\mathcal{L}$ is given by

$$\begin{aligned}
\mathcal{L}\left(\int_0^x K(x-y)f(y)\,\mathrm{d}y\right) &= \int_0^\infty e^{-sx}\int_0^x K(x-y)f(y)\,\mathrm{d}y\mathrm{d}x \\
&= \int_0^\infty \int_y^\infty e^{-sx}K(x-y)f(y)\,\mathrm{d}x\,\mathrm{d}y \\
&= \int_0^\infty \underbrace{\left(\int_y^\infty e^{-s(x-y)}K(x-y)\,\mathrm{d}x\right)}_{\equiv \hat{K}(s)} e^{-sy}f(y)\,\mathrm{d}y \\
&= \hat{K}(s)\underbrace{\int_0^\infty e^{-sy}f(y)\,\mathrm{d}y}_{\equiv \hat{f}(s)} \\
&= \hat{K}(s)\hat{f}(s).
\end{aligned}$$

The Volterra equation is given by

$$f(x) = g(x) + \lambda\int_0^x K(x-y)f(y)\,\mathrm{d}y.$$

Taking the Laplace transform of this then gives

$$\begin{aligned}\hat{f}(s) &= \hat{g}(s) + \lambda \hat{K}(s)\hat{f}(s) \\ \Rightarrow \hat{f}(s) &= \frac{\hat{g}(s)}{1+\lambda\hat{K}(s)},\end{aligned}$$

which is reminiscent of the solution to the Fourier transformed equations. As before, in order to obtain $f(x)$ one must inverse transform, this time using the Bromwich integral, given by

$$f(x) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{zx}\hat{f}(z)\,\mathrm{d}z.$$

Example 4.4

Consider the integral equation

$$f(x) = x - \int_0^x (x-y)f(y)\,\mathrm{d}y.$$

Comparing to the Volterra equation $f(x) = g(x) + \int_0^x K(x-y)f(y)\,\mathrm{d}y$, one sees that $g(x) = x$ and $K(x-y) = -(x-y)$, thus

$$\begin{aligned}\hat{g}(s) &= \int_0^\infty xe^{-sx}\,\mathrm{d}x, \\ \hat{K}(x-y) &= \int_0^\infty (-x+y)e^{-sx}\,\mathrm{d}x.\end{aligned}$$

In general $\mathcal{L}(t^n) = \frac{n!}{s^{n+1}}$, thus these become

$$\begin{aligned}\hat{g}(s) &= \frac{1!}{s^{1+1}} = \frac{1}{s^2} \\ \hat{K}(x-y) &= \int_0^\infty -xe^{-sx} + \int_0^\infty ye^{-sx}\,\mathrm{d}x \\ &= -\frac{1}{s^2} + 0,\end{aligned}$$

and hence the solution is given by

$$\begin{aligned}
\hat{f}(s) &= \frac{1}{s^2} - \frac{1}{s^2}\hat{f}(s) \\
\rightarrow \hat{f}(s) &= \frac{1}{s^2+1} \\
&= \frac{\frac{1}{s-i} - \frac{1}{s+i}}{2i} \\
&= \frac{\mathcal{L}(e^{ix}) - \mathcal{L}(e^{-ix})}{2i} \\
&= \mathcal{L}\left(\frac{e^{ix} - e^{-ix}}{2i}\right) \\
&= \mathcal{L}(\sin(x)) \\
\Rightarrow f(x) &= \sin(x).
\end{aligned}$$

4.3.3 Problems Reducible to a Differential Equation

It is often useful to reduce integral equations to ordinary differential equations, however this is not always possible and so one must look for clues as to whether it is possible, e.g. the kernel becomes simpler when differentiated (polynomial) or the kernel moves into itself after being differentiated enough times (trigonometric functions, exponentials etc). A useful result of integration is the **fundamental theorem of calculus**:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\int_0^x h(x,y)\,\mathrm{d}y\right) = h(x,x) + \int_0^x \frac{\partial h}{\partial x}\,\mathrm{d}y. \tag{4.1}$$

Theorem 4.3

Example 4.5

Consider the same integral equation as Example 4.4:

$$f(x) = x - \int_0^\infty (x-y)f(y)\,\mathrm{d}y.$$

The differentials of this are then

$$\frac{\mathrm{d}f}{\mathrm{d}x} = f'(x) = 1 - (x-x)f(x) - \int_0^x f(y)\,\mathrm{d}y = 1 - \int_0^x f(y)\,\mathrm{d}y$$
$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} = f''(x) = -f(x).$$

This has a general solution

$$f(x) = A\cos(x) + B\sin(x),$$

and since $f(0) = 0 \to A = 0$ and $f'(0) = 1 \to B = 1$, then

$$f(x) = \sin(x),$$

as before.

Example 4.6

Now consider the integral equation

$$f(x) = x + \int_0^x xyf(y)\,\mathrm{d}y.$$

Using a rearrangement of this ($\int_0^x yf(y) = \frac{f(x)-x}{x}$) and Equation (4.1) gives the first derivative as

$$\begin{aligned}\frac{\mathrm{d}f}{\mathrm{d}x} = f'(x) &= 1 + xxf(x) + \int_0^x yf(y)\,\mathrm{d}y \\ &= 1 + x^2 f(x) + \frac{f(x)-x}{x} \\ &= x^2 f(x) + \frac{f(x)}{x}.\end{aligned}$$

Solving this first order differential equation then gives the solution as

$$\begin{aligned}\frac{1}{f}\,\mathrm{d}f &= \left(x^2 + \frac{1}{x}\right)\,\mathrm{d}x \\ \ln(f) &= \frac{1}{3}x^3 + \ln(x) + \text{const.} \\ \Rightarrow f(x) &= Axe^{\frac{1}{3}x^3}.\end{aligned}$$

Using the fact that $f'(0) = 1 \rightarrow A = 1$, the final solution is thus

$$\Rightarrow f(x) = xe^{\frac{1}{3}x^3}.$$

Example 4.7

Consider the integral equation

$$f(x) = \lambda \int_0^{1-x} f(y)\,\mathrm{d}y = \lambda f(1-x).$$

This is of the form $\lambda \int_0^1 K(x,y)f(y)\,\mathrm{d}y$, which has kernel values $K = 0$ for $y > 1 - x, y < 0$ and $K = 1$ for $y < 1 - x, y > 0$. The derivatives of this are then

$$\begin{aligned}\tfrac{\mathrm{d}f}{\mathrm{d}x} &= f'(x) = \lambda(-1)f(1-x) = -\lambda\left(\lambda\int_0^x f(y)\,\mathrm{d}y\right) \\ \tfrac{\mathrm{d}^2f}{\mathrm{d}x^2} &= f''(x) = -\lambda^2 f(x).\end{aligned}$$

The general solution to this is

$$f(x) = A\sin(\lambda x) + B\cos(\lambda x).$$

It is known that $f(1) = 0$ and $f'(0) = -\lambda f(1) = 0$, thus $A = 0$. Also $f'(1) = -\lambda f(0)$, hence

$$\begin{aligned}-\lambda\sin(\lambda) &= -\lambda \\ \rightarrow \sin(\lambda) &= 1 \\ \Rightarrow \lambda &= \frac{\pi}{2} + 2n\pi. \qquad\qquad n = 0, \pm1, \pm2\ldots\end{aligned}$$

Analytic solutions are not usually possible, however numeric methods are often easy and well-behaved. If the kernel is separable (or can be approximated as a separable kernel) the integral equation reduces to a matrix equation. For other cases discretisation is usually a good strategy, e.g. a Fredholm equation of the second kind

$$f(x) = g(x) + \int_a^b K(x, y) f(y)\,\mathrm{d}y$$

can be split into N parts and evaluated at these discrete points, i.e. $x_j = a + \frac{j(b-a)}{N-1}$, $f(x_j) = f_j$ and $g(x_j) = g_j$, giving

$$\begin{aligned} f_i &= g(x_i) + \int_a^b K(x_i, y) f(y)\,\mathrm{d}y \\ &\approx g(x_i) + \left(\frac{b-a}{N-1}\right) \sum_{j=0}^{N-1} K(x_i, y_j) f(x_j). \end{aligned}$$

Defining $K_{ij} \equiv \frac{b-a}{N-1} K(x_i, y_j)$, then the solution becomes

$$\begin{aligned} f_i &\approx g_i + \sum_j K_{ij} f_j \\ \mathbf{f} &\approx \mathbf{g} + K\mathbf{f}. \end{aligned}$$

4.4 Neumann Series Solution (Perturbation Theory)

Sometimes the parameter λ may be considered as small, so one might hope to obtain a solution as a series of powers of λ, e.g. the Born approximation for scattering. Starting from the general integral equation form

$$f(x) = g(x) + \lambda \int K(x, y) f(y)\,\mathrm{d}y,$$

integrating $f(y)$ introduces a new function $f(z)$, which when integrated introduces another function $f(a)$, ad infinitum, i.e.

$$\begin{aligned} f(x) &= g(x) + \lambda \int K(x,y) f(y)\,\mathrm{d}y \\ &= g(x) + \lambda \int K(x,y) \left(g(y) + \lambda \int K(y,z) f(z)\,\mathrm{d}z \right) \mathrm{d}y \\ &= g(x) + \lambda \int K(x,y) \left(g(y) + \lambda \int K(y,z) \left(g(z) + \lambda \int K(z,a) f(a)\,\mathrm{d}a \right) \mathrm{d}z \right) \mathrm{d}y \end{aligned}$$

etc.

By generalising this to subscripts the solution to $f(x)$ becomes an infinite series, i.e.

$$f(x) = g(x) + \lambda \int K(x,y_1) g(y_1)\,\mathrm{d}y_1 + \lambda^2 \int K(y_1,y_2) \int K(y_2,y_3) g(y_2)\,\mathrm{d}y_1\,\mathrm{d}y_2 + \ldots$$

The question now is whether this sequence converges or diverges.

