Mathematical Methods for Physics

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March 21, 2022

Contents

1. Second Order ODEs and Sturm-Liouville theory

1.1 General 2nd Order ODEs

Arfken 7.4, 7.6
(Riley 15.0,15.2)

1.1.1 Introduction

Consider a general linear second order differential equation:[1]

$$p_0(x)y''(x) + p_1(x)y'(x) + q(x)y(x) = f(x). \tag{1.1}$$

It is linear because each term on the LHS contains only y, y' or y'', not for instance y^2 or yy'. The functions p_0, p_1, q, and f are assumed to be given and may be complex (but usually are real), and we want to find y. Usually the functions are defined on a given domain $a \leq x \leq b$.

We often write this schematically as

$$\mathcal{L}y(x) = f(x), \tag{1.2}$$

where $\mathcal{L}$ is a differential operator that acts on one function to produce another.

The space of functions we will be interested in is that of complex functions of the real variable x which are square-integrable on the interval $x \in [a, b]$, denoted $L_2[a, b]$. These form a vector space with an inner product (a Hilbert space). We will usually require them to be at least twice differentiable, except possibly at isolated points, and will not constantly refer to such restrictions.

If $f(x) \neq 0$ the equation is inhomogeneous; if $f(x) = 0$ the equation is homogeneous:

$$p_0(x)y''(x) + p_1(x)y'(x) + q(x)y(x) = 0. \tag{1.3}$$

Linearity implies that if y_1 and y_2 are both solutions of the homogeneous equation, then so is $Ay_1 + By_2$ for (complex) constants A and B.

Often we divide (1.1) by $p_0(x)$ to get the alternate form of the equation

$$y''(x) + P(x)y'(x) + Q(x)y(x) = F(x). \tag{1.4}$$

or for the homogeneous case

$$y''(x) + P(x)y'(x) + Q(x)y(x) = 0. \tag{1.5}$$

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[1]Most of the time after this introductory section we will be concerned with problems in which $p_0' = p_1$, in which case we will denote p_0 and q_0 by $-p$ and q.

At most values of x, $P(x)$ and $Q(x)$ are finite; such points are ordinary points of the equation. If, in the vicinity of some point x_0, $P(x)$ or $Q(x)$ diverges, but $(x - x_0)P(x)$ and $(x - x_0)^2Q(x)$ are finite, x_0 is called a *regular singular point*. If $P(x)$ diverges faster than $1/(x - x_0)$ and/or $Q(x)$ diverges faster than $1/(x - x_0)^2$ we speak of an irregular singular point. The relevance of this classification for the solutions is as follows: at an ordinary point solutions are analytic and have Taylor expansions with a radius of convergence governed by the distance to the nearest singular point in the complex plane. At a regular singular point a solution may be analytic or at worst will have a pole or a branch point; at least one solution will exist of the form $y(x) = (x - x_0)^s u(x)$ where $u(x)$ is analytic and s is a number called the indicial exponent. (This is called Fuchs' theorem.) We will meet this again when we seek series solutions of common differential equations.

1.1.2 Linear independence and second solutions

It is useful to have a way to check if a set of n functions $\{u_i(x)\}$ are linearly independent. By definition if they not, we can find a set of coefficients c_i, not all zero, such that for all x in the domain, $\sum_i^n c_i u_i(x) = 0$. Assuming the functions to be differentiable at least $n - 1$ times, we can obtain further equations for the coefficients by differentiating this equation multiple times; writing the mth derivative of u_i as $u_i^{(m)}$, we can combine the first $n - 1$ equations formed that way with the original to get:

$$\begin{pmatrix} u_1 & u_2 & \dots & u_n \\ u_1' & u_2' & \dots & u_n' \\ \vdots & \vdots & \vdots\vdots\vdots & \vdots \\ u_1^{(n-1)} & u_2^{(n-1)} & \dots & u_n^{(n-1)} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = 0 \tag{1.6}$$

For any given x this is just a matrix equation, and it can only hold, for c_i not all zero, if the determinant of the matrix vanishes. This determinant is called the Wronskian of the functions (the "W" is silent).

So if a set of functions is not linearly independent over a domain, their Wronskian vanishes for all x in the domain. The converse is true also true in all cases of interest to us: a vanishing Wronskian implies linear dependence. Linearly-independent functions will have a Wronskian which does not vanish (except possibly at isolated points).

The Wronskian allows us to determine that there are at most two independent solutions of a homogeneous 2nd order equation. Consider three solutions of the homogeneous equation (1.5), y_1, y_2 and y_3. Then

$$W(x) = \begin{vmatrix} y_1 & y_2 & y_3 \\ y_1' & y_2' & y_3' \\ y_1'' & y_2'' & y_3'' \end{vmatrix} = - \begin{vmatrix} y_1 & y_2 & y_3 \\ y_1' & y_2' & y_3' \\ Py_1' + Qy_1 & Py_2' + Qy_2 & Py_3' + Qy_3 \end{vmatrix} = 0. \tag{1.7}$$

The determinant vanishes because its third row is a linear combination of the first two. So there cannot be three independent solutions; one of the three must be a linear combination of the others. (The proof generalises to n solutions of an nth-order equation, and to a single solution of a first-order one.)

Given one solution y_1, we can always construct another linearly independent one. We have $W[y_1(x), y_2(x)] = y_1y_2' - y_2y_1'$, and

$$\frac{\mathrm{d}W}{\mathrm{d}x} = y_1y_2'' - y_2y_1''$$
$$= -y_1(Py_2' + Qy_2) + y_2(Py_1' + Qy_1) = -P(x)W(x),$$

and so, since $\int (W'/W)\,\mathrm{d}x = \ln W$, we obtain

$$W(x) = \exp\left(-\int^x P(x')\mathrm{d}x'\right). \tag{1.8}$$

Furthermore we can rewrite

$$W = y_1 y_2' - y_2 y_1' = y_1^2 \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{y_2}{y_1}\right) \qquad \Rightarrow \qquad \frac{y_2}{y_1} = \int^x \frac{W(x')}{y_1^2(x')}\mathrm{d}x' \tag{1.9}$$

So finally

$$y_2(x) = y_1(x)\int^x \frac{\exp\left(-\int^{x'} P(z)\mathrm{d}z\right)}{y_1^2(x')}\mathrm{d}x'. \tag{1.10}$$

Thus (except at singular points) we can construct a second solution. It may not be orthogonal to the first, but we can make it so by subtracting off the appropriate amount of y_1 (Gram-Schmidt orthogonalisation). The general solution of the homogeneous equation is $Ay_1 + By_2$, where y_1 an y_2 are two linearly independent solutions.

An example is a second solution to the differential equation $(1 - x^2)y'' - 2xy' + 2y = 0$ (Legendre's equation with $l = 1$) for which $y_1 = x$ is clearly a solution. Dividing by $(1 - x^2)$ we have $P = -2x/(1 - x^2)$. The second solution is then

$$y_2(x) = x\int^x \frac{\exp\left(-\int^u \frac{-2z}{1-z^2}\mathrm{d}z\right)}{u^2}\mathrm{d}u = x\int^x \frac{1}{(1-u^2)u^2}\mathrm{d}u = \frac{x}{2}\log\left(\frac{1+x}{1-x}\right) - 1 \tag{1.11}$$

where we have dropped a term cx which would arise from the final constant of integration, since that is a multiple of y_1. This solution diverges at the regular singular points $x = \pm 1$. For future reference we note that this function is given the symbol $Q_1(x)$, while the polynomial solution is $P_1(x) = x$.

Returning to the *inhomogeneous* equation $\mathcal{L}u = f$, if u and v are both solutions we have $\mathcal{L}(u - v) = 0$. So $u - v$ is a solution of the homogeneous equation. We can write the general solution to the inhomogeneous equation as $u(x) + Ay_1(x) + By_2(x)$, where u is *any* solution of the inhomogeneous equation. $u(x)$ is called the *particular integral* and the rest the *complementary function*.

1.1.3 Boundary conditions

Up till now we have not mentioned boundary conditions. As we only have two unknown constants in our general solution, we only get to specify two conditions to give a unique solution. We have to distinguish between *homogeneous* and *inhomogeneous* boundary conditions: a homogeneous condition is one such that if functions u and v satisfy it, so will $Cu + Dv$ for constants C and D. Examples are $u(a) = 0$ or $u'(b) = 0$. Inhomogeneous conditions set a scale, eg $u(a) = 1$. *Initial value* conditions specify $u(a)$ and $u'(a)$ (or similarly at b) and are necessarily inhomogeneous (or else we will force $u = 0$ everywhere) while *separated boundary conditions* give one condition at each of a and b and can be either homogeneous or inhomogeneous. *Periodic boundary conditions* relate u and u' at a and b, and are homogeneous.

If we have both a homogeneous equation and homogeneous boundary conditions, there is nothing in either to set a scale and $Cu + Dv$ will be a solution if u and v are. However, with a homogeneous equation we cannot in fact impose arbitrary homogeneous boundary conditions at a and b. For example if $\mathcal{L}y = y'' + y$, the solutions are $y = A\cos x + B\sin x$. If we want

boundary conditions $y(0) = 0$ and $y(1) = 0$, we find $A = 0$ from the first condition, but also $B = 0$ from the second.

However there is a class of homogeneous equations that have undetermined parameters in q, eg

$$y'' + \lambda y = 0, \qquad (1.12)$$

where λ, a constant, is not known. Then we can ask for what values of λ the desired boundary conditions can be satisfied. In this case, we know the answer is $\lambda = (n\pi)^2$ for integer n, and the solution is $y = B \sin(n\pi x)$.

In these problems we separate the term with the undetermined parameter from qy and rewrite the equation as

$$p_0(x)y''(x) + p_1(x)y'(x) + q_0(x)y(x) = \lambda\rho(x)y(x) \qquad \text{or} \qquad \mathcal{L}y(x) = \lambda\rho(x)y(x). \qquad (1.13)$$

Written in this form it is clearly an eigenvalue equation (or a generalised eigenvalue equation if $\rho \neq 1$), and we will see much more of such equations. If the homogeneous equation and given boundary conditions does have a solution, then the corresponding eigenvalue problem has $\lambda = 0$ as an eigenvalue.

Section A.4 collects the principal equations that we will consider in this part of the course, with notes on their physical origin and (where appropriate) parameters and eigenvalues; it should be read now though some of the details will only be clarified subsequently.

1.2 Sturm-Liouville theory

Arfken 8.1-3
Riley 17.1-4

1.2.1 Sturm-Liouville and Hermitian operators

A particularly useful class of equations have a more restricted form of Eq. (1.3) with $p_1 = p_0'$:

$$-\frac{\mathrm{d}}{\mathrm{d}x}\Big(p(x)y'(x)\Big) + q(x)y(x) = 0 \qquad \Rightarrow \qquad \mathcal{L}y \equiv -(py')' + qy \qquad (1.14)$$

with $q(x)$ real, and $p(x)$ positive for $x \in (a, b)$. $\mathcal{L}$ is called a Sturm-Liouville operator.

Why are these interesting?

Consider, for a Sturm-Liouville operator and two functions u and v defined on $x \in [a, b]$,

$$\begin{aligned}
\int_a^b v^*(x)\mathcal{L}u(x)\,\mathrm{d}x &= \int_a^b -v^*(pu')' + v^*qu\,\mathrm{d}x \\
&= \left(\int_a^b -u^*(pv')' + u^*qv\,\mathrm{d}x\right)^* + \Big[p(uv^{*\prime} - v^*u')\Big]_a^b \\
&= \left(\int_a^b u^*(x)\mathcal{L}v(x)\,\mathrm{d}x\right)^* + \Big[p(uv^{*\prime} - v^*u')\Big]_a^b. \qquad (1.15)
\end{aligned}$$

where we have integrated the first term twice by parts.

Ignoring the boundary terms, this is very reminiscent of the definition of a *Hermitian* operator

$$\langle v|\hat{H}u\rangle = \langle \hat{H}v|u\rangle \equiv \langle u|\hat{H}v\rangle^*. \qquad (1.16)$$

Hermitian operators have many useful properties and we would like to prove the same for Sturm-Liouville operators. However a Sturm-Liouville operator is only Hermitian (or *self-adjoint*) if the space of functions on which it acts is restricted to those which satisfy appropriate boundary conditions, such that the term $[p(uv^{*\prime} - v^*u')]_a^b$ vanishes.

This can only be satisfied by homogeneous boundary conditions, either periodic where the values of $p(uv^{*\prime} - v^*u')$ at a and b are non-zero but equal and so cancel, or separated where $p(uv^{*\prime} - v^*u')$ vanishes at both a and b. A *regular* SL equation has the form of Eq. (1.14), with $p(x) > 0$ for $x \in [a, b]$, and with separated homogeneous boundary conditions.[2]

Suitable separated boundary conditions have the general homogeneous form (applicable to both u and v):

$$\alpha_a u'(a) + \beta_a u(a) = 0 \qquad \text{and} \qquad \alpha_b u'(b) + \beta_b u(b) = 0 \qquad (1.17)$$

where α_a etc are finite constants and at least one of (α_a, β_a) and of (α_b, β_b) are non-zero. If p itself vanishes at a or b we don't need to specify a condition on u and v there, except that they and their first derivatives should be finite; however in this case a or b (or both) is a singular point.

These boundary conditions include the commonly-met cases of either the function or its derivative vanishing at the boundaries, but also a fixed ratio of the function and its derivative, that is a fixed value of the log derivative $(\ln u)'$.

1.2.2 Sturm-Liouville eigenvalue equations

As in Eq. (1.13), we consider equations in which $q(x)$ has an undetermined constant λ in it, which we separate out to write

$$-\frac{\mathrm{d}}{\mathrm{d}x}\Big(p(x)y'(x)\Big) + q(x)y(x) = \lambda\rho(x)y(x) \qquad \text{or} \qquad \mathcal{L}y = \lambda\rho y \qquad (1.18)$$

with $q(x)$ real, and $p(x)$ and $\rho(x)$ positive for $x \in (a, b)$ (This time we don't bother to relabel q as q_0, it will be clear from the context.) This is a Sturm-Liouville equation, and we will assume boundary conditions such that $\mathcal{L}$ is Hermitian.

As already discussed, for an arbitrarily chosen λ we have a homogeneous equation and homogeneous boundary conditions, and there will be no solution in general. So the problem becomes that of finding both the values of λ for which solutions exist, the eigenvalues, and the corresponding eigenfunctions.

A number of results follow directly.

Reality of eigenvalues, generalised orthogonality of eigenfunctions

If y_i and y_j are both eigenfunctions satisfying $\mathcal{L}y_n = \lambda_n\rho y_n$ (ρ being positive), we have

$$\int_a^b y_j^* \mathcal{L}y_i \, \mathrm{d}x = \left(\int_a^b y_i^* \mathcal{L}y_j \mathrm{d}x\right)^* \qquad \Rightarrow \qquad (\lambda_i - \lambda_j^*)\int_a^b y_j^* \rho y_i \, \mathrm{d}x = 0. \qquad (1.19)$$

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[2] We will use "Hermitian" and "self-adjoint" interchangeably. In the more mathematical literature, "self-adjoint" is more restrictive: if the operator is self-adjoint then the vanishing of the boundary term $[...]_a^b$ requires *both* u and v to satisfy the boundary conditions. For a regular Sturm-Liouville operator, with separated homogeneous boundary conditions and $p > 0$, this will obviously be true, since eg $u(a) = u(b) = 0$ is not sufficient without $v(a) = v(b) = 0$ also. The properties of the spectrum of eigenvalues and form of the corresponding eigenvectors that we describe later require self-adjointness. In the physics literature the distinction is rarely made, and the current editions of both Riley and Arfken use "Hermitian". Somewhat confusingly, they use "self-adjoint" for the property of the operator where I have used "Sturm-Liouville", with Hermiticity requiring appropriate boundary conditions on u and v in addition.

If we set $i = j$, the integral is positive definite so we have $\lambda_i - \lambda_i^* = 0$, ie the eigenvalues of $\mathcal{L}$ are real. Conversely if they belong to different eigenvalues, we need the integral to vanish. So the eigenfunctions belonging to different eigenvalues satisfy a generalised orthogonality condition

$$\int_a^b y_j^*(x)\rho(x)y_i(x)\,\mathrm{d}x = 0 \qquad \text{for } \lambda_i \neq \lambda_j. \tag{1.20}$$

(Note we will often refer to this simply as "orthogonality", the "generalised" being implied if $\rho \neq 1$.)

Reality of eigenfunctions

Although up to now we have allowed for the eigenfunctions to be complex, we now see that we can choose them to be real. Recall the functions p, q and ρ are real, so if $y_i = u_i + iv_i$, u_i and v_i both being real, then u_i and v_i must separately be real eigenfunctions of $\mathcal{L}$ with the same eigenvalue. If this eigenvalue is non-degenerate, this means u_i and v_i are just multiples of the same function, and $y_i = Cu_i$, C being a constant; we can then take the (real) u_i in place of y_i as the eigenfunction for this eigenvalue. If there is degeneracy, ie a second eigenfunction for the same eigenvalue $\tilde{y}_i = \tilde{u}_i + i\tilde{v}_i$, then $\tilde{u}_i$ and $\tilde{v}_i$ are solutions as well, but only two of u_i, v_i, $\tilde{u}_i$ and $\tilde{v}_i$ are linearly independent (see next subsection) and we can chose an orthogonal pair to be our two real eigenfunctions for this eigenvalue.

Degeneracy of eigenfunctions

We can easily show that a regular SL problem has only one independent solution for a given eigenvalue λ, while periodic boundary conditions allow for two.

Suppose that y_1 and y_2 are (real) solutions corresponding to the same λ. We write $\tilde{\mathcal{L}} = \mathcal{L} - \rho\lambda$, and note that as λ and ρ are real, $\tilde{\mathcal{L}}$ is also Hermitian, so we can treat this as a simple homogeneous equation: $\tilde{\mathcal{L}}y = 0$.

First, we note that the expression that enters the boundary term in (1.15) can be written in terms of the Wronskian, $p(y_1y_2' - y_2y_1') = pW[y_1, y_2]$, and so with separated bcs and positive p, Hermiticity requires that $W(a) = W(b) = 0$.

Now comparing the SL equation (1.14) with the form of Eq. (1.5), the function we called P corresponds to p'/p, and so from Eq. (1.8) the Wronskian of two independent solutions is given by

$$W[y_i(x), y_2(x)] \propto \exp\left(-\int^x \frac{p'(x')}{p(x')}\mathrm{d}x'\right) = \frac{W_0}{p(x)} \tag{1.21}$$

where W_0 is a constant. But $p(x) > 0$, so the vanishing of W at the boundaries requires $W_0 = 0$. Hence $W(x) = 0$ for all $x \in [a, b]$. So a regular SL equation with a given eigenvalue λ cannot have two independent solutions. (Recall the problem above, (1.12), where only the $\sin(n\pi x)$ solution survived after the bcs were imposed.)

This assumes separated boundary conditions; the other possibility for Hermiticity is that $W(b)p(b)$ and $W(a)p(a)$ cancel, so $W(a)$ need not vanish. This is exactly what we get from Eq. (1.21): if two solutions do exist their Wronskian satisfies $W(x)p(x) = \text{const}$. The periodic boundary conditions $y(a) = y(b)$ and $p(a)y'(a) = p(b)y'(b)$ are consistent with this and thus two solutions can indeed exist (cf $\cos(n\pi x)$ and $\sin(n\pi x)$). These two solutions can be chosen to be orthogonal to one another, so in fact we can arrange that all eigenfunctions, not just those corresponding to different eigenvalues, are orthogonal and we can replace the condition in (1.20) with "$i \neq j$".

Eigenfunctions as a basis; classification of eigenfunctions by the number of nodes

For Hermitian operators in a finite N-dimensional space, N orthogonal eigenvectors automatically form a basis, and any vector in the space can be expressed as a sum over the eigenvectors. For an infinite-dimensional function space this is not obvious, but it is true. We will prove it in the final section of the course if time permits. For the particular case $\mathcal{L}y \equiv -y''$, the eigenfunctions are sines and/or cosines (depending on the boundary conditions) and the fact that they form a basis leads to Fourier analysis. As another example, Legendre polynomials form a complete set on the interval $[-1, 1]$ with the boundary condition $(py')(\pm 1) = 0$, where $p = (1 - x^2)$, which in practice just requires "well-behaved" (finite) functions.[3] The expansion of a function $f(x)$ in a complete set of orthonormal functions $\{\phi_i(x)\}$ obeying $\int_a^b \phi_j^* \rho \phi_i \mathrm{d}x = \delta_{ij}$ is

$$f(x) = \sum_{i=1}^{\infty} f_i \phi_i(x) \qquad \text{where} \qquad f_i = \int_a^b \phi_i^*(x) \rho(x) f(x)\, \mathrm{d}x. \tag{1.22}$$

Convergence of the series is taken to be convergence "in the mean", which implies that

$$\lim_{n \to \infty} \int_a^b \left| f(x) - \sum_{i=1}^{n} f_i \phi_i(x) \right|^2 \rho(x) \mathrm{d}x = 0 \tag{1.23}$$

and which is still satisfied if there are a finite number of discontinuities, though the "Gibbs phenomenon" (a failure to reproduce the function in the immediate vicinity of the discontinuity) occurs.