Assuming that g and K are bounded, i.e. $|g| \leq g_{\max}$ and $|K| \leq K_{\max}$, and the ranges of the integrations are finite, one may obtain the upper bound on each term by replacing g and K by their maximal values, i.e.

$$\begin{aligned} |f(x)| \leq g_{\max} &+ |\lambda| K_{\max} g_{\max} \int \mathrm{d}y_1 \\ &+ |\lambda|^2 K_{\max}^2 g_{\max} \iint \mathrm{d}y_2\,\mathrm{d}y_1 \\ &+ |\lambda|^3 K_{\max}^3 g_{\max} \iiint \mathrm{d}y_3\,\mathrm{d}y_2\,\mathrm{d}y_1 \\ &\vdots \\ &+ |\lambda|^m K_{\max}^m g_{\max} \iint \ldots \int \mathrm{d}y_m\,\mathrm{d}y_{m-1} \ldots \mathrm{d}y_1. \end{aligned}$$

The limits thus far have been left undefined but are important. There is an interesting difference when the Neumann series is applied to the Volterra equation as compared to a general Fredholm equation.

4.4.1 The Volterra Equation

Suppose that the lower limit of integration is zero with a generalised upper limit, i.e.

$$\begin{aligned}
\int \mathrm{d}y_1 &= \int_0^x \mathrm{d}y_1 = x \\
\iint \mathrm{d}y_1\,\mathrm{d}y_2 &= \int_0^x \int_0^{y_2} \mathrm{d}y_1\,\mathrm{d}y_2 = \int_0^x y_2\,\mathrm{d}y_2 = \frac{x^2}{2} \\
\iiint \mathrm{d}y_1\,\mathrm{d}y_2\,\mathrm{d}y_3 &= \int_0^x \int_0^{y_3} \int_0^{y_2} \mathrm{d}y_1\,\mathrm{d}y_2\,\mathrm{d}y_3 = \int_0^x \frac{y_3^2}{2}\,\mathrm{d}y_3 = \frac{x^3}{6} \\
&\vdots \\
\iint \ldots \int \mathrm{d}y_1 \ldots \mathrm{d}y_n &= \frac{x^n}{n!}.
\end{aligned}$$

Using these in the Neumann series solution, $|f(x)|$ is thus

$$\begin{aligned}
|f(x)| &\leq g_{\max} + \sum_{m=1}^{\infty} \frac{|\lambda|^m K_{\max}^m x^m}{m!} g_{\max} \\
&\leq \left(\sum_{m=0}^{\infty} \frac{|\lambda|^m K_{\max}^m x^m}{m!} \right) g_{\max} \\
&\leq e^{|\lambda| K_{\max} x} g_{\max}.
\end{aligned}$$

Therefore the Neumann series always converges for a Volterra equation with bounded g and K.

4.4.2 Fredholm Series

Taking general limits of a and b, the Neumann series become

$$\begin{aligned}
\int \mathrm{d}y_1 &= \int_a^b \mathrm{d}y_1 = (b-a) \\
\iint \mathrm{d}y_1\,\mathrm{d}y_2 &= \int_a^b \int_a^b \mathrm{d}y_1\,\mathrm{d}y_2 = (b-a)^2 \\
&\vdots \\
\iint \ldots \int \mathrm{d}y_1\,\mathrm{d}y_2 \ldots \mathrm{d}y_m &= \int_a^b \int_a^b \ldots \int_a^b \mathrm{d}y_1\,\mathrm{d}y_2 \ldots \mathrm{d}y_m = (b-a)^m.
\end{aligned}$$

As such, $|f(x)|$ is given by

$$|f(x)| \leq g_{\max} + \sum_{m=1}^{\infty} |\lambda|^m K_{\max}^m (b-a)^m g_{\max} = \sum_{m=0}^{\infty} |\lambda|^m K_{\max}^m (b-a)^m g_{\max}.$$

This is simply a geometric series, thus it converges if the terms in the sum are less than one, i.e.

$$\begin{aligned}
&|\lambda| K_{\max}(b-a) < 1 \\
&\qquad \Rightarrow |\lambda| < \frac{1}{K_{\max}(b-a)}.
\end{aligned}$$

If this condition is violated then the series may or may not converge - it depends on the form of the kernel. If a solution to the integral equation is of the form

$$f(x) = g(x) - \lambda \int R(x,y;\lambda) g(y)\,\mathrm{d}y$$

then it defines the so-called **resolvent kernel**, $R(x,y;\lambda)$.

Consider the Volterra equation

$$f(x) = g(x) + \lambda \int_0^x K(x,y) f(y)\,\mathrm{d}y$$

and perform a Neumann solution

$$f(x) = g(x) + \lambda \int_0^x K(x,y)g(y)\,\mathrm{d}y + \lambda \int_0^x K(x,y)\left(\lambda \int_0^y K(y,z)f(z)\,\mathrm{d}z\right)\,\mathrm{d}y$$

$$= g(x) + \lambda \int_0^x K(x,y)g(y)\,\mathrm{d}y + \lambda \int_0^x \left(\lambda \int_z^x K(x,y)K(y,z)\,\mathrm{d}y\right) f(z)\,\mathrm{d}z$$

$$= g(x) + \lambda \int_0^x K_1(x,y)g(y)\,\mathrm{d}y + \lambda \int_0^x K_2(x,z)f(z)\,\mathrm{d}z,$$

where $K_1(x,y) = K(x,y)$ and the "iterated" kernel $K_2(x,z) = \int_z^x K(x,y)K(y,z)\,\mathrm{d}y$. One may continue these expansions and form a general summation, i.e.

$$f(x) = g(x) + \sum_{m=1}^{N-1} \lambda^m \int_0^x K_m(x,y)g(y)\,\mathrm{d}y + \lambda^N \int_0^x K_N(x,y)f(y)\,\mathrm{d}y,$$

where

$$\begin{aligned}\int K_n(x,y)g(y)\,\mathrm{d}y &= \int K(x,z)\int K_{n-1}(z,y)g(y)\,\mathrm{d}y\,\mathrm{d}z \\ &= \iint K(x,z)K_{n-1}(z,y)\,\mathrm{d}z g(y)\,\mathrm{d}y \\ \Rightarrow K_n(x,y) &= \int K(x,z)K_{n-1}(z,y)\,\mathrm{d}z.\end{aligned}$$

In terms of K_n, the resolvent kernel is given by

$$\begin{aligned}-\lambda R(x,y;\lambda) &\equiv \sum_{m=1}^{\infty} \lambda^m K_m(x,y) \\ \Rightarrow R(x,y;\lambda) &= -\sum_{m=1}^{\infty} \lambda^{m-1} K_m(x,y),\end{aligned}$$

which holds if the series converges.

Example 4.8

Consider the integral equation

$$f(x) = g(x) + \lambda \int_0^1 xyf(y)\,\mathrm{d}y.$$

Firstly one finds the resolvent for any $g(x)$. The iterated kernels are given by

$$\begin{aligned}
K_1(x,y) &= K(x,y) = xy;\\
K_2(x,y) &= \int_0^1 K(x,z)K_1(z,y)\,\mathrm{d}z\\
&= \int_0^1 (xz)(zy)\,\mathrm{d}z\\
&= \frac{1}{3}xy;\\
K_3 &= \int_0^1 K(x,z)K_2(z,y)\,\mathrm{d}z\\
&= \int_0^1 (xz)\left(\frac{1}{3}zy\right)\,\mathrm{d}z\\
&= \frac{1}{3^2}xy;\\
&\dots\\
K_m &= \frac{1}{3^{m-1}}xy.
\end{aligned}$$

The resolvent kernel is then given by

$$\begin{aligned}
R(x,y;\lambda) &= -\sum_{m=1}^{\infty} \lambda^{m-1}K_m(x,y)\\
&= -\sum_{m=1}^{\infty} \lambda^{m-1}\left(\frac{1}{3^{m-1}}xy\right)\\
&= -\sum_{m=1}^{\infty} \left(\frac{\lambda}{3}\right)^{m-1} xy.
\end{aligned}$$

This is a geometric series with a ratio $r = \frac{\lambda}{3}$, thus by the relation $\sum_{m=0}^{\infty} ar^m = \frac{a}{1-r}$, the resolvent kernel is

$$R(x, y; \lambda) = -\frac{xy}{1 - \frac{\lambda}{3}}.$$

Example 4.9

Now instead consider the general integral equation $f(x) = g(x) + \lambda \int_0^x K(x, y) f(y)\,\mathrm{d}y$ with a kernel given by $K(x, y) = \left(\frac{x}{y}\right)^{\frac{1}{2}}$. This

takes the form of a Volterra equation, thus the integrated kernels are

$$
\begin{aligned}
K_2(x,y) &= \int_y^x K(x,z)K_1(z,y)\,\mathrm{d}z \\
&= \int_y^x \left(\frac{x}{z}\right)^{\frac{1}{2}} \left(\frac{z}{y}\right)^{\frac{1}{2}} \mathrm{d}z \\
&= \int_y^x \left(\frac{x}{y}\right)^{\frac{1}{2}} \mathrm{d}z \\
&= \left(\frac{x}{y}\right)^{\frac{1}{2}} (x-y); \\
K_3(x,y) &= \int_y^x K(x,z)K_2(z,y)\,\mathrm{d}z \\
&= \int_y^x \left(\frac{x}{z}\right)^{\frac{1}{2}} \left(\frac{z}{y}\right)^{\frac{1}{2}} (z-y)\,\mathrm{d}z \\
&= \int_y^x \left(\frac{x}{y}\right)^{\frac{1}{2}} (z-y)\,\mathrm{d}z \\
&= \left(\frac{x}{y}\right)^{\frac{1}{2}} \left[\frac{1}{2}(z-y)^2\right]_y^x \\
&= \left(\frac{x}{y}\right)^{\frac{1}{2}} \cdot \frac{1}{2}(x-y)^2; \\
&\vdots \\
K_m(x,y) &= \left(\frac{x}{y}\right)^{\frac{1}{2}} \frac{(x-y)^{m-1}}{(m-1)!}.
\end{aligned}
$$