Completeness of a set of orthonormal vectors $\{|n\rangle\}$ in N dimensions can be written

$$\sum_{n=1}^{N} |n\rangle\langle n| = \hat{I}; \tag{1.24}$$

the equivalent in functional form is

$$\delta(x - x') = \sum_{i=1}^{\infty} \phi_i(x) \phi_i^*(x') \rho(x'). \tag{1.25}$$

This can be verified by multiplying both sides of (1.25) by $f(x')$ and integrating wrt x' to get $\sum_{i=1}^{\infty} f_i \phi_i(x) = f(x)$.

In the above the numbering $\phi_1, \phi_2 \ldots$ is arbitrary. But in fact sets of eigenfunctions of a regular SL operator have a natural ordering, because the eigenfunctions can be classified by the number of nodes (excluding any at a and b). This isn't completely obvious, and will not be proved in full. But it can be shown that if we have a pair of eigenvalues λ and μ with corresponding solutions y_λ and y_μ, and if $\lambda > \mu$, then y_λ has at least one zero between each pair of zeros of y_μ, and also between each end-point and the nearest (first or last) zero of y_μ, and hence has more zeros than y_μ. This shows that the eigenvalues are not continuous (an infinitesimal change in λ can't change the function to the point where develops a new node[4]) but have a discrete spectrum. We can therefore list the eigenvalues in ascending order

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[3]For analytic functions there is a unique Taylor-Laurent series about $x = 0$ which can be re-expressed as a sum over Legendre polynomials, which establishes completeness in that particular case.

[4]The exception would be if the function had a local minimum which dropped through zero to created two new nodes at once, but for analytic p and q it is easy to show that it is not possible for y and y' to vanish at the same point. Otherwise all higher derivatives would vanish and the function itself would be zero for all x.

$\lambda_1 < \lambda_2 < \lambda_3 \dots$ starting with the eigenvalue λ_1 for which the eigenfunction has the fewest nodes, and each subsequent eigenfunction has more nodes than the one before. In fact the number of interior nodes of y_n is exactly $n-1$, and the eigenfunctions are oscillatory in nature. (This is why we chose to write $\mathcal{L}y = -(py')' + qy$ with $p > 0$; had we not included the initial minus sign the eigenvalues would have formed a descending set). The sine or cosine solutions we obtain from $-y'' = \lambda y$ are in fact a very good picture of the solutions for the complicated case, except that in general the nodes are not perfectly evenly spaced.

1.2.3 Application to quantum mechanics and casting equations in Sturm-Liouville form

The properties above (real eigenvalues, discrete spectrum with a lowest or "ground state" eigenvalue, oscillatory solutions with an extra node each time we go up a level) are exactly those that we have frequently met before in quantum-mechanical problems. In one-dimension the Schrödinger equation is clearly an example of an SL equation (where $p(x) = \hbar^2/2m =$const and $q(x) = V(x)$) and the boundary conditions we impose are always homogeneous to preserve the important principle of superposition. However when we separate the Schrödinger equation in plane or spherical polar coordiates we obtain radial equations which are not SL in form, for instance in a 2D infinite square well, for solutions with angular dependence $e^{in\phi}$, we obtain the radial equation

$$r^2 R''(r) + r R'(r) + (k^2 r^2 - n^2) R(r) = 0 \qquad \text{with } k = \sqrt{2mE}/\hbar \text{ and } R(a) = 0. \qquad (1.26)$$

Comparing with the general form of Eq. (1.13), we have $p_0 = r^2$, $q_0 = -n^2$ and $p_1 = r \neq p_0'$. (Note n^2 is just a parameter in the radial equation, related to the angular momentum.) This is a (generalised) eigenvalue problem with $\lambda = k^2$, but it is not of SL form.[5] Can we salvage anything?

The answer is yes. Any 2nd-order linear differential operator such as the LHS of Eq. (1.13) can be cast in SL form by multiplying throughout by an integrating factor $w(x)$, chosen so that $wp_1 = (wp_0)'$. This gives

$$w' = w\left(\frac{p_1}{p_0} - \frac{p_0'}{p_0}\right) \qquad \Rightarrow \qquad w(x) = \frac{1}{p_0(x)} \exp\left(\int^x \frac{p_1(x')}{p_0(x')} dx'\right). \qquad (1.27)$$

In this case $p_1/p_0 = 1/r$ and $w(r) = 1/r$, giving a new equation with the same eigenvalues and eigenfunctions as before, but now in manifestly SL form:

$$-(rR')' + \frac{n^2}{r}R = k^2 r R. \qquad (1.28)$$

The point $r = 0$ is a regular singular point. The boundary condition is $R(a) = 0$; because $p(0) = 0$ the condition at the origin is just that $R(0)$ is finite.

This transformation lets us see that all the desirable properties of an SL equation still hold. The only thing to note is that there is a weight function $\rho = r$ in the orthogonality relation. Of course, this is exactly what we expect from the physical problem, with the element of area being $dS = 2\pi r\,dr$. (The corresponding 3D problem has r^2 as the weight function.) If the nodes of the nth Bessel function are $z_i^{(n)}$, the solutions are $J_n(k_i r)$, where $k_i = z_i^{(n)}/a$.

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[5]Setting $z = kr$ allows us to write this as Bessel's equation, with solution $R(r) = J_n(kr)$, which is very useful except that it no longer looks like an eigenvalue equation.

Another examples of an equation that occurs in QM is Hermite's:

$$y''(z) - 2zy'(z) + 2ny(z) = 0. \tag{1.29}$$

Again it is not in SL form. The integrating factor $w(z)$, and hence the weight factor $\rho(z)$, is e^{-z^2}. For the 1D Schrödinger equation with a quadratic potential, if the full wave function is expressed as a polynomial times the function $e^{-z^2/2}$ which gives the right long-distance behaviour (in suitably-scaled coordinates),[6] some manipulation yields the Hermite equation for the polynomials. Hence the weight factor e^{-z^2} in the orthogonality relation for the polynomials means that the full wave functions do obey the expected orthogonality conditions. See PHYS30201 A.4 for more details.

In the general case we need to check that the new weight function is finite and positive on $x \in (a, b)$.

In the background section of these notes, you will find a list of many of the second-order ODEs that you have met, including all that we will be assuming familiarity with in the next sections, so if you haven't already, you should read section A.4 now. Most of them are not in SL form as presented there, but as we have just seen, that is easily remedied. For the ones that are eigen equations, you should now have a better understanding of the general properties of their eigenvalues and eigenfunctions.

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[6]For the quadratic potential $V = \frac{1}{2}m\omega^2 x^2$ the scaling is the usual $z = x/x_0$ with $x_0 = \sqrt{\hbar/m\omega}$ and $E = (n + \frac{1}{2})\hbar\omega$. The boundary conditions require n to be an integer.

1.3 Generating functions

Arfken 12.1,14.1, 15.1,15.3
Riley 18.1,18.5

1.3.1 Legendre polynomials

Consider the problem in electrostatics of finding the potential at a point $\mathbf{r}$ near the origin of a charge placed on the z-axis at $\mathbf{r}_0 = r_0 \mathbf{e}_z$. We know the answer of course:

$$\Phi(\mathbf{r}) \propto \frac{1}{|\mathbf{r} - \mathbf{r}_0|} = \frac{1}{\sqrt{r^2 + r_0^2 - 2rr_0 \cos\theta}}. \tag{1.30}$$

However we also know that the electric potential must satisfy the Laplace equation $\nabla^2 \Phi(\mathbf{r}) = 0$ except at $\mathbf{r} = \mathbf{r}_0$, and that the general axially-symmetric solution is

$$\Phi(r,\theta) \propto \sum_l \left(A_l\, r^l + \frac{B_l}{r^{l+1}} \right) P_l(\cos\theta) \tag{1.31}$$

(omitting the same constants as in (1.30)). Now it will not be possible to find a single solution of this form valid everywhere: Φ has to be finite both at $r = 0$ and at $r \to \infty$, and only $A_l = B_l = 0$ would allow that. But we are familiar with the idea that a series expansion may have a restricted radius of convergence. In this case, the expression in Eq. (1.30), for any fixed $\cos\theta$, can be expanded as a Taylor series about the the origin, involving only positive powers of r, but that series will have radius of convergence r_0—the distance to the position of the charge.[7] For $r > r_0$ we would need a Laurent series, in this case involving only negative powers of r, instead.

So we have (working in units where $r_0 = 1$ for simplicity)

$$\frac{1}{\sqrt{1 + r^2 - 2r\cos\theta}} = \sum_{l=0}^{\infty} A_l\, r^l\, P_l(\cos\theta) \qquad \text{for } |r| < 1.$$

It remains to find the constants A_l which we do by considering the expression for $\cos\theta = 1$, recalling that with the conventional normalisation $P_l(1) = 1$. Since $(1 - r)^{-1} = 1 + r + r^2 + \dots$ for $|r| < 1$, we see that $A_l = 1$ for all l: So we have

$$\frac{1}{\sqrt{1 + r^2 - 2r\cos\theta}} = \sum_{l=0}^{\infty} r^l\, P_l(\cos\theta) \qquad \text{for } |r| < 1.$$

This expression is called the generating function $g(\cos\theta, r)$ for the Legendre polynomials: Usually the two variable are relabelled, $r \to t$ and $\cos\theta \to x$: then

$$g(x,t) = \frac{1}{\sqrt{1 + t^2 - 2xt}} = \sum_{n=0}^{\infty} t^n\, P_n(x) \qquad \text{for } |t| < 1. \tag{1.32}$$

By constructing the Taylor series in t for the LHS we can read off expressions for the P_l. Formally,[8]

$$P_n(x) = \frac{1}{n!} \frac{\mathrm{d}^n}{\mathrm{d}t^n} g(x,t) \bigg|_{t=0}, \tag{1.33}$$

---

[7]Mathematically, Eq. (1.30), regarded as a function of complex r at fixed real $\cos\theta$, has non-analytic points at $r = \mathrm{e}^{\pm i\theta}$; for $\theta = 0, \pi$ these merge to give a simple pole at $r = \pm 1$, otherwise there are two branch points.