The resolvent kernel is then

$$\begin{aligned} R(x,y;\lambda) &= -\sum_{m=1}^{\infty} \lambda^{m-1} K_m(x,y) \\ &= -\sum_{m=1}^{\infty} \lambda^{m-1} \left(\frac{x}{y}\right)^{\frac{1}{2}} \frac{(x-y)^{m-1}}{(m-1)!} \\ &= -\left(\frac{x}{y}\right)^{\frac{1}{2}} e^{\lambda(x-y)}, \end{aligned}$$

and so the final solution is given by

$$f(x) = g(x) + \lambda \int_0^x \left(\frac{x}{y}\right)^{\frac{1}{2}} e^{\lambda(x-y)} g(y)\,\mathrm{d}y.$$

4.5 Summary

4.6 Hilbert-Schmidt Theory

Hilbert-Schmidt theory offers a general approach to Hermitian kernels, i.e. those that satisfy

$$K(x,y) = K(y,x)^*.$$

The theory is based on the sets of eigenfunctions $\{u_i\}$ and eigenvalues $\{\lambda_i\}$ of the kernel, which are related by

$$u_i(x) = \lambda_i \int_a^b K(x,y) u_i(y)\,\mathrm{d}y,$$

where K is required to be bounded (defined over a finite range). The main result of Hilbert-Schmidt theory is that under certain circumstances these eigenfunctions can be proved to exist and can be used as a basis to expand any "source representative" function $phi(x)$, which is to say that for a function which can be written in terms of a "source" ρ as

$$\phi(x) = \int_a^b K(x,y)\rho(y)\,\mathrm{d}y,$$

Table 4.1: Methods for solving integral equations corresponding to integral forms.

Condition	**Method**	**Description**
$K(x,y) = \sum_{i=1}^{N} \phi_i(x)\psi(x)$	Degenerate kernel	1. Find form of separated kernel 2. Use this form for f 3. Carry through equation 4. Equate terms of coefficient 5. Use to find f
$\int_{-\infty}^{\infty} K(x,y)f(y)\,\mathrm{d}y$	Displacement kernel	1. Take Fourier transforms of all terms 2. Use $\tilde{f}(k) = \frac{\tilde{g}(k)}{1+\lambda_{\tilde{k}}(k)}$ 3. Inverse Fourier result
$\int_{0}^{x} K(x,y)f(y)\,\mathrm{d}y$	Displacement kernel	1. Take Laplace transform 2. Use $\hat{f}(k) = \frac{\hat{g}(k)}{1+\hat{k}(s)}$ 3. Inverse Laplace result
	Neumann series	

the function $\phi(x)$ is square integrable and the source ρ is not necessarily unique.

4.7 Eigenvalue Problems

Provided the kernel $K(x, y)$ is Hermitian, the eigenvalues are real.

Theorem 4.4: Eigenvalues of Hermitian kernels are real

$$\begin{aligned}\lambda(u_n, u_n) &= (\lambda u_n, u_n) \\ &= (K u_n, u_n) \\ &= (u_n, K^* u_n) \\ &= (u_n, \lambda^* u_n) \\ &= \lambda^* (u_n, u_n) \\ \Rightarrow \lambda &= \lambda^*.\end{aligned}$$

For different eigenvalues the eigenfunctions are orothogonal.

Theorem 4.5: Orthogonality of eigenfunctions

Knowing that

$$\begin{aligned}(u_n, K u_m) &= \lambda_m (u_n, u_m) \\ (u_n, K u_m) &= (K u_n, u_m) = \lambda_n (u_n, u_m)\end{aligned}$$

the difference of these is then

$$0 = (\lambda_m - \lambda_n)(u_n, u_m).$$

Given that the eigenvalues are different, i.e. $\lambda_m \neq \lambda_n$, then (u_n, u_m) and thus the eigenfunctions are orthogonal.

The source representative equation may be represented by a convergent eigen-

function expansion, i.e.

$$\begin{aligned} f(x) &= \int_a^b K(x,y)g(y)\,\mathrm{d}y \\ \Rightarrow f(x) &= \sum_i (u_i, f)u_i(x). \end{aligned}$$

The term *source representative* derives from electrostatics, in that the potential can be written in terms of its source ρ, where the Coulomb potential takes on the role of the kernel, i.e.

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}^3\mathbf{r}'.$$

One can seek an eigenfunction expansion of the kernel:

$$\begin{aligned} K(x,y) &= \sum_i K_i^*(y)u_i(x) \\ &= K(x,y)^* \\ &= \sum_i K_i(y)u_i^*(x), \end{aligned}$$

which makes use of the kernel's hermiticity. Using this expansion in the eigenfunction equation gives

$$\begin{aligned} u_n(x) &= \lambda \int_a^b \left(\sum_m K_m(x)u_m^*(y)\right) u_n(y)\,\mathrm{d}y \\ &= \lambda_n \sum_m K_m(x) \underbrace{\int_a^b u_m^*(y)u_n(y)\,\mathrm{d}y}_{=\delta_{mn}} \\ &= \lambda_n \sum_m K_m(x)\delta_{mn} \\ &= \lambda_n K_n(x) \\ \Rightarrow K(x,y) &= \sum_n \frac{u_n(x)u_n^*(y)}{\lambda_n}. \end{aligned}$$

This is in the form of the Green's function expansion for a Hermitian operator, i.e.

$$Lu_m = \lambda_n u_n \Leftrightarrow u_n(x) = \lambda \int G(x,y)u_n(y)\,\mathrm{d}y.$$

A Fredholm equation of the second kind is usually written

$$f(x) = g(x) + \lambda \int_a^b K(x,y) f(y)\,\mathrm{d}y,$$

and may therefore be written as

$$f(x) - g(x) = \lambda \int_a^b K(x,y) f(y)\,\mathrm{d}y.$$

This may then be rewritten in terms of expansions, i.e. $f(x) - g(x) = \sum_n c_n u_n(x)$, where

$$\begin{aligned}
\sum_n c_n u_n(x) &= \lambda \int_a^b K(x,y) f(y)\,\mathrm{d}y \\
&= \lambda \int_a^b K(x,y) \big(f(y) - g(y) + g(y)\big)\,\mathrm{d}y \\
&= \lambda \int_a^b K(x,y) \big(f(y) - g(y)\big)\,\mathrm{d}y + \lambda \int_a^b K(x,y) g(y)\,\mathrm{d}y \\
&= \lambda \int_a^b K(x,y) \sum_n c_n u_n(y)\,\mathrm{d}y + \lambda \int_a^b K(x,y) g(y)\,\mathrm{d}y \\
&= \lambda \int_a^b \sum_m \frac{u_m(x) u_m^*(y)}{\lambda_m} \sum_n c_n u_n(y)\,\mathrm{d}y + \lambda \int_a^b \sum_n \frac{u_n(x) u_n^*(y)}{\lambda_n} g(y)\,\mathrm{d}y \\
&= \lambda \int_a^b \sum_m \sum_n \frac{c_n}{\lambda_m} u_m(x) u_m^*(y) u_n(y)\,\mathrm{d}y + \lambda \sum_n \frac{u_n(x)}{\lambda_n} \int_a^b u_n^*(y) g(y)\,\mathrm{d}y \\
&= \lambda \sum_m \sum_n \frac{c_n}{\lambda_m} u_m(x) \delta_{mn} + \lambda \sum_n \frac{u_n(x)}{\lambda_n} (u_n^*, g) \\
&= \lambda \sum_n \frac{c_n}{\lambda_n} u_n(x) + \lambda \sum_n \frac{u_n(x)}{\lambda_n} (u_n^*, g) \\
&= \lambda \sum_n \left(\frac{c_n + (u_n, g)}{\lambda_n} \right) u_n(x).
\end{aligned}$$

Comparing coefficients of u_n gives

$$\begin{aligned} c_n &= \frac{\lambda}{\lambda_n}\left(c_n + (u_n, g)\right) \\ \Rightarrow c_n &= \frac{\lambda}{\lambda_n - \lambda}\left(u_n, g\right). \end{aligned}$$

This can now be used to solve the integral equation:

$$\begin{aligned} f(x) - g(x) &= \sum_n \frac{\lambda}{\lambda_n - \lambda}\left(u_n, g\right) u_n(x) \\ &= \sum_n \frac{\lambda}{\lambda_n - \lambda} u_n \int_a^b u_n^*(y) g(y)\,\mathrm{d}y, \end{aligned}$$

however from earlier it is known that $f(x) - g(x) = -\lambda \int_a^b R(x, y; \lambda) g(y)\,\mathrm{d}y$, and so

$$R(x, y; \lambda) = \sum_n \frac{u_n(x) u_n^*(y)}{\lambda - \lambda_n}.$$

The solutions for R are finite provided $|\lambda| < |\lambda_0|$, where λ_0 is the eigenvalue with the smallest magnitude. FOr any λ the smallest denominator is λ_n, from which we can deduce that the Neumann series solution of the Fredholm equation converges only for $|\lambda| < |\lambda_1|$, the smallest eigenvalue.