[8]We will meet generating functions for other special functions below; note that the normalisation may vary so that, for instance, for Hermite polynomials the $n!$ is missing from the analogue of (1.33).

but below we will use the known expansion of a binomial series $(1+z)^n$ as a shortcut:

$$
\begin{aligned}
g(x,t) &= (1-(2tx-t^2))^{-\frac{1}{2}} = 1 + \tfrac{1}{2}(2tx - t^2) + \tfrac{3}{8}(2tx - t^2)^2 + \tfrac{5}{16}(2tx - t^2)^3 + \tfrac{35}{128}(2tx - t^2)^4 + \dots \\
&= 1 + \tfrac{1}{2}(2tx - t^2) + \tfrac{3}{8}(4t^2x^2 - 4xt^3 + t^4) + \tfrac{5}{16}(8t^3x^3 - 12t^4x^2 + \dots) + \tfrac{35}{128}(16t^4x^4 + \dots) + \dots \\
&= 1t^0 + xt + \left(\tfrac{3}{2}x^2 - \tfrac{1}{2}\right)t^2 + \left(\tfrac{5}{2}x^3 - \tfrac{3}{2}x\right)t^3 + \left(\tfrac{35}{8}x^4 - \tfrac{15}{4}x^2 + \tfrac{3}{8}\right)t^4 + \dots
\end{aligned}
$$

where in the last two lines we have dropped all terms of order t^5 or higher. From this we can read off the first five Legendre polynomials, eg $P_4(x) = \left(\tfrac{35}{8}x^4 - \tfrac{15}{4}x^2 + \tfrac{3}{8}\right)$.

This provides one way of obtaining the polynomials, but it is more useful for obtaining what are called recurrence relations which relate polynomials of different orders. If for instance we differentiate $g(x,t)$ with respect to t we get

$$
\frac{\partial g}{\partial t} = \frac{x - t}{(1 - 2tx + t^2)^{3/2}} = \frac{x - t}{1 - 2tx + t^2}\, g(x,t)
$$

$$
\Rightarrow \quad \sum_{n=0}^{\infty} n\, t^{n-1} P_n(x) = \frac{x - t}{1 - 2tx + t^2} \sum_{n=0}^{\infty} t^n P_n(x)
$$

$$
\Rightarrow \quad \sum_{n=0}^{\infty} \left(n(t^{n-1} - 2xt^n + t^{n+1}) + (t^{n+1} - xt^n) \right) P_n(x) = 0
$$

$$
\Rightarrow \quad \sum_{n=0}^{\infty} nt^{n-1} P_n(x) - \sum_{n=0}^{\infty}(2n + 1)t^n x\, P_n(x) + \sum_{n=0}^{\infty}(n + 1)t^{n+1} P_n(x) = 0.
$$

By shifting the summation variable $n \to n \pm 1$ in the first and last terms, and regrouping, we get

$$
\sum_{n=0}^{\infty} \Big((n + 1)P_{n+1}(x) - (2n + 1)x\, P_n(x) + nP_{n-1}(x) \Big) t^n = 0. \tag{1.34}
$$

By collecting powers of t, we get from t^0, $P_1(x) = xP_0(x)$, which we know to be correct, and from t^n for $n \geq 1$, the three-term recurrence relation

$$
(n + 1)P_{n+1}(x) - (2n + 1)x\, P_n(x) + nP_{n-1}(x) = 0 \tag{1.35}
$$

which we can easily check holds for $n = 1, 2, 3$ from the forms we deduced above.

Differentiating with respect to x gives another type of relation, one involving the derivatives of the polynomials. By a method similar to the above, we get

$$
\sum_{n=0}^{\infty} t^n P_n'(x) = \frac{t}{1 - 2tx + t^2} \sum_{n=0}^{\infty} t^n P_n(x)
$$

$$
\Rightarrow \quad \sum_{n=0}^{\infty}(t^n - 2t^{n+1}x + t^{n+2})P_n'(x) - t^{n+1} P_n(x) = 0
$$

$$
\Rightarrow \quad P_{n-1}'(x) - 2xP_n'(x) + P_{n+1}'(x) = P_n(x) \qquad \text{for } n > 0, \tag{1.36}
$$

or combining with the derivative of Eq. (1.35), we also get (among other relations)

$$
P_{n+1}'(x) - P_{n-1}'(x) = (2n + 1)P_n(x) \tag{1.37}
$$
$$
xP_n'(x) - P_{n-1}'(x) = nP_n(x) \tag{1.38}
$$
$$
xP_n'(x) - P_{n+1}'(x) = -(n + 1)P_n(x) \tag{1.39}
$$
$$
(1 - x^2)P_n'(x) = nP_{n-1}(x) - nxP_n(x). \tag{1.40}
$$

In addition differentiating (1.40) and combining with n times (1.38) gives Legendre's equation

$$(1 - x^2)P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0 \tag{1.41}$$

which is a further check on the approach. Some textbook *define* the Legendre polynomials via the generating function and derive the equation that they satisfy; we have used the opposite approach as more physically motivated. Legendre polynomials arise in many problems where the equations have spherical symmetry and the solutions are axially symmetric about the z-axis; further solutions which break the axial symmetry involve associated Legendre polynomials (spherical harmonics). If the boundaries are such that poles ($\cos\theta = \pm 1$) are not in the domain, the second solutions $Q_n(\cos\theta)$ will enter as well; we found $Q_1(x)$ above (see Eq. (1.11)) and we will discuss these further in section 1.4.1.

1.3.2 Bessel functions of integer order

For Bessel functions, (solutions to Eq. (1.26)) we use a similar approach. In the 2-d x-y plane, one solution to the wave equation is the plane wave $e^{i(ky-\omega t)}$, with $\omega/c = k$. However we can equate that to the form we obtain if we separate first in time and space and then in plane polar coordinates to give the general solution to the wave equation, in a region containing the origin, as follows:

$$e^{i(ky-\omega t)} = \left(A_0 J_0(kr) + \sum_{n=1}^{\infty} \left(A_n e^{in\phi} + B_n e^{-in\phi} \right) J_n(kr) \right) e^{-i\omega t} \tag{1.42}$$

where the sum is over integer n. Dividing out $e^{-i\omega t}$, substituting $y = r\sin\phi = r(e^{i\phi} - e^{-i\phi})/(2i)$ in the plane wave, setting $e^{i\phi} = t$ and $kr = z$, and equating the two forms gives

$$\exp\left(\tfrac{z}{2}(t - \tfrac{1}{t})\right) = A_0 J_0(z) + \sum_{n=1}^{\infty} \left(A_n t^n + B_n t^{-n} \right) J_n(z). \tag{1.43}$$

Symmetry under $t \to -1/t$ means that $B_n = (-1)^n A_n$, and the value at $z = 0$ sets $A_0 = 1$ if $J_0(0) = 1$, as is conventional (all the other J_n vanish at the origin). This time, the conventional normalisation of all the Bessel functions is *defined* such that $A_n = 1$ for all n, and hence we have the generating function $g(z,t)$ obeying

$$g(z,t) = \exp\left(\tfrac{z}{2}(t - \tfrac{1}{t})\right) = J_0(z) + \sum_{n=1}^{\infty} (t^n + (-1)^n t^{-n}) J_n(z) = \sum_{n=-\infty}^{\infty} t^n J_n(z). \tag{1.44}$$

Recall that Bessel's equation only depends on n^2 so we are free to define $J_{-n}(z) = (-1)^n J_n(z)$, which then allows us to rewrite the sum as in the second form above.

Bessel functions are not terminating polynomials, but we can obtain a Taylor series expansion of the solution directly from Eq. (1.44). For instance taking the Taylor expansion in z of the LHS and gathering terms independent of t gives

$$J_0(z) = \sum_{j=0,2\ldots}^{\infty} \frac{(-1)^{j/2} z^j}{((j/2)!)^2 2^j} = \sum_{m=0,1\ldots}^{\infty} \frac{(-1)^m}{(m!)^2} \left(\frac{z}{2}\right)^{2m} \tag{1.45}$$

which is even in z and has vanishing derivative at the origin; this series has an infinite radius of convergence.

Differentiating wrt z or t gives the useful recurrence relations

$$J_{n-1}(z) - J_{n+1}(z) = 2J_n'(z) \qquad \text{and} \qquad J_{n+1}(z) + J_{n-1}(z) = \frac{2n}{z}J_n(z). \tag{1.46}$$

The first of these gives $J_1(z) = -J_0'(z)$, which tells us that $J_1(z)$ is odd and linear about the origin. In general the first term in the expansion of J_n is proportional to z^n, and is odd (even) for odd (even) n.

As with the Legendre case, these recurrence relations can be manipulated till they take the form of Bessel's equation. This obvious fact is of more relevance in this case, because in the next section we will see that Bessel functions of non-integer order are also of interest; this shows that they also obey the recurrence relations.

1.3.3 Hermite polynomials

Here we state without proof a generating function for Hermite polynomials:

$$g(x,t) = \mathrm{e}^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}. \tag{1.47}$$

1.3.4 Rodrigues' Formula

Rodrigues' Formula gives different form of generating function for a restricted class of equations of the form (see Eq. (1.13))

$$p_0(x)y''(x) + p_1(x)y'(x) = -\lambda y(x) \tag{1.48}$$

where the p_i are polynomial, p_0 being at most quadratic and p_1, linear in x. In that case the integrating function $w(x)$ defined in Eq. (1.27) will be calculable. Then it can be shown that the nth regular eigenfunction is given by

$$y_n \propto \frac{1}{w(x)}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(w(x)\big(p_0(x)\big)^n\right) \tag{1.49}$$

(where we have used "$\propto$" rather than "$=$" as a multiplicative constant may be needed to get the conventional normalisation). So for example for Hermite's equation (1.29), $p_0 = 1$, $p_1 = -2x$, $w = \mathrm{e}^{-x^2}$ and

$$H_n(x) = (-1)^n \mathrm{e}^{x^2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \mathrm{e}^{-x^2} \tag{1.50}$$

and for Legendre's equation (1.41) (with conventional normalisation)

$$P_n(x) = \frac{(-1)^n}{2^n n!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n (1-x^2)^n \tag{1.51}$$

The general proof of Rodrigues' formula is given in Arfken 12.1 and (for specific cases) Riley 18.1, 18.9, and will not be given here though it is not too complicated.

Such equations (Laguerre's is another) have terminating polynomial solutions. Bessel's function is not of this form, though it might initially appear so at least for $n = 0$, as when the weight function x^2 is divided out, $p_0 = 1$ and $p_1 = 1/x$.