Example 4.10: Find the resolvent $f(x) = g(x) + \lambda \int_0^1 xy f(y)\,\mathrm{d}y$

In order to solve this, one must first find the eigenfunctions satisfying

$$u_i(x) = \lambda_i \int_a^b K(x, y) u_i(y)\,\mathrm{d}y.$$

The kernel is $K(x, y) = xy$, and so the eigenfunctions are

$$\begin{aligned} u_i(x) &= \lambda \int_a^b xy u_i(y)\,\mathrm{d}y \\ &= x\left(\lambda_i \int_a^b y u_i(y)\,\mathrm{d}y\right) \\ &= Cx, \end{aligned}$$

where C is a constant, and so there is only one eigenfunction. The corresponding eigenvalue is then

$$\begin{aligned} u_1(x) = Cx &= \lambda_1 \int_0^1 xy(Cy)\,\mathrm{d}y \\ &= \lambda \int_0^1 Cxy^2\,\mathrm{d}y \\ &= \frac{1}{3}\lambda_1 Cx \\ \Rightarrow \lambda_1 &= 3. \end{aligned}$$

Normalisation requires that the eigenfunction is unitary over this range, hence

$$\begin{aligned} 1 &= \int_0^1 |u_1(x)|^2\,\mathrm{d}x \\ &= \int_0^1 |Cx|^2\,\mathrm{d}x \\ &= \frac{1}{3}|C|^2 \\ \Rightarrow |C| &= \sqrt{3}. \end{aligned}$$

The resolvent kernel is therefore

$$\begin{aligned} R(x,y;\lambda) = \frac{u_1(x)u_1^*(y)}{\lambda-\lambda_1} &= \frac{\left(\sqrt{3}x\right)\left(\sqrt{3}y\right)}{\lambda-3} \\ &= \frac{3xy}{\lambda-3}. \end{aligned}$$

Chapter 5

Calculus of Variations

There are many problems in mathematical physics that require the minimisation of a function involving an integral of a function over some region. Some examples of this include:

- Hamilton's principle (mechanics)
  A mechanical system described by coordinates $q_i(t)$ follows a trajectory $q_i^0(t)$ which makes the action stationary, i.e.

  $$S = \int_{t_i}^{t_f} (T - V)\,\mathrm{d}t,$$

  where T is the kinetic energy and V is the potential energy. These are expressed in terms of $q_i(t)$ and $\dot{q}_i(t)$.

- Fermat's principle (optics)
  A ray of light passes between two points whose travel time is given by

  $$T = \int \frac{\mathrm{d}s}{\left(\frac{c}{n}\right)} = \frac{1}{c}\int n\,\mathrm{d}s.$$

- Electrostatics
  Finding the minimised electrostatic potential energy U by using $\phi(\mathbf{r})$:

  $$U = \frac{\epsilon_0}{2}\int_V (\boldsymbol{\nabla}\phi)^2\ \mathrm{d}^3\mathbf{r} + \int \rho(\mathbf{r})\phi(\mathbf{r})\,\mathrm{d}^3 r.$$

These examples all involve a **functional** of some function.

Definition 5.1: Functional

Akin to how a function $f(x)$ takes a variable argument x to output a number, a **functional** $F[y]$ takes an function argument y to output a number, where the square bracket notation is used to distinguish between functions and functionals. Phrased more formally, a functional maps a function onto a number. Definite integrals are examples of functionals, i.e.

$$I[y] = \int_a^b y(x)\,\mathrm{d}x.$$

Example 5.1

Consider a functional over a range $[0, \pi]$ given by

$$I[y] = \int_0^\pi y(x)\,\mathrm{d}x,$$

then some function values give functional values

$y(x)$	$I[y]$
$\sin(x)$	2
$\cos(x)$	0
x	$\frac{\pi^2}{2}$
x^2	$\frac{\pi^3}{3}$.

5.1 Functionals

5.1.1 Stationary Points and the Euler-Lagrange Equation

A stationary state of a function is the point at which the function does not change under small variations in its argument, i.e. taking $x \to x + \delta x$ then

$f(x) \to f(x) + \delta f(x)$ and if $\delta f = 0$ to first order of δx the point is stationary. These stationary states are paramount for functionals.

A functional has a stationary point for any function y such that a small change $y(x) \to y(x) + \varepsilon(x)$ leads to no change in $I[y]$ to first order in $\varepsilon(x)$. The smallness of $\varepsilon(x)$ only implies that as a function it is uniformly (everywhere) close to zero, but may vary arbitrarily. One may identify stationary points as those at which the first terms vanish, regardless of choice of the small quantities $\{\varepsilon_i\}$.

For a functional $F[y(t)]$, replace $y(t)$ by $y(t) + \varepsilon(t)$ and expand to first order in ε:

$$F[y(t) + \varepsilon(t)] = F[y(t)] + \int \varepsilon(t) A([y], t)\, \mathrm{d}t + \mathcal{O}(\varepsilon^2).$$

One can then identify

$$A([y], t) \equiv \frac{\delta F}{\delta y(t)}$$

as the functional derivative of F with respect to the function $y(t)$. An important class of functionals is given by

$$F[y(x)] = \int_a^b f(y, y_x; x)\, \mathrm{d}x \qquad (y_x = \tfrac{\mathrm{d}y}{\mathrm{d}x})$$

One may now calculate the functional derivative of this:

$$\begin{aligned} F[y + \varepsilon] &= \int_a^b f(y + \varepsilon, y_x + \varepsilon, x)\, \mathrm{d}x \\ &= \int_a^b f(y, y_x, x) + \varepsilon(x) \frac{\partial f}{\partial y} + \varepsilon_x \frac{\partial f}{\partial y_x} + \mathcal{O}(\varepsilon^2)\, \mathrm{d}x \\ &= F[y] + \int_a^b \varepsilon(x) \frac{\partial f}{\partial y}\, \mathrm{d}x + \left[\varepsilon \frac{\partial f}{\partial y_x}\right]_a^b - \int_a^b \varepsilon \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial f}{\partial y_x}\, \mathrm{d}x + \mathcal{O}(\varepsilon^2) \\ &= F[y] + \int_a^b \varepsilon(x) \left(\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial f}{\partial y_x}\right) \mathrm{d}x + \left[\varepsilon \frac{\partial f}{\partial y_x}\right]_a^b. \end{aligned}$$

Often the problem is to minimise F, subject to given values $y(a)$ and $y(b)$, hence the preservation of these boundary conditions imples $\varepsilon(a) = \varepsilon(b) = 0$. Since $\varepsilon(x)$ is allowed to vary arbitrarily, the integral is only zero if the quantity multiplying ε is zero at every point x, though one may choose ε to

peak at a particular value of x. Therefore for the functional to be stationary all terms proportional to ε must vanish, hence

$$\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial f}{\partial y_x} = 0,$$

which is the Euler-Lagrange equation.

Notes:

- Often the explicit dependence upon x is not written, but it instead assumes that the reader understands that it is a functional equation
- One uses the functional derivative location $\frac{\delta I[y]}{\delta y}$ for the term in the functional $I[y + \delta y]$ proportional to δy:

$$I[y + \delta y] = I[y] + \int \mathrm{d}x \delta y(s) \frac{\delta I[y]}{\delta y}(x) + \ldots$$

- The functional is NOT an integral, e.g. the functional $I[y] = y(0)$ can be turned into an integral by inserting a delta function:

$$I[y] = \int y(x)\delta(x)\,\mathrm{d}x.$$

Example 5.2

Suppose that one wished to find the shortest path between two point, $x = a$ and $x = b$, in a plane. One must minimise the path length L in terms of a norm infinitesimal $(\mathrm{d}s)^2 = (\mathrm{d}x)^2 + (\mathrm{d}y)^2$:

$$\begin{aligned} L[y(x)] &= \int_a^b \frac{\mathrm{d}s}{\mathrm{d}x}\,\mathrm{d}x \\ &= \int_a^b \sqrt{1 + y_x^2}\,\mathrm{d}x. \end{aligned}$$

From here minimisation requires the form of $y(x)$. For a general function the Euler-Lagrange equation is given by $\frac{\delta I[y]}{y} = 0$, thus *sdf*

However, as f does not explicitly depend on y then $\frac{\partial f}{\partial y} = 0$ and so

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y_x}\right) &= 0 \\ \rightarrow \frac{\partial f}{\partial y_x} &= c \\ = \frac{y_x}{\sqrt{1-y_x^2}} & \\ \rightarrow \frac{y_x^2}{1-y_x^2} &= c^2 \\ y_x &= \sqrt{\frac{1}{1+c^2}}. \end{aligned}$$

Since all terms on the right side are constant, set equal to a general constant, m. Therefore

$$\begin{aligned} \frac{\mathrm{d}y}{\mathrm{d}x} &= m \\ \Rightarrow y &= mx + d, \end{aligned}$$

where the constants m and d are chosen to suit boundary conditions. One should note that this is the classic equation for a straight line between two points.

5.1.2 Special Cases

No explicit dependence on y

If f has no explicit dependence on y then $\frac{\partial f}{\partial y} = 0$ and so the Euler-Lagrange equation reads $\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y_x}\right) = 0$, which results in $\frac{\partial f}{\partial y_x} =$ constant, i.e. $\frac{\partial L}{\partial \dot{q}}$ in Lagrangian dynamics.

No explicit dependence on x

If $f(y, y_x; x) = f(y, y_x)$ then there is no dependence on x. As such the derivatives become

$$\begin{aligned}\frac{\mathrm{d}f}{\mathrm{d}x} &= \frac{\partial f}{\partial x} + y_x \frac{\partial f}{\partial y} + y_{xx} \frac{\partial f}{\partial y_x} \\ &= 0 + y_x \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y_x}\right) + y_{xx} \frac{\partial f}{\partial y_x} \\ &= \frac{\mathrm{d}}{\mathrm{d}x}\left(y_x \frac{\partial f}{\partial y_x}\right) \\ \Rightarrow f - y_x \frac{\partial f}{\partial y_x} &= \text{const.}\end{aligned}$$

5.2 Fermat's Principle

Fermat's principle of geometrical optics states that light always travels between two points along the path that takes the least time. Equivalently, light takes the shortest optical path which implies Snell's law.

The time t to travel along an arbitrary path $y(x)$ at a speed c is given by

$$\begin{aligned}t[y] &= \int \frac{1}{v}\,\mathrm{d}s \\ &= \frac{1}{c}\int n(x,y)\,\mathrm{d}s \\ &= \frac{1}{c}\int n(y)\sqrt{1+y'^2}\,\mathrm{d}x,\end{aligned}$$

or in terms of path length p;

$$p[y] = \int \underbrace{n(y)\sqrt{1+y'^2}}_{=f(y,y_x)}\,\mathrm{d}x,$$

which has no dependence on x. The equation for the special case of no

x-dependence is thus

$$\begin{aligned} f - y_x \frac{\partial f}{\partial y_x} &= n(y)\sqrt{1+y_x^2} - y_x \left(\frac{n(y) y_x}{\sqrt{1+y_x^2}} \right) \\ &= \frac{n(y)}{\sqrt{1+y_x^2}} \left(1 + y_x^2 - y_x^2\right) \\ &= \frac{n(y)}{\sqrt{1+y_x^2}}. \end{aligned}$$

To interpret this geometrically draw a triangle, as shown in Figure 5.1. From

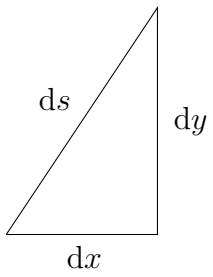

Figure 5.1

the diagram one sees that $\frac{\mathrm{d}x}{\mathrm{d}s} = \sin(\theta)$ and $\frac{\mathrm{d}x}{\mathrm{d}s} = \frac{1}{\sqrt{1+y_x^2}}$, hence $n(y)\sin(\theta) =$ const., which is Snell's law.

5.3 The Brachistochrone

The term "brachistrochrone" derives from the Ancient Greek brakhistos khronos, meaning *shortest time*. In physics the brachistochrone is the curve along which a particle slides the fastest between two points under the influence of gravity. Let the ends of the path be at $(0,0)$ and (x_f, y_f), with the particle starting from rest. The time of descent T at a constant speed v is given by

$$T = \int_A^B \mathrm{d}t = \int_A^B \frac{\mathrm{d}t}{\mathrm{d}s}\,\mathrm{d}s = \int_A^B \frac{1}{v}\,\mathrm{d}s,$$

which is what is to be minimised. From energy conservation $\frac{1}{2}mv^2 = mgy \Rightarrow v = \sqrt{2gy}$. As before with Fermat's $\mathrm{d}s = \sqrt{1 - y_x^2}\,\mathrm{d}x$, and so

$$T[y(x)] = \int \frac{1}{\sqrt{y}}\sqrt{1 + y_x^2}\,\mathrm{d}x,$$

where the factor of $2g$ has been ignored because it [...]. As with Snell's law $n = \frac{1}{\sqrt{y}}$, and so $\frac{1}{\sqrt{y}}\sin(\theta) = \frac{1}{\sqrt{c}}$ (const.). Therefore $y = c\sin^2(\theta) = \frac{1}{2}c\big(1 - \cos(2\theta)\big)$. Working through the algebra one then sees that the solution is a parametrised equation of a cycloid:

$$\begin{aligned}
\frac{\mathrm{d}x}{\mathrm{d}\theta} &= \frac{\mathrm{d}x}{\mathrm{d}y}\,\frac{\mathrm{d}y}{\mathrm{d}\theta} \\
&= \tan(\theta)\cdot 2c\sin(\theta)\cos(\theta) \\
&= 2c\sin^2(\theta) \\
&= c\big(1 - \cos(2\theta)\big) \\
\Rightarrow x &= c\left(\theta - \frac{1}{2}\sin(2\theta)\right) \\
&= \frac{1}{2}c\big(2\theta - \sin(2\theta)\big) \\
\Rightarrow y &= \frac{1}{2}c\big(1 - \cos(2\theta)\big)\,.
\end{aligned}$$

5.4 Generalisation to more Functions and Variables

5.4.1 Generalisation 1

So far the only functionals encountered have been of the form

$$\delta I[y] = \delta\int_a^b F(y, y_x; x)\,\mathrm{d}x = 0,$$

however this is not necessarily the case. Consider the problem of minimisation but with one end free (unconstrained), i.e.

$$F[y] = \int_a^b f(y, y_x; x)\,\mathrm{d}x,$$

where $y(x)$ may be chosen freely for $x > a$, including $x = b$. Previously the substitution $y(x) \to y(x)+\varepsilon(x)$ was made, then the functional was expanded to first order in ε with the condition $\varepsilon(a) = \varepsilon(b) = 0$, however now there is no boundary condition for $\varepsilon(b)$.

From before

$$F[y+\varepsilon] = F[y] + \int_a^b \left(\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial f}{\partial y_x}\right)\varepsilon\,\mathrm{d}x + \left[\varepsilon(x)\frac{\partial f}{\partial y_x}\right]_a^b + \mathcal{O}(\varepsilon^2),$$

and from the Euler-Lagrange equation this becomes

$$F[y+\varepsilon] = F[y] + \varepsilon(b)\frac{\partial f}{\partial y_x}(b) - \varepsilon(a)\frac{\partial f}{\partial y_x}(a).$$

However, $\varepsilon(a) = 0$ and so

$$F[y+\varepsilon] = F[y] + \varepsilon(b)\frac{\partial f}{\partial y_x}(b).$$

For $y = 0$, $F[y] = 0$ as a boundary condition, hence

$$F[0+\varepsilon] = \varepsilon(b)\frac{\partial f}{\partial y_x}(b).$$

For this to be a stable solution $F[y+\varepsilon] = 0$ and so

$$\varepsilon(b)\frac{\partial f}{\partial y_x}(b) = 0.$$

Example 5.3

Reconsider the brachistochrone problem, instead with y_f free to vary. Now the boundary conditions are

$$\begin{aligned} \frac{\partial f}{\partial y_x} &= 0 && x = x_f \\ \Rightarrow \frac{1}{\sqrt{y}} \frac{y_x}{\sqrt{1+y_x^2}} &= 0 \\ \Rightarrow \frac{\mathrm{d}y}{\mathrm{d}x} &= 0 \text{ at } x = x_f \\ \Rightarrow \theta &= \frac{\pi}{2} \text{ at } x = x_f \\ \therefore x_f = \frac{1}{2}c\left(2\theta - \sin(2\theta)\right) &= \frac{1}{2}c(\pi - 0) \\ \Rightarrow c &= \frac{2}{\pi}x_f. \end{aligned}$$

5.4.2 Generalisation 2

If there is more than one variable $\{y_i\}$, i.e.

$$F[\{y_i\}] = \int_a^b f(\{y_i, y_{x_i}\}; x)\,\mathrm{d}x,$$

then one must instead look for a stationary point with respect to all y_i. The ends are fixed for this. Generalising the technique used thus far must be used on each variable, i.e.

$$\frac{\delta F}{\delta y_i} = \frac{\partial f}{\partial y_i} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y_{x_i}}\right) = 0.$$

There are many examples of this in mechanics.

5.4.3 Generalisation 3

If F is the functional of a field, it may depend on multiple variables, i.e.

$$F[\psi] = \int f(\psi, \boldsymbol{\nabla}\psi; r)\, \mathrm{d}^3\mathbf{r},$$

where F is the free energy, f is the free energy density and ψ is the condensate wavefunction, e.g. $f = \frac{1}{2}\frac{\hbar^2}{2m_e}|\boldsymbol{\nabla}\psi|^2 - a(T)|\psi|^2 + b(T)|\psi|^4$. Some examples of this include

- Derivation of field equations in electromagnetism
- Gravitation from an action principle

5.5 Hamilton's Principle

Definition 5.2: Hamilton's principle

Hamilton's principle or **Hamilton's principle of least action** is a general principle that states that the dynamics of a system evolve as a stationary point of the action functional $\mathcal{S}$ given by

$$\mathcal{S}[q] \overset{\text{def}}{=} \int_{t_1}^{t_2} L\left(q(t), \dot{q}(t)\right)\, \mathrm{d}t,$$

where L is the Lagrangian of the system.