1.4 Series solutions to differential equations

Arfken 8.3, 14.1, 14.3, 15.6
Riley 16

Series solutions to differential equations were introduced in PHYS20171 Maths of Waves and Fields. This section is mostly revision, but we comment on the results in the light of our previous work. In particular we find that we need to use a different method if we are expanding about a regular singular point, and that other singular points will restrict the radius of convergence of the series. Note that we start without imposing boundary conditions and hence expect to find two solutions for each equation.

1.4.1 Series solutions about ordinary points

Given a differential equation we can expand the solution about an ordinary point of the equation $x = x_0$ as a Taylor series which will in general have a radius of convergence governed by the distance to the nearest singular point. For example for the **classical equation of SHM**,

$$- y''(x) = y, \tag{1.52}$$

expanding about the origin we write

$$y(x) = \sum_{n=0}^{\infty} a_n x^n, \tag{1.53}$$

and plugging this into the differential equation and equating powers of x gives, for $n \geq 2$,

$$a_n = -\frac{1}{n(n-1)} a_{n-2} \qquad \Rightarrow \qquad \begin{cases} a_n = \frac{(-1)^{n/2}}{n!} a_0 & \text{n even,} \\ a_n = \frac{(-1)^{(n-1)/2}}{n!} a_1 & \text{n odd.} \end{cases} \tag{1.54}$$

Hence $y(x) = a_0 \cos x + a_1 \sin x$ as expected. The ratio test shows that as

$$\left| \frac{a_{n+2} x^{n+2}}{a_n x^n} \right| = \left| \frac{x^2}{(n+1)(n+2)} \right| \tag{1.55}$$

for any given finite x, the ratio of successive terms tends to zero as $n \to \infty$ and the series converges. This illustrates useful points that are often met: until we specify boundary conditions there are two independent solutions. As the equation is symmetric under $x \to -x$, the solutions are either odd or even and the recurrence relation is a two-term relation between odd or even terms only. There are no singular points except $|x| = \infty$ so we can expand about any point (here we used the origin) and the radius of convergence is infinite, that is a single series solution is valid everywhere.

For **Legendre's equation**

$$(1 - x^2)y'' - 2xy' + l(l+1)y = 0 \tag{1.56}$$

(where to begin with we should not assume anything about l) the recurrence relation for an expansion about the origin (an ordinary point) is

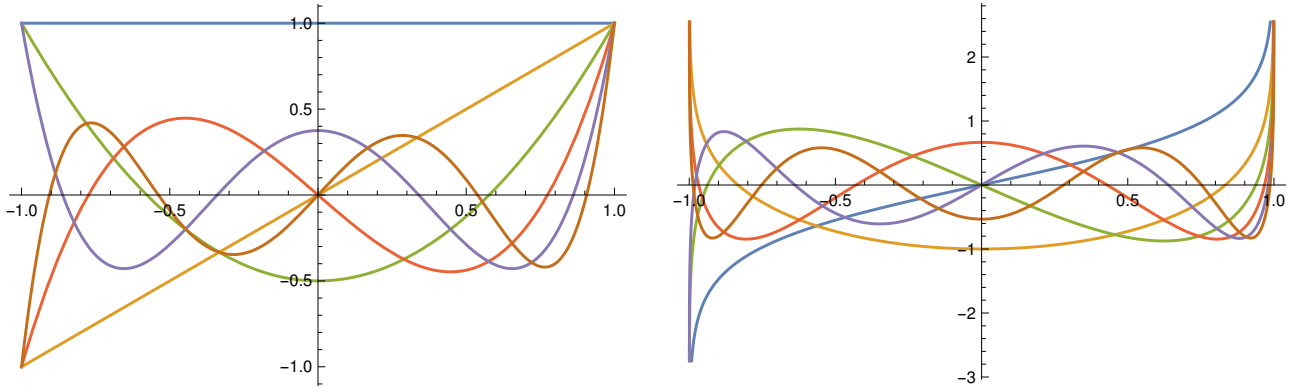$$a_{n+2} = -\frac{l(l+1) - n(n+1)}{(n+1)(n+2)} a_n, \tag{1.57}$$

Figure 1.1: Regular (Left) and irregular (right) solutions of Legendre's equation for integer $l = 0 - 6$

This time the ratio of successive terms tends to x^2 as $n \to \infty$, so it converges for $|x| < 1$ and diverges for $|x| > 1$. Since the equation has regular singular points at $x = \pm 1$ this is as expected. However the ratio test does not tell what happens to the solution at those points; for that we need Gauss's test[9] which looks at sub-leading terms in the ratio as a function of n. We need to be careful with the meaning of n when the series has missing terms, so let us instead consider $\sum_{j=0} b_j (x^2)^j$ with $n = 2j$ and $b_j = a_{2j}$:

$$\frac{b_j}{b_{j+1}} = \frac{(2j+1)(2j+2)}{2j(2j+1) - l(l+1)} \xrightarrow[j \to \infty]{} 1 + \frac{1}{j} + \mathcal{O}\left(\frac{1}{j^2}\right) \tag{1.58}$$

Since the coefficient of $1/j$, 1, is not greater than 1, the series diverges at $|x| = 1$. (We get the same result if we let $n = 2j + 1$ for the odd series.)

We know the way out: for integer even (odd) l the even (odd) series will have $a_{l+2} = 0$ and the series terminates. The resulting finite polynomial $P_l(x)$ converges for all finite x. The odd (even) series, $Q_l(x)$, does not terminate and only converges for $|x| < 1$; boundary conditions requiring well-behaved solutions at $x = \pm 1$ then excludes this second solution. In a familiar pattern, therefore, requiring solutions with certain boundary conditions quantises the eigenvalues—in this case, this corresponds to the quantisation of orbital angular momentum. The full solution in a region excluding $|x| = 1$ is

$$y(x) = a_0 P_l(x) + a_1 Q_l(x) \quad \text{for } l = 0, 2, 4 \ldots, \qquad y(x) = a_0 Q_l(x) + a_1 P_l(x) \quad \text{for } l = 1, 3, 5 \ldots \tag{1.59}$$

Of course we saw near the start of this section that we can always construct a second solution given one solution. We constructed $Q_1(x)$ (Eq. (1.11)), which can be shown to have the Taylor expansion

$$Q_1(x) = -1 + \sum_{n=2,4\ldots} \frac{x^n}{(n-1)} \tag{1.60}$$

in accordance with the recurrence relation (1.57).

On a domain $x \in [a, b]$ with $|a|, |b| < 1$, with separable homogeneous boundary conditions, Legendre's equation is a regular SL problem with eigenvalue λ which it is not particularly useful to write as $l(l+1)$. We know therefore that the spectrum will be non-degenerate (the solutions

---

[9]see Arfken, example 1.1.7 and text above

will can be written as superpositions of P_l and Q_l for non-integer l), there will be a lowest eigenvalue corresponding to a solution with no nodes, and higher eigenvalues correspond to more and more nodes, without bound. If $|a|$ or $|b| = 1$ the problem is no longer regular ($p(\pm 1)$ is not finite and ± 1 are regular singular points) but the same properties persist.

Hermite's equation presents nothing fundamentally new; the origin is an ordinary point and the series solution converges for all finite x; however the function grows as $e^{x^2/2}$ for $x \to \infty$, a problem which is solved if the eigenparameter n is an even or odd integer, in which case the even or odd series terminates. See PHYS30201 A.4 for more details.

1.4.2 Frobenius's method and Bessel functions

Bessel's equation

$$x^2 y'' + xy' + (x^2 - n^2)y = 0 \tag{1.61}$$

is more interesting, because the origin is a regular singular point and one might expect problems. Note we write the parameter as n^2 and will not necessarily assume integer n, but we will take it non-negative. If n is known to be non-integer, we write it as ν.[10]

For this case we will use the more general form of a series solution due to Frobenius [11], and write

$$y(x) = x^s \sum_{j=0}^{\infty} a_j x^j \tag{1.62}$$

where s is the lowest power of x in the expansion and its coefficient a_0 is by definition non zero. (Note a_0 is no longer necessarily the coefficient of x^0, which can cause confusion.) This allows for a pole or branch point at $x = 0$ if $s < 0$, but also for a solution that starts with x or a higher power of x. Substituting (1.62) in (1.61) gives

$$\sum_{j=0} \left((j+s)(j+s-1) + (j+s) - n^2 \right) a_j x^{j+s} + \sum_{j=0} a_j x^{j+s+2} = 0$$

$$\Rightarrow \quad (s^2 - n^2)a_0 x^s + ((s+1)^2 - n^2)a_1 x^{s+1} + \sum_{j=2} \left(\left((j+s)^2 - n^2 \right) a_j + a_{j-2} \right) x^{j+s} = 0$$

The recurrence relation is

$$a_j = \frac{1}{n^2 - (j+s)^2} \, a_{j-2} \quad \text{for } j \geq 2, \tag{1.63}$$

but in addition we need the first two terms to vanish. The first gives

$$s^2 - n^2 = 0 \tag{1.64}$$

which is called the indicial equation, and requires $s = \pm n$. (Recall that $a_0 \neq 0$ by definition: x^s is the lowest power in the series.) In general the vanishing of the second term requires $a_1 = 0$,[12]

---

[10]It should be noted that while Bessel's equation looks like an eigenvalue equation with $\lambda = -\nu^2$, this is not how it arises in physics; rather ν is an externally-imposed parameter related to the single-valued, finite angular part of the solution (for instance in 2D $\nu = m$, an integer, or as we will see, in 3D $\nu = l + \frac{1}{2}$, hence half integer). It becomes an eigenvalue problem in k when the substitution $x = kr$ is made, exactly as the homogeneous ODE $y'' = -y$ becomes the eigenvalue equation $y'' = -k^2 y$ under a similar substitution. See Eq. (A.18).

[11]See the end of this section for a comment on what happens if we use this more general form when the simpler one of the previous section would have worked.