For a scalar field $\phi(t, \mathbf{r})$:

$$\int[\phi] = \int \underbrace{\int \underbrace{\Lambda(\phi, \boldsymbol{\nabla}\phi, \frac{\partial\phi}{\partial t}; t, \mathbf{r})}_{\text{Lagrange density}}\, \mathrm{d}^3\mathbf{r}}_{\text{Lagrangian}}\, \mathrm{d}t.$$

This can be rewritten with $\left(\frac{\partial\phi}{\partial t}, \boldsymbol{\nabla}\phi\right) = \partial_\mu\phi$ and $(t, \mathbf{r}) = x^\mu \to \mathrm{d}t\, \mathrm{d}^3\mathbf{r} = \mathrm{d}^4x$:

$$\int[\phi] = \int \Lambda\left(\phi, \partial_\mu\phi; x\right)\, \mathrm{d}^4x.$$

In order to derive the new Euler-Lagrange equation, consider a minimalisation problem again with $\phi \to \phi + \delta\phi$:

$$\begin{aligned}
\delta s &= \int \delta\Lambda \, \mathrm{d}^4 x \\
&= \int \left(\delta\phi \, \frac{\partial \Lambda}{\partial \phi} + \delta\left(\partial_\mu \phi\right) \frac{\partial \Lambda}{\partial\left(\partial_\mu \phi\right)} \right) \mathrm{d}^4 x \\
&= \int \left(\delta\phi \, \frac{\partial \Lambda}{\partial \phi} + \partial_\mu(\delta\phi) \, \frac{\partial \Lambda}{\partial\left(\partial_\mu \phi\right)} \right) \mathrm{d}^4 x \\
&= \int \left(\delta\phi \, \frac{\partial \Lambda}{\partial \phi} + \partial_\mu \left(\delta\phi \, \frac{\partial \Lambda}{\partial\left(\partial_\mu \phi\right)} \right) \right) \mathrm{d}^4 x - \int \delta\phi \, \partial_\mu \left(\frac{\partial \Lambda}{\partial\left(\partial_\mu \phi\right)} \right) \mathrm{d}^4 x \\
&= \int \delta\phi \left(\frac{\partial \Lambda}{\partial \phi} - \partial_\mu \left(\frac{\partial \Lambda}{\partial\left(\partial_\mu \phi\right)} \right) \right) \mathrm{d}^4 x + \underbrace{\int \partial_\mu \left(\delta\phi \, \frac{\partial \Lambda}{\partial\left(\partial_\mu \phi\right)} \right) \mathrm{d}^4 x}_{\substack{\text{These are surface terms} \\ \text{which are unimportant} \\ \text{for field equations.}}} .
\end{aligned}$$

To first order in $\delta\phi$, $\delta s = 0$ thus the Euler-Lagrange is

$$\frac{\delta s}{\delta \phi} = \frac{\partial \Lambda}{\partial \phi} - \partial_\mu \left(\frac{\partial \Lambda}{\partial\left(\partial_\mu \phi\right)} \right) = 0.$$

Example 5.4

Describe the motion of an elastic stretched string with fixed endpoints, assuming a small deformation.
The kinetic energy T_k is given by

$$T_k = \frac{1}{2} \int_0^L \mu \left(\frac{\partial y}{\partial t} \right)^2 \mathrm{d}x.$$

As before, the deformation $\mathrm{d}s$ is given by

$$\begin{aligned}(\mathrm{d}s)^2 &= (\mathrm{d}x)^2 + (\mathrm{d}y)^2 \\ &= \left(1 + \left(\frac{\partial y}{\partial x}\right)^2\right)(\mathrm{d}x)^2 \\ \Rightarrow \mathrm{d}s &= \sqrt{1+y_x^2}\,\mathrm{d}x \\ &\approx \left(1 + \frac{1}{2}y_x^2\right)\,\mathrm{d}x\end{aligned}$$

for small deformations. The work done in stretching the string is proprtional to its tension T:

$$\begin{aligned}\mathrm{d}W &= T\,(\mathrm{d}s - \mathrm{d}x) \\ &\approx T\left(\frac{1}{2}y_x^2\right)\mathrm{d}x.\end{aligned}$$

The potential energy V is then

$$V[y] = \int_0^L \frac{1}{2}Ty_x^2\,\mathrm{d}x.$$

The Lagrangian is therefore

$$L = T_k - V = \int_0^L \underbrace{\frac{1}{2}\mu\left(\frac{\partial y}{\partial t}\right)^2 - \frac{1}{2}T\left(\frac{\partial y}{\partial x}\right)^2}_{\text{Lagrange density, }\Lambda}\,\mathrm{d}x.$$

By the new Euler-Lagrange equation

$$\frac{\delta s}{\delta y} = \frac{\partial \Lambda}{\partial y} - \frac{\partial}{\partial t}\left(\frac{\partial \Lambda}{\partial\left(\frac{\partial y}{\partial t}\right)}\right) - \frac{\partial}{\partial x}\left(\frac{\partial \Lambda}{\partial\left(\frac{\partial y}{\partial x}\right)}\right) = 0.$$

Therefore

$$\begin{aligned}0 &= 0 + \mu\,\frac{\partial}{\partial t}\left(\frac{\partial y}{\partial t}\right) + \frac{\partial}{\partial x}\left(-T\,\frac{\partial y}{\partial x}\right) \\ \Rightarrow \frac{\partial^2 y}{\partial t^2} &= \frac{T}{\mu}\frac{\partial^2 y}{\partial x^2}\end{aligned}$$

Functionals that depend on second derivatives and higher can be treated by very similar methods to those seen previously, however more integration by parts is necessary to obtain the Euler-Lagrange equation.

Example 5.5

Consider a flexible bar clamped at one end ($x = 0$) with a transverse force applied to the other end ($x = L$). From being clamped, the boundary conditions are $y(0) = 0$ and $y_x(0) = 0$. The potential energy U of the bar is

$$U[y] = \frac{1}{2} \underbrace{K}_{\text{stiffness}} \int_0^L \underbrace{(y_{xx})^2}_{\text{curvature}} \, \mathrm{d}x.$$

The potential energy is minimised when $\delta u = 0$ (equilibrium). One can now derive the Euler-Lagrange equation at the free end:

$$\begin{aligned}
\delta U[y] &= \frac{1}{2} K \int_0^L \delta \left(y_{xx}^2 \right) \, \mathrm{d}x + W \delta y(L) \\
&= \frac{1}{2} K \int_0^L 2 \left(\delta y_{xx} \right) y_{xx} \, \mathrm{d}x + W \delta y(L) \\
&= K \left[\delta y_{xx} \cdot y_{xx} \right]_0^L - K \int_0^L y_x \cdot y_{xxx} \, \mathrm{d}x + W \delta y(L) \\
&= K \left(\delta y_x(L) y_{xx}(L) - \delta y(L) y_{xxx}(L) - \delta y_x(0) \ldots + \delta y(0) \right) \\
&+ K \int_0^L \delta y(x) \frac{\mathrm{d}^4 y}{\mathrm{d}x^4} \, \mathrm{d}x + W \delta y(L) \\
&= 0.
\end{aligned}$$

From the coefficients of $\delta y(x)$, the Euler-Lagrange equation is

$$\frac{\delta U}{\delta y} = K \frac{\mathrm{d}^4 y}{\mathrm{d}x^4} = 0.$$

From the coefficients of $\delta y(L)$ and $\delta y_x(L)$ one can read off the boundary conditions:

$$\begin{aligned}
\delta y(L): \quad & -K y_{xxx}(L) + W = 0 \quad && \Rightarrow y_{xxx}(L) = \tfrac{W}{K} \\
\delta y_x(L): \quad & K y_{xx}(L) = 0 && \Rightarrow y_{xx}(L) = 0.
\end{aligned}$$

Integrating the Euler-Lagrange then gives

$$y = 6Ax^3 + 2Bx^2 + Cx + D,$$

however $y(0) = 0$, $y_x(0) = 0$ and so $C = D = 0$, thus

$$y = 6Ax^3 + 2Bx^2 = 0.$$

From this $B = -3Ax$, and so

$$\begin{array}{l|l} y_{xxx}(L) = \frac{W}{K} & y_{xx}(L) = B = -3AL \\ 6A = \frac{W}{K} & \\ \Rightarrow A = \frac{W}{6K} & \end{array}$$

$$\Rightarrow y(x) = \frac{W}{4K}\left(x^3 - 3Lx^2\right).$$

5.6 Constrained Variational Problems

There are often subsidiary conditions on a minimsation problem, i.e. minimising a value provided other conditions are held. For example, one might wish to minimise the functional $(\delta I)_c = \int \frac{\delta I}{\delta y}\delta y_x \,\mathrm{d}x = 0$ provided δy_c satisfies the constraint $(\delta J)_c = \int \frac{\delta J}{\delta y}\,\mathrm{d}y_c \,\mathrm{d}x = 0$.

A major example of the usage of constrained variational problems is in quantum mechanics when attempting to find the energy of a particle, requiring that it is normalised, i.e.

$$I[\phi] = \int \phi \hat{H} \phi \,\mathrm{d}x, \quad \text{provided}$$
$$J[\phi] = \int |\phi|^2 \,\mathrm{d}x = 1.$$

To find the stationary points $f(x)$ subject to constraints $g_k(x) = c_k$ $(k = 1, 2, \ldots)$, it may be possible to solve an auxiliary problem. One now attempts to find the stationary points of the modified function

$$F(x, \lambda_1, \lambda_2, \ldots) = f(x) - \lambda_1 g_1(x) - \lambda_2 g_2(x) - \ldots,$$

where λ_i are **Lagrange multipliers**.

5.6.1 Lagrange's Undetermined Multipliers

Definition 5.3: Lagrange multipliers

In mathematical optimisation **Lagrange multipliers** are used to find local maxima and minima of a function.

The solutions, if they exist, depend on λ, i.e. $y(x, \lambda)$ with λ chosen such that $J[y(x, \lambda)] = c$.

Proof 5.1

Take $\delta k = \int \frac{\delta k}{\delta y} \delta y \, \mathrm{d}x = 0$, which must also satisfy for δy_c:

$$\begin{aligned} (\delta k)_c &= \int \frac{\delta k}{\delta y} \delta y_c \, \mathrm{d}x \\ &= \int \frac{\delta x}{\delta y} \delta y_c \, \mathrm{d}x - \lambda \underbrace{\int \frac{\delta J}{\delta y} \delta y_c \, \mathrm{d}x}_{=0 \text{ by constraint}} . \end{aligned}$$

One now has

$$(\delta I)_c = \int \frac{\delta x}{\delta y} \delta y_c \, \mathrm{d}x = 0,$$

which is the initial problem to be solved.

5.7 The Isoperimetric Problems

Definition 5.4: Isoperimetric

Deriving from the Ancient Greek prefix **iso-**, meaning *equal*, and suffix **-perimetros**, meaning *the length of a boundary*, the term **isoperimetric** relates to shapes with the same length perimeter. In mathematics this is applied to problems of finding plane figures with the largest possible area, provided the boundaries have a specified length.

Example 5.6: Maximise the area of a region in the xy-plane whose boundary has a fixed length L

Parametrising the problem into $x(t)$ and $y(t)$, where $t \in [0,1]$ is the fraction of the total path subtended. As the shape must be closed $x(0) = x(1)$ and $y(0) = y(1)$. The area S and length L of the shape are given by

$$\begin{aligned} S[x,y] &= \oint y\,\mathrm{d}x = \int_0^1 y\dot{x}\,\mathrm{d}t \\ L[x,y] &= \oint \sqrt{\mathrm{d}x^2 + \mathrm{d}y^2} \\ &= \int_0^1 \sqrt{\dot{x}^2 + \dot{y}^2}\,\mathrm{d}t \\ &= L_0 = \text{const.} \end{aligned}$$

Introducing an auxiliary functional $G[x,y]$ such that

$$\begin{aligned} G[x,y] &= S - \lambda L \\ &= \int_0^1 \underbrace{y\dot{x} - \lambda\sqrt{\dot{x}^2 + \dot{y}^2}}_{=g(y,\dot{y};\dot{x})}\,\mathrm{d}t. \end{aligned}$$

As $g(y,\dot{y};\dot{x})$ has no explicit dependence on x then $\frac{\partial g}{\partial x} = 0$. The derivative with respect to $\dot{x}$ is given by

$$\begin{aligned} \frac{\partial g}{\partial \dot{x}} &= y - \frac{\lambda\dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = Q \text{ (const.)} \\ \Rightarrow -(Q - y) &= \frac{\lambda\dot{x}}{\sqrt{\dot{x}^2 + \dot{y}^2}}. \end{aligned}$$

The Euler-Lagrange equation for y is then

$$\begin{aligned} \frac{\delta G}{\delta y} &= \frac{\partial g}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial g}{\partial \dot{y}}\right) \\ &= \dot{x} - \frac{\mathrm{d}}{\mathrm{d}t}\left(-\frac{\lambda\dot{y}}{\sqrt{\dot{x}^2 + \dot{y}^2}}\right) = 0. \end{aligned}$$

Integrating this with respect to time, then

$$x + \frac{\lambda \dot{y}}{\sqrt{\dot{x}^2 + \dot{y}^2}} = P \text{ (const.)}$$
$$\Rightarrow P - x = \frac{\lambda \dot{y}}{\sqrt{\dot{x}^2 + \dot{y}^2}}.$$

By the chain rule the ratios of the rates of change in y and x is then the rate of change in y with respect to x, hence

$$\frac{\dot{y}}{\dot{x}} = \frac{\mathrm{d}y}{\mathrm{d}x} = -\frac{P - x}{Q - y}.$$

Performing the appropriate integrals then solves the equation:

$$\int (Q - y)\,\mathrm{d}y = -\int (P - x)\,\mathrm{d}x$$
$$\rightarrow (Q - y)^2 = -(P - x)^2 + R^2$$
$$\Rightarrow (P - x)^2 + (Q - y)^2 = R^2,$$

which is the equation of a circle centred at (P, Q).

5.7.1 Generalisations of functionals

There may be multiple constraints, i.e. $J_i[y] = c_i$. In order to solve this, introduce an auxiliary functional K:

$$K([y], \lambda) = I[y] - \sum_i \lambda_i J_i[y]$$

and then solve $\delta K = \delta I - \lambda \delta J = 0$. There may also be a family of constraints, i.e. $J([y], a) = c(a)$, wjere a varies continuously. In this case the auxiliary is then

$$K[y] = I[y] - \int \lambda(a) J([y], a)\,\mathrm{d}a.$$

Example 5.7

Consider a pendulum moving under gravity with constraint $r(t) = R$, where R is a constant. The action $\mathcal{S}$ for an unconstrained particle would be given by

$$\mathcal{S}[r, \phi] = \int \frac{1}{2} m\dot{r}^2 + \frac{1}{2} m r^2 \dot{\phi}^2 + mgr\cos(\phi)\,\mathrm{d}t.$$

Taking into account a constraint, the modified action $\tilde{\mathcal{S}}$ will be

$$\tilde{\mathcal{S}}[r, \phi] = \int \frac{1}{2} m\dot{r}^2 + \frac{1}{2} m r^2 \dot{\phi}^2 + mgr\cos(\phi) - \lambda(t)\left(r(t) - R\right)\,\mathrm{d}t.$$

The Euler-Lagrange equation in r for this modified action is then

$$\begin{aligned}\frac{\delta\tilde{\mathcal{S}}}{\delta r} &= \frac{\partial L^*}{\partial r} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L^*}{\partial \dot{r}} \\ &= \left(0 + mr\dot{\phi} + mg\cos(\phi) - \lambda\right) - \frac{\mathrm{d}}{\mathrm{d}t}\left(m\dot{r}\right) \\ &= mr\dot{\phi}^2 + mg\cos(\phi) - \lambda - m\ddot{r}.\end{aligned}$$

For a minimum this must be equal to zero, and hence one forms an equation of motion:

$$m\ddot{r} = \underbrace{mr\dot{\phi}^2}_{\substack{\text{centrifugal} \\ \text{force}}} + \underbrace{mg\cos(\phi)}_{\substack{\text{projection of weight} \\ \text{along the rod}}} - \underbrace{\lambda.}_{\substack{\text{tension in} \\ \text{pendulum rod,} \\ \text{constraining } r \\ \text{to be } R}}$$

The parameter $\lambda(t)$ is chosen such that the constraint is satisfied, i.e. $r(t) = R$ thus $\dot{r} = \ddot{r} = 0$, hence

$$\Rightarrow \lambda = mr\dot{\phi}^2 + mg\cos(\phi).$$

The Euler-Lagrange equation in ϕ is

$$\begin{aligned}\frac{\delta\tilde{\mathcal{S}}}{\delta\phi} &= \frac{\partial L^*}{\partial \phi} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L^*}{\partial \dot{\phi}} \\ &= -mgr\sin(\phi) - \frac{\mathrm{d}}{\mathrm{d}t}\left(mr^2\dot{\phi}\right).\end{aligned}$$

Again, at minimum this must be equal to zero and so

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(r^2\dot{\phi}\right) = -gr\sin(\phi).$$

From the constraint $r = R \to \dot{r} = 0$, and thus

$$\begin{aligned} R^2\ddot{\phi} &= -gR\sin(\phi) \\ \Rightarrow \ddot{\phi} &= -\frac{g}{R}\sin(\phi). \end{aligned}$$

Example 5.8

Consider an isperimetric problem in terms of an arc length $S \in [0, L]$, where L is a fixed value of path length. The are enclosed by the path is

$$S = \oint y\,\mathrm{d}x = \int_0^L y\,\frac{\mathrm{d}x}{\mathrm{d}s}\,\mathrm{d}s,$$

where the functions $x(s)$ and $y(s)$ are not independent, i.e.

$$\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}s}\right)^2 = 1.$$

The auxiliary functional is then

$$S[x,y] = \int \underbrace{\left(y\,\frac{\mathrm{d}x}{\mathrm{d}s} - \lambda(s)\left(\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}s}\right)^2\right)\right)}_{=g(y,x_s,y_s;s)}\,\mathrm{d}s.$$

There is no explicit dependence on x so

$$\begin{aligned} \frac{\partial g}{\partial x} &= 0 \\ \frac{\partial g}{\partial x_s} &= y - 2\lambda x_s = Q = \text{const.} \end{aligned}$$

The Euler-Lagrange equation in y is then

$$\begin{aligned}\frac{\delta S}{\delta y} &= \frac{\partial g}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}s}\frac{\partial g}{\partial y_s} \\ &= x_s - \frac{\mathrm{d}}{\mathrm{d}s}\left(-2\lambda y_s\right).\end{aligned}$$

As before, for this to be minimised set it equal to zero:

$$\begin{aligned}x_s + \frac{\mathrm{d}}{\mathrm{d}s}\left(2\lambda y_s\right) &= 0 \\ x = -2\lambda y_s &= P = \text{const.}\end{aligned}$$

Using the equations for P and Q to get

$$\begin{aligned}\frac{x-P}{y-Q} = \frac{-2\lambda y_s}{2\lambda x_s} = -\frac{y_s}{x_s} &= -\frac{\mathrm{d}y}{\mathrm{d}x} \\ \rightarrow (x-P)\,\mathrm{d}x &= -(y-Q)\,\mathrm{d}y \\ (x-P)\,\mathrm{d}x + (y-Q)\,\mathrm{d}y &= 0 \\ \Rightarrow (x-P) + (y-Q) &= \text{const.} = R^2,\end{aligned}$$

which is again the equation for a circle.