[12] If $n = \pm\frac{1}{2}$ and $s = -\frac{1}{2}$, $a_1 \neq 0$ is allowed though not required, otherwise we need $a_1 = 0$. For $s = -\frac{1}{2}$, the series built on a_1 will start with $x^{\frac{1}{2}}$. However if $s = -\frac{1}{2}$ is one possibility, so is $s = \frac{1}{2}$ and this already gives a series starting at $x^{\frac{1}{2}}$; we don't get anything new. So even here we can set a_1 to zero.
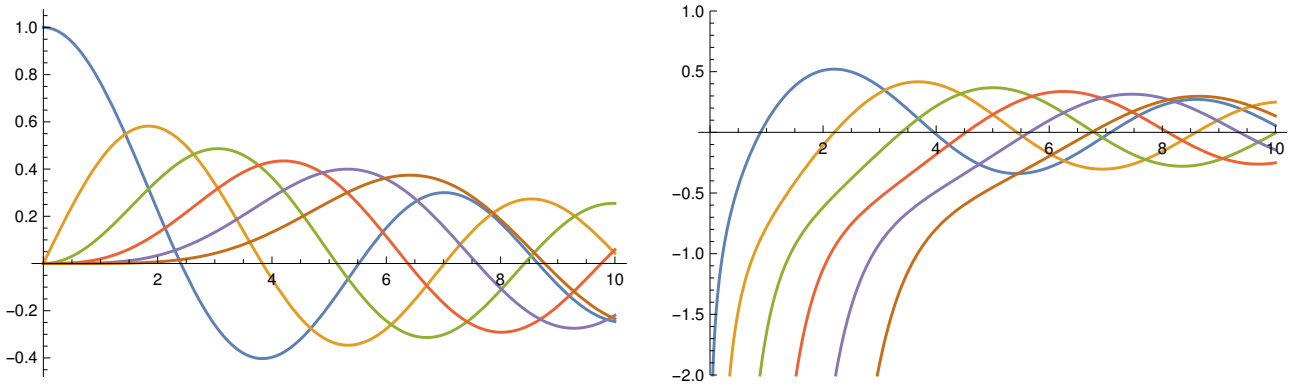
Figure 1.2: Regular (left) and irregular (right) solutions of Bessel's equation for integer $n = 0-5$

and we obtain the two solutions (if they exist) from the two values of s. Unless $s = n = 0$, one of these by definition will be divergent at the origin, the other will start with the power x^n—as indeed we already found to be true for integer n.

Starting with the case $n = 0$, $s = 0$, (1.63) is simply $a_j = -\frac{1}{j^2} a_{j-2}$. Setting $a_0 = 1$,

$$J_0(x) = \sum_{j=0,2\ldots} \frac{(-1)^{j/2}}{(j!!)^2} x^j \tag{1.65}$$

where $j!! = j(j-2)(j-4)\ldots = 2^{j/2}(j/2)!$ for even j. This is the same as we found before, see Eq. (1.45). But there is no other series solution!

For other integer $n > 0$, if we take $s = n$ the solution will be of the form $x^n f(x^2)$, $f(0)$ being finite, which will be odd or even as n is odd or even, and with $a_j = -a_{j-2}/j(j+2n)$ for $j \geq 2$,

$$J_n(x) = \sum_{m=0,1\ldots} \frac{(-1)^m}{m!(m+n)!} \left(\frac{x}{2}\right)^{n+2m} \tag{1.66}$$

where the normalisation matches that obtained from the generating function. Now if we take $s = -n$, the other solution of the indicial equation, we might expect to get a second solution, albeit one that is not regular at the origin. However the recurrence relation is $a_j = -a_{j-2}/j(j-2n)$ which fails when $j = 2n$. So again we do not get a second series solution.

Of course a second solution must exist, and is denoted $Y_n(x)$ or $N_n(x)$, but its behaviour at the origin must not be describable by a power series, even one with negative powers. $\log x$ is such a function (though not one of the solutions itself).

Note that we assumed positive n and found a solution for $s = n$; if we assume negative n we have a solution for (positive) $s = -n$. As the equation only depends on n^2 the two cases are not independent. Recall above we chose to define $J_{-n}(z) = (-1)^n J_n(z)$ for integer n.

Moving on to non-integer $n = \nu$, with $\nu > 0$, we can in fact reuse much of the analysis above. We have to define $\Gamma(\alpha)$ which has the value $(\alpha - 1)!$ for integer $\alpha > 0$, and which for any integer N satisfies

$$\Gamma(\alpha) = (\alpha - 1)(\alpha - 2)(\alpha - 3)\ldots(\alpha - N)\Gamma(\alpha - N) \tag{1.67}$$

For $s = \nu$, and using conventional normalisation in the second step,

$$J_\nu(x) = A_\nu x^\nu \sum_{m=0,1\ldots} \frac{(-1)^m \Gamma(\nu + 1)}{2^{2m} m! \Gamma(m + \nu + 1)} x^{2m} = \sum_{m=0,1\ldots} \frac{(-1)^m}{m! \Gamma(m + \nu + 1)} \left(\frac{x}{2}\right)^{\nu+2m}. \tag{1.68}$$

Replacing $\nu \to -\nu$ gives $J_{-\nu}$ which is an independent solution, albeit one which is not regular at the origin.

All of the series given above clearly converge for all $x > 0$.

For non-integer ν it is actually conventional to define the second solution via

$$N_\nu = \frac{\cos(\nu\pi)J_\nu - J_{-\nu}}{\sin(\nu\pi)} \tag{1.69}$$

which clearly forms a linearly-independent pair with J_ν since it contains $J_{-\nu}$. For integer $\nu = n$ both the numerator and denominator vanish (recall $J_{-n} = (-1)^n J_n$) but the expression can be evaluated using l'Hôpital's rule (in ν) and used to define N_n as well. As expected it is (logarithmically) divergent at the origin.

Finally for $n = \nu = \frac{1}{2}$, we note that for integer m,

$$m!\Gamma(m + 1 + \tfrac{1}{2}) = m!\Gamma(\tfrac{1}{2})\tfrac{1}{2} \cdot \tfrac{3}{2} \cdot \tfrac{5}{2} \dots \tfrac{2m+1}{2}$$
$$= (2m)!!(2m+1)!!2^{-(2m+1)}\Gamma(\tfrac{1}{2}) = (2m+1)!2^{-(2m+1)}\Gamma(\tfrac{1}{2})$$

so

$$J_{\frac{1}{2}}(x) = \frac{2^{\frac{1}{2}}}{\Gamma(\tfrac{1}{2})x^{\frac{1}{2}}} \sum_{m=0,1\dots} \frac{(-1)^m}{(2m+1)!}x^{2m+1} \propto \frac{\sin x}{\sqrt{x}}. \tag{1.70}$$

and $J_{-\frac{1}{2}}(x) \propto \cos x/\sqrt{x}$.

Bessel functions of half-integer order turn out to be useful for the solution of the wave equation in spherical polar coordinates. The radial wave function satisfies

$$r^2 R''(r) + 2r R'(r) + (k^2 r^2 - l(l+1))R(r) = 0, \tag{1.71}$$

and with the substitution $R(r) = u(r)/r$, for $l = 0$, we obtain $u(r) = A\cos(kr) + B\sin(kr)$. However the alternative substitution $R(r) = u(kr)/\sqrt{kr}$ transforms the equation into Bessel's equation with $\nu = l + \frac{1}{2}$. For $l = 0$ that gives the same as the simpler substitution, but we also now have a way of finding solutions for higher l. These occur enough that they are called spherical Bessel functions and given special symbols:

$$j_l(x) = \sqrt{\frac{\pi}{2x}}\, J_{l+\frac{1}{2}}(x), \qquad n_l(x) = \sqrt{\frac{\pi}{2x}}\, J_{-l-\frac{1}{2}}(x). \tag{1.72}$$

A final comment on Frobenius's method: if we use if when we don't need to, that is for an expansion about an ordinary point, we will find that the indicial equation has solutions $s = 0$ and $s = 1$. If, further, the equation has symmetry under $x \to -x$, such that we expect odd or even solutions, the solution we obtain for $s = 1$ will be the same as the one built on a_1 for $s = 0$.

1.5 Transform methods

1.5.1 Fourier Transforms: differential equations defined on an infinite interval

Arfken 20.2-4
Riley 13.1
Background A.9

Frequently met boundary conditions are that the solution to a differential equation be square integrable, vanishing at $x = \pm\infty$. Assuming suitable conditions on its continuity, such a solution $y(x)$ will have a Fourier transform $\tilde{y}(k)$ defined as

$$\tilde{y}(k) = \int_{-\infty}^{\infty} e^{-ikx} y(x) \mathrm{d}x, \tag{1.73}$$

with the inverse being given by

$$y(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} \tilde{y}(k) \mathrm{d}k, \tag{1.74}$$

Contrary to usage in, for instance, QM, it proves more useful to distribute the factor of 2π asymmetrically in this course.

Now the Fourier transform of the derivative of $y(x)$ has a simple form:

$$\mathrm{F.T.}[y'] = \int_{-\infty}^{\infty} e^{-ikx} \frac{\mathrm{d}y}{\mathrm{d}x} \mathrm{d}x = -\int_{-\infty}^{\infty} \left(\frac{\mathrm{d}}{\mathrm{d}x} e^{-ikx} \right) y(x) \mathrm{d}x = ik\tilde{y}(k) \tag{1.75}$$

and similarly the FT of the second derivative is $-k^2\tilde{y}(k)$. Thus a differential equation with (positive) constant coefficients can be turned into an algebraic equation for $\tilde{y}(k)$. So

$$y'' + 2ay' + by = f(x) \quad \Rightarrow \quad \tilde{y}(k) = \frac{\tilde{f}(k)}{b + 2ika - k^2} \tag{1.76}$$

The issue of course is to find the inverse transform:

$$y(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} \frac{\tilde{f}(k)}{b + 2ika - k^2} \mathrm{d}k \tag{1.77}$$

There will be particular functions $\tilde{f}(k)$ for which we can actually do the integral. More generally though, we recall the convolution theorem, that the FT or inverse FT of a product is a convolution. The IFT of $\tilde{f}(k)$ is of course $f(x)$; let us define the other IFT as

$$G(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} \frac{1}{b + 2ika - k^2} \mathrm{d}k \tag{1.78}$$

so

$$y(x) = \int_{-\infty}^{\infty} G(x - z) f(z) \, \mathrm{d}z. \tag{1.79}$$

The calculation of $G(x)$ may be often done using methods from complex variables, by considering an integral in the complex k plane over a semi-circular contour of radius R, such that the desired integral is the limit as $R \to \infty$ of the straight section. (See A.7, contour A.)

We invoke Jordan's lemma to say that if $x > 0$, the contribution from a semicircle in the upper half plane will tend to 0 as $R \to \infty$. Thus the desired real integral can be equated to the full contour integral, which is evaluated from the residues of the enclosed poles. For $x < 0$ the contour must instead be closed in the lower half plane. Here the poles are at $ia \pm \sqrt{b - a^2}$ and assuming $b > a^2$ these are both in the upper half plane; the result is

$$G(x) = \Theta(x)\mathrm{e}^{-ax}\frac{\sin\left(\sqrt{b - a^2}x\right)}{\sqrt{b - a^2}} \tag{1.80}$$

Recall $\Theta(x - x_0)$ is a unit step function at x_0 and its inclusion here ensures that $G(x)$ vanishes for $x < 0$. This is continuous and falls off exponentially as $x \to \infty$, so any reasonable driving term $f(x)$ will give a well defined solution, which we can rewrite as

$$y(x) = \int_{-\infty}^{x} G(x - z)f(z)\,\mathrm{d}z. \tag{1.81}$$

Even if the integral cannot be done analytically, it can be done numerically. This is a general method of finding the particular integral. The complementary function is absent, because in this case it contains e^{-ax} and so is not finite at $x \to -\infty$.