Consider the problem of finding the stationary point of a certain functional of the form

$$I[\phi] = (\phi, L\phi) = \int_a^b \phi^* L\phi \,\mathrm{d}x,$$

where L is Hermitian, i.e. $L = L^\dagger$. This system is subject to a constraint

$$J[\phi] = (\phi, \rho\phi) = \int_a^b \phi^* \rho\phi \,\mathrm{d}x,$$

where ρ is real and non-negative. Taking the auxiliary equation $K[\phi] =$

$I[\phi] - \lambda J[\phi]$ which must satisfy $\delta k = \delta I - \lambda \delta J = 0$ then

$$\begin{aligned}
\delta K &= \delta I - \lambda \delta J = 0 \\
&= \delta\left(\phi, L\phi\right) - \lambda \delta\left(\phi, \rho\phi\right) \\
&= \int_a^b \delta\left(\phi^* L\phi\right)\, \mathrm{d}x - \lambda \int_a^b \delta\left(\phi^* \rho\phi\right)\, \mathrm{d}x \\
&= \int_a^b \delta\left(\phi^*\right) L\phi\, \mathrm{d}x + \int_a^b \phi^* L\delta\left(\phi\right)\, \mathrm{d}x - \lambda \int_a^b \delta\left(\phi^*\right) \rho\phi\, \mathrm{d}x - \lambda \int_a^b \phi^* \rho\delta\left(\phi\right)\, \mathrm{d}x \\
&= \int_a^b \left(\delta\phi^*\right)\left(L\phi - \lambda\rho\phi\right) + \left(\phi^* L - \lambda\phi^*\rho\right)\left(\delta\phi\right)\, \mathrm{d}x.
\end{aligned}$$

For this to be zero it would be easiest if the coefficients of $\delta\phi$ and $\delta\phi^*$ were equal but $\delta\phi^* \equiv (\delta\phi)^*$ and so there is no guarantee that they will be independent functions. Instead using

$$f\delta\phi^* + g\delta\phi = 0$$

and expanding $\delta\phi^{(*)}$ as real and complex components, i.e. $\delta\phi = \delta u + i\delta v$ and $\delta\phi^* = \delta u - i\delta v$, then now there are usable independent functions δu and δv. Therefore

$$\begin{aligned}
f\delta\phi^* + g\delta\phi &= f\left(\delta u - i\delta v\right) + g\left(\delta u + i\delta v\right) \\
&= \left(f + g\right)\delta u - i\left(f - g\right)\delta v.
\end{aligned}$$

These were the coefficients of $\delta\phi^*$ and $\delta\phi$ so it is as if $\delta\phi^*$ and $\delta\phi$ could be regarded as independent. Within the integral one now has

$$\begin{aligned}
f = L\phi - \lambda\rho\phi = 0 &\rightarrow L\phi = \lambda\rho\phi; \\
g = \left(L\phi\right)^* - \lambda\rho\phi^* = 0 &\rightarrow \left(L\phi\right)^* = \lambda\rho\phi^* \\
&\rightarrow L\phi = \lambda^*\rho\phi.
\end{aligned}$$

The two equations in λ are consistent for λ being real, which is true for Hermitian operators, which is what was assumed. If the operator L were not Hermitian then the equations may be inconsistent, so the trick of regarding $\delta\phi^*$ and $\delta\phi$ as being independent is only true in the Hermitian case. If L is the Sturm-Liouville operator there is an infinite number of solutions, i.e. $\lambda = \lambda_0, \lambda_1, \ldots$.

5.8 The Catenary

Definition 5.5: Catenary

Deriving from the Latin *catena*, meaning in relation to a chain, the **catenary** problem in mathematics concerns a chain or inextensible rope being fixed at either end and allowed to hang freely.

5.9 The Rayleigh-Ritz Method

The Rayleigh-Ritz method is used to calculate the smallest eigenvalue of a Sturm-Liouville equation, i.e. equations of the form

$$Lu_0 = \lambda_0 \rho u_0,$$

where λ_0 is the smallest eigenvalue. Taking the scalar product of both sides with the eigenfunction u_0

$$\begin{aligned}(u_0, Lu_0) = (u_0, \lambda_0 \rho u_0) = \lambda_0 (u_0, \rho u_0) \\ \Rightarrow \lambda_0 = \frac{(u_0, Lu_0)}{(u_0, \rho u_0)} = \frac{I[u_0]}{J[u_0]}.\end{aligned}$$

This suggests that one should study the functional of the form

$$\overline{K}[\phi] = \frac{I[\phi]}{J[\phi]},$$

where the overline has been used to distinguish the functional from a kernel and ϕ is a general variable which satisfies the same boundary conditions as u_0. ϕ can be expanded in terms of the eigenfunctions u_n, i.e.

$$\phi(x) = \sum_{n=0}^{\infty} c_n u_n(x),$$

where $Lu_n = \lambda_n u_n$ and $(u_n, \rho u_n) = 1$, i.e. ρ is normalised. From earlier, one can use the form to find $I[\phi]$;

$$\begin{aligned} I[\phi] &= (\phi, L\phi) \\ &= \sum_{n=0}^{\infty} c_n^* u_n^* \lambda_n c_n u_n \\ &= \sum_{n=0}^{\infty} |c_n|^2 \geq \sum_{n=0}^{\infty} \lambda_0 |c_n|^2, \end{aligned}$$

with equality holding for $c_n = 0 \; \forall \; n \neq 0$, and $J[\phi]$;

$$\begin{aligned} J[\phi] &= (\phi, \rho\phi) \\ &= \sum_{n=0}^{\infty} c_n^* u_n^* \rho c_n u_n \\ &= \sum_{n=0}^{\infty} |c_n|^2 u_n^* \rho u_n \\ &= \sum_{n=0}^{\infty} |c_n|^2. \end{aligned}$$

The functional then becomes

$$\overline{K} = \frac{I[\phi]}{J[\phi]} \geq \frac{\sum_{n=0}^{\infty} |c_n|^2 \lambda_0}{\sum_{n=0}^{\infty} |c_n|^2} = \lambda_0,$$

and thus by inserting any ϕ into $\overline{K}$ gives an upper bound on the smallest eigenvalue. This is to say that if one were to choose some ϕ which depends on a variable x and a set $\{\alpha_i\}$, i.e. $[\phi(x, \{\alpha_i\})]$, then

$$\overline{K}[\phi(x, \{\alpha_i\})] = \kappa(\{\alpha_i\}) \geq K_0.$$

The Rayleigh-Ritz method is to choose the parameters $\{\alpha_i\}$ such that it minimises $\kappa(\{\alpha_i\})$ and providing a close upper limit on λ_0.

Example 5.9

Consider oscillations on a circular drum head of radius 1. The transverse displacement u obeys the scalar Helmholtz equation, i.e.

$$\nabla^2 u + k^2 u = 0.$$

This is subject to boundary conditions $u(1) = 0$ and $u(0)$ is finite, i.e. the rim is fixed and $\frac{1}{r} \not\to \infty$ at the centre. In polar coordinates, for $u = u(r)$

$$\begin{aligned} \nabla^2 u = \frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}u}{\mathrm{d}r} &= -k^2 u \\ \to -\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}u}{\mathrm{d}r}\right) &= k^2 r u \\ \Rightarrow -u\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}u}{\mathrm{d}r}\right) &= k^2 r u^2. \end{aligned}$$

From this one sees that $\rho(r) = r$, and so

$$I[u] = -\int_0^1 u\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}u}{\mathrm{d}r}\right)\mathrm{d}r = -\underbrace{[\ldots]_0^1}_{=0 \text{ by b.c.'s}} + \int_0^1 r\left(\frac{\mathrm{d}u}{\mathrm{d}r}\right)\mathrm{d}r$$

$$J[u] = \int_0^1 r u^2 \,\mathrm{d}r.$$

Making a trial function that satisfies the boundary conditions of $u(r) =$

$1 - r^{2\alpha}$ where $\alpha > 0$, then

$$\begin{aligned} I[u] &= \int_0^1 r \left(\frac{\mathrm{d}u}{\mathrm{d}r}\right)^2 \mathrm{d}r \\ &= \int_0^1 r \left(\frac{\mathrm{d}}{\mathrm{d}r}\left(1 - r^{2\alpha}\right)\right)^2 \mathrm{d}r \\ &= \int_0^1 r \left(-2\alpha r^{2\alpha-1}\right)^2 \mathrm{d}r \\ &= 4\alpha^2 \int_0^1 r^{4\alpha-1} \,\mathrm{d}r \\ &= \frac{4\alpha^2}{4\alpha} = \alpha \end{aligned}$$

$$\begin{aligned} J[u] &= \int_0^1 r u^2 \,\mathrm{d}r \\ &= \int_0^1 r \left(1 - r^{2\alpha}\right)^2 \mathrm{d}r \\ &= \int_0^1 \left(r - 2r^{2\alpha+1} + r^{4\alpha+1}\right) \mathrm{d}r \\ &= \left[\frac{1}{2}r^2 - \frac{2r^{2\alpha+2}}{2\alpha+2} + \frac{r^{4\alpha+2}}{4\alpha+2}\right]_0^1 \\ &= \frac{1}{2} - \frac{2}{2\alpha+2} + \frac{1}{4\alpha+2} \\ &= \frac{\alpha^2}{(\alpha+1)(2\alpha+1)}. \end{aligned}$$

Therefore

$$\kappa(\alpha) = \overline{K}[u] = \frac{I[u]}{J[u]} = \frac{\alpha}{\left(\frac{\alpha^2}{(\alpha+1)(2\alpha+1)}\right)} = 2\alpha + 3 + \frac{1}{\alpha}.$$

In order to find the smallest eigenvalue, find the turning point of this functional, i.e.

$$\frac{\mathrm{d}\overline{K}}{\mathrm{d}\alpha} = 2 - \frac{1}{\alpha^2} \Rightarrow \alpha = \pm\sqrt{\frac{1}{2}}.$$

Using this one can estimate the smallest eigenvalue:

$$\begin{aligned} K_0^2 &< K\left(\alpha = \frac{1}{\sqrt{2}}\right) \\ &< \frac{2}{\sqrt{2}} + 3 + \sqrt{2} \\ &< 2\sqrt{2} + 3 \approx 5.828. \end{aligned}$$

The true solution to the problem is a Bessel function whose value is $K_0^2 = 5.783$, thus the simple trial solution gives a good approximation.

5.9.1 Application to Quantum Mechanics

5.10 The Completeness Theorem for Hermitian Sturm-Liouville Operators