While we have used x as the variable here, the interpretation is simpler if we think of time; in particular if we replace $a \to \gamma/2$ and $b \to \omega_0^2$, we see the problem is the classical underdamped harmonic oscillator with a driving term. Let's pursue this a little further. First we note that, conventionally, we swap the signs in the Fourier transform and inverse transform if the variables are t and ω compared with x and k, so

$$G(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-i\omega t}\frac{1}{\omega_0^2 - i\gamma\omega - \omega^2}\,\mathrm{d}\omega = \Theta(t)\mathrm{e}^{-\frac{1}{2}\gamma t}\frac{\sin\left(\sqrt{\omega_0^2 - \frac{1}{4}\gamma^2}\,t\right)}{\sqrt{\omega_0^2 - \frac{1}{4}\gamma^2}}. \tag{1.82}$$

with, for a source $f(t)$,

$$y(t) = \int_{-\infty}^{t} G(t - t')f(t')\,\mathrm{d}t'. \tag{1.83}$$

Note that this solution incorporates *causality*: only the behaviour of the source at times $t' < t$ influences the solution at t.

Consider the very simple case of an oscillatory driving term, $f(t) = f_0\,\mathrm{e}^{-i\omega_d t}$. Writing $\omega_r = \sqrt{\omega_0^2 - \frac{1}{4}\gamma^2}$, we have

$$\begin{aligned}
y(t) &= f_0\int_{-\infty}^{t} \mathrm{e}^{-\frac{1}{2}\gamma(t-t')}\frac{\mathrm{e}^{i\omega_r(t-t')} - \mathrm{e}^{-i\omega_r(t-t')}}{2i\omega_r}\mathrm{e}^{-i\omega_d t'}\,\mathrm{d}t' \\
&= \frac{f_0}{\omega_r}\left[\frac{\mathrm{e}^{-\frac{1}{2}\gamma(t-t')+i\omega_r(t-t')-i\omega_d t'}}{\frac{1}{2}\gamma - i\omega_r - i\omega_d} - \frac{\mathrm{e}^{-\frac{1}{2}\gamma(t-t')-i\omega_r(t-t')-i\omega_d t'}}{\frac{1}{2}\gamma + i\omega_r - i\omega_d}\right]_{-\infty}^{t} \\
&= \frac{f_0\mathrm{e}^{-i\omega_d t}}{\omega_0^2 - \omega_d^2 - i\gamma\omega_d} \tag{1.84}
\end{aligned}$$

This is exactly what we would have obtained in first year, with the amplitude having the familiar Lorentzian form with a peak where the driving and undamped natural frequencies coincide. It is the steady-state solution, obtained if the source was switched on sufficiently

far in the past that any "transients" (solutions of the homogeneous equation) induced by the sudden switch-on on the source have died away.

Our derivation of G required a damping term (else the poles would have been on the real axis), and that same damping term ensures the vanishing of the integral at $t' \to -\infty$. It turns out (as we shall see later, 2.2.3) that the result for G does hold even if $\gamma = 0$, and, provided $\omega_d \neq \omega_0$, Eq. (1.84) does represent the "particular integral" corresponding to the source. But in the absence of damping, "transients" don't die away. And if we replace the lower limit by $-T$ to reflect a source switched on in the distant past, we will obtain terms proportional to $e^{i(\omega_0 \pm \omega_d)T}e^{\pm i\omega_0 t}$, which indeed have the form of solutions of the homogeneous equation with phases that depend on the switch-on time. The solution in the absence of transients is obtained simply by dropping such terms, or as sometimes phrased, taking $\lim_{T \to \infty} e^{i\alpha T} = 0$. If the source has "always" been on, there should be no transients induced by the switch-on.

Of course if $\omega_d = \omega_0$ we hit a problem—but we knew that already. For completeness we note that in that case, returning to the first line of Eq. (1.84), with $\gamma = 0$ and $\omega_r = \omega_d = \omega_0$,

$$y(t) = f_0 \int_{-T}^{t} \frac{e^{i\omega_0(t-2t')} - e^{-i\omega_0 t}}{2i\omega_0} dt' = -\frac{f_0}{2i\omega_0}(T+t)e^{-i\omega_0 t}, \qquad (1.85)$$

(dropping the "transient") which is indeed the relevant particular integral for this case. This reflects an amplitude that grows linearly with time since switch-on at $-T$.

1.5.2 Laplace Transforms: differential equations with initial conditions

Arfken 20.7-10
Riley 13.2, 25.5

Though we are less concerned with these in this course, problems in the time domain are almost always specified by initial conditions rather than boundary conditions, that is we do not usually specify conditions on a solution at some future time t. Rather we set it up and want to see how it evolves.

For such problems the Laplace transform is more useful than the Fourier Transform:

$$F(s) = \int_{0}^{\infty} e^{-st} f(t)\, dt. \qquad (1.86)$$

Unlike with the F.T. it is hard to assign a physical meaning to the conjugate variable s (sometimes called p or other names).

Convergence of the integral may require restrictions on s; for instance if $f(t) = e^{at}$, $F(s) = 1/(s-a)$ only for $s > a$.

The Laplace transform is insensitive to $f(t)$ for $t < 0$. It will be unchanged if we replace $f(t)$ by $\Theta(t)f(t)$.

In practice the inverse is normally found via look-up tables such as Table 1.1. If $F(s)$ is the L.T. of $f(t)$, then $\Theta(t)f(t)$ is the inverse Laplace transform of $F(s)$. The $\Theta(t)$ is important!

The shift theorems are particularly useful:

$$F(s - s_0) \to e^{s_0 t} f(t)\Theta(t) \quad \text{and} \quad e^{-st_0}F(s) \to f(t-t_0)\Theta(t-t_0) \qquad (1.87)$$

For Laplace transforms, the convolution $h(t)$ of two functions $f(t)$ and $g(t)$ is given by

$$h(t) = (f * g)(t) = \int_{0}^{t} f(u)g(t-u)\, du. \qquad (1.88)$$

This agrees with the previous definition (with an integral from $-\infty \to \infty$) if both functions vanish for negative values of their argument. The inverse Laplace transform of a product $H(s) = F(s)G(s)$ is the convolution $h(t) = f * g$.

The inverse Laplace transform may be computed using the Bromwich integral, in which s is treated as a complex variable lying on a line parallel to the imaginary axis:

$$f(t) = \frac{1}{2\pi i} \int_{\lambda - i\infty}^{\lambda + i\infty} e^{st} F(s) \, ds. \tag{1.89}$$

The offset λ must be positive, and large enough so that the line of integration lies to the right of all poles of $F(s)$. (For proof, see Arfken 20.10 or Riley 25.5)
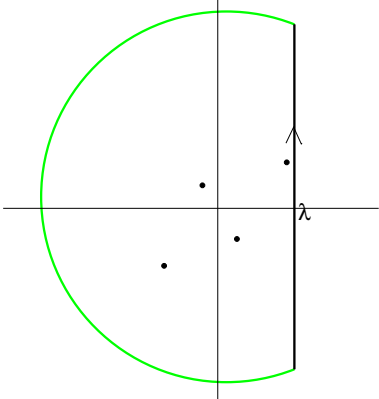
If $F(s)$ has only poles, and no more complicated analytic structure such as branch points, we can close the contour of integration as shown in the diagram (green arc). Provided $F(s)$ tends to zero as $|s| \to \infty$, for $t > 0$ Jordan's Lemma ensures that contribution of the arc vanishes as the radius is taken to infinity. For $t < 0$, we close the contour to the right instead and as no poles are enclosed the integral vanishes. Hence $f(t)$ is just given by $\Theta(t)$ times the sum of the residues of $e^{st} F(s)$. If $F(s)$ has a branch cut the contour will be more complicated.

The expressions for the Laplace transforms of the derivatives of $f(t)$,

$$f'(t) \to sF(s) - f(0) \quad \text{and} \quad f''(t) \to s^2 F(s) - sf(0) - f'(0). \tag{1.90}$$

allow us to recast differential equations for $f(t)$ as algebraic ones for $F(s)$. An important feature is that the initial conditions on $f(t)$ are incorporated directly. Higher derivatives can also be included. As before the challenge is to invert $F(s)$; as before the general solution can be cast as a convolution, but for specific cases it may also be possible to use the look-up table or the Bromwich integral to do the inversion directly. As a fairly trivial example to illustrate the problem, consider

$$\frac{\mathrm{d}f}{\mathrm{d}t} + f(t) = \Theta(t)(1 - \Theta(t - 2)), \qquad f(0) = 1 \tag{1.91}$$

that is a unit driving term which lasts for 2 time units—and could also be written $\Theta(t)\Theta(2 - t)$. This gives

$$sF(s) - 1 + F(s) = \int_0^2 e^{-st} \mathrm{d}t = \frac{1}{s}(1 - e^{-2s})$$

$$\Rightarrow F(s) = \frac{1}{s} - \frac{e^{-2s}}{s} + \frac{e^{-2s}}{s + 1}$$

$$\Rightarrow f(t) = \Theta(t)\left(1 - \Theta(t - 2) + \Theta(t - 2) e^{-(t-2)}\right) = \Theta(t)\Theta(2 - t) + e^2 \Theta(t - 2) e^{-t}.$$

$$\tag{1.92}$$

To reach the second line we used partial fractions to separate $1/s(s+1)$ and for the third line we used the lookup table including the shift theorem (1.87). The solution is a constant until the driving term ceases, then it decays with the natural decay time of the undriven solution e^{-t}.

Coupled differential equations can also be handled with Laplace methods, since one obtains simultaneous algebraic equations for the corresponding transforms. Laplace methods have been extensively used to analyse the propagation of signals though electrical circuits, with the convolution method allowing for efficient calculation of numerical solutions for a variety of inputs.

$f(t)$	$F(s) = \int_0^\infty e^{-st} f(t)dt$	Restrictions
1	$\dfrac{1}{s}$	$s > 0$
e^{at}	$\dfrac{1}{s-a}$	$s > a$
t^n	$\dfrac{n!}{s^{n+1}}$	$s > 0$, n a positive integer
$t^{-1/2}$	$\sqrt{\dfrac{\pi}{s}}$	$s > 0$
$\sin(at)$	$\dfrac{a}{s^2 + a^2}$	$s > 0$
$\cos(at)$	$\dfrac{s}{s^2 + a^2}$	$s > 0$
$\sinh(at)$	$\dfrac{a}{s^2 - a^2}$	$s > a$
$\cosh(at)$	$\dfrac{s}{s^2 - a^2}$	$s > a$
$t^n f(t)$	$(-1)^n \dfrac{d^n}{ds^n}\left(F(s)\right)$	$s > 0$, n a positive integer
$\frac{f(t)}{t}$	$\int_s^\infty F(y)dy$	$s > 0$
$f(at)$	$\frac{1}{a}F(\frac{s}{a})$	$s > 0$
$f'(t)$	$sF(s) - f(0)$	$s > 0$
$f''(t)$	$s^2 F(s) - sf(0) - f'(0)$	$s > 0$
$\Theta(t - t_0)$	$\dfrac{e^{-st_0}}{s}$	$t_0, s > 0$
$\Theta(t - t_0)f(t - t_0)$	$e^{-st_0}F(s)$	$t_0, s > 0$
$e^{s_0 t}f(t)$	$F(s - s_0)$	$s > s_0$
$\delta(t - t_0)$	e^{-st_0}	$t_0, s > 0$

Table 1.1: Table of common Laplace transforms and useful relations

2. Green's Functions

2.1 Introduction

In the previous chapter we were largely concerned with homogeneous ODEs, including eigenvalue problems. In this chapter we will consider inhomogeneous problems, and particularly the method of solution that involves constructing a function, unique to the linear operator on the LHS, which can be applied to any driving term on the RHS to give a solution. This called the Green's function of the operator (subject to relevant boundary conditions). We had a brief preview of a Green's function in the last section, Eq. (1.79).

Consider in particular the problem in electrostatics of finding the electric potential due to charges. Starting from the potential at $\mathbf{r}$ due to a single charge q_0 at $\mathbf{r}_0$,

$$\Phi(\mathbf{r}) = \frac{q_0}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}_0|} \tag{2.1}$$

and using the principle of superposition, we have for a series of charges q_i, or for a region V of charge density $\rho(\mathbf{r})$,

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_i \frac{q_i}{|\mathbf{r} - \mathbf{r}_i|} \qquad \text{or} \qquad \Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \mathrm{d}^3\mathbf{r}'. \tag{2.2}$$

The potential is a solution to Poisson's equation, $-\nabla^2\Phi(\mathbf{r}) = \rho(\mathbf{r})/\epsilon_0$, which is an inhomogeneous ODE with a source term. The Green's function we are looking for that enables us to construct the solution from the source term is, by inspection,

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|}, \tag{2.3}$$

with

$$\Phi(\mathbf{r}) = \int G(\mathbf{r}, \mathbf{r}') \frac{\rho(\mathbf{r}')}{\epsilon_0} \mathrm{d}^3\mathbf{r}'. \tag{2.4}$$

On its own the Green's function is (ϵ_0 times) the potential due to a unit point charge at $\mathbf{r}'$, and it satisfies the Laplace equation (as a function of $\mathbf{r}$) everywhere except at $\mathbf{r} = \mathbf{r}'$; it also satisfied the boundary condition that Φ vanishes as $|\mathbf{r}| \to \infty$. Note $\mathbf{r}'$ is considered just as a parameter in this interpretation, but mathematically the Green's function is a function of both $\mathbf{r}$ and $\mathbf{r}'$.

Writing

$$\frac{\rho(\mathbf{r})}{\epsilon_0} = -\nabla_{\mathbf{r}}^2 \Phi(\mathbf{r}) = -\int \nabla_{\mathbf{r}}^2 G(\mathbf{r}, \mathbf{r}') \frac{\rho(\mathbf{r}')}{\epsilon_0} \mathrm{d}^3\mathbf{r}' \tag{2.5}$$

implies that

$$-\nabla_{\mathbf{r}}^2 G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \tag{2.6}$$

which can in fact be taken as the equation that defines the Green's function, and again makes clear that it is the response to a point source. (The subscript on $\nabla_{\mathbf{r}}^2$ just reminds us that it acts on functions of $\mathbf{r}$.)

Returning to one dimension and considering a general linear differential operator $\mathcal{L}$ (or $\mathcal{L}_x$) subject to certain boundary conditions, we define $G(x, z)$ as the function which satisfies the following equation together with the the boundary conditions in x:

$$\mathcal{L}_x G(x, z) = \delta(x - z). \tag{2.7}$$

Thus for some function $f(x)$ on an interval $[a, b]$, we can write

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

$$= \int_a^b \mathcal{L}_x G(x, z) f(z) \, \mathrm{d}z = \mathcal{L}_x \int_a^b G(x, z) f(z) \, \mathrm{d}z \tag{2.8}$$

and hence

$$\mathcal{L} y(x) = f(x) \quad \Rightarrow \quad y(x) = \int_a^b G(x, z) f(z) \, \mathrm{d}z \tag{2.9}$$

(x', y, z and t are all commonly-used alternatives for the integration variable/second argument of the Green's function.)

Numerically, integration is much easier than the solution of differential equations, so if we can find a Green's function we have a very efficient way to proceed, and to deal with any source term. We will consider three methods: the continuity method, the eigenfunction expansion and Fourier transform methods.

2.2 Ordinary differential equations

Arfken 10.1
Riley 15.2.5

2.2.1 Continuity method

Consider the Green's function $G(x, z)$, for an operator $\mathcal{L}$ subject to homogeneous boundary conditions at $x = a$ and $x = b$. For definiteness we assume a Hermitian second-order differential operator of the form $\mathcal{L} v \equiv -(pv')' + qv$ and assume there are only ordinary points for $x \in (a, b)$.

The first thing to note is that for $x < z$ and for $x > z$ (but not at $x = z$), $G(x, z)$ satisfies $\mathcal{L}_x G(x, z) = 0$. Let y_1 and y_2 be solutions of $\mathcal{L} y = 0$, and let y_1 satisfy the boundary condition at a and y_2 that at b. (Recall that in general there will be no solution that satisfies both. If there is, the solution to the inhomogeneous equation is not unique.) The normalisation of y_1 and y_2 is not fixed by the homogeneous boundary conditions, and in what follows we allow it to depend on the second variable z.

Then a Green's function of the form

$$G(x, z) = \begin{cases} y_1(x) u_1(z) & \text{for } x < z \\ y_2(x) u_2(z) & \text{for } x > z, \end{cases} \tag{2.10}$$

where u_1 and u_2 are as-yet undetermined functions, satisfies the boundary conditions and $\mathcal{L}_x G(x, z) = 0$ for $x \neq z$. What we need is to find the two functions $u_{1,2}$ so that the behaviour at $x = z$ is correct.
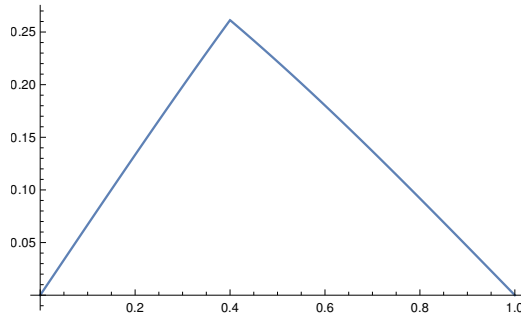
Figure 2.1: Green's function for $\mathcal{L}y \equiv -y'' + y$ with $y(0) = 0$ and $y(1) = 0$, plotted as a function of x for $z = 0.4$. The line segments are not in fact straight but sections of sine curves.

Furthermore if $\mathcal{L}$ is a second-order operator we need $G(x,z)$ to be continuous at $x = z$; the first derivative at least must be finite there. Thus $y_1(z)u_1(z) = y_2(z)u_2(z)$, which in turn requires $u_1/u_2 = y_2/y_1$, and

$$G(x,z) = \begin{cases} A(z)y_2(z)y_1(x) & \text{for } x < z \\ A(z)y_1(z)y_2(x) & \text{for } x > z. \end{cases} \tag{2.11}$$

To find the function $A(z)$, we integrate across the point $x = z$:

$$\int_{z-\epsilon}^{z+\epsilon} \mathcal{L}_x G(x,z)\mathrm{d}x = \int_{z-\epsilon}^{z+\epsilon} \delta(x-z) = 1 \tag{2.12}$$

So

$$1 = -[p(x)\tfrac{\mathrm{d}}{\mathrm{d}x}G(x,z)]_{z-\epsilon}^{z+\epsilon} + \int_{z-\epsilon}^{z+\epsilon} q(x)G(x,z)\mathrm{d}x \tag{2.13}$$

$G(x,z)$, and hence $q(x)G(x,z)$, are finite and continuous at $x = z$, so as $\epsilon \to 0$ the second term on the RHS vanishes. The x-derivative $G'(x,z)$ is finite but different on either side of $x = z$, with a finite discontinuity at $x = z$; thus the first term does not vanish. So

$$\begin{aligned} 1 &= \lim_{\epsilon \to 0} (-A(z))\big(y_1(z)y_2'(z+\epsilon)p(z+\epsilon) - y_2(z)y_1'(z-\epsilon)p(z-\epsilon)\big) \\ &= -A(z)p(z)\big(y_1(z)y_2'(z) - y_2(z)y_1'(z)\big) \tag{2.14} \\ &= -A(z)\,p(z)W\big(y_1(z), y_2(z)\big) \tag{2.15} \end{aligned}$$

where we have used the continuity of the y_i and of p to replace $z \pm \epsilon$ with z as $\epsilon \to 0$.

Now we have seen before, (1.21), that the Wronskian of two solutions of a Sturm-Liouville equation is proportional to $1/p$, and so $A(z)$ is in fact a constant,

$$A(z) \equiv A = -\frac{1}{p(z)W\big(y_1(z), y_2(z)\big)}. \tag{2.16}$$

This expression substituted into (2.11) gives our final result for $G(x,z)$. We note that it is symmetric under $x \leftrightarrow z$, something that does not persist if the problem is not Hermitian (see the end of this subsection).

For example, with $\mathcal{L}y \equiv -y'' - y$ subject to boundary conditions $y(0) = 0$ and $y(1) = 0$, which is Hermitian, the two solutions are $y_1 = \sin x$ and $y_2 = \sin(1-x)$. The Wronskian is

$-\sin(1)$ and so $A = 1/\sin(1)$ and

$$G(x, z) = \begin{cases} \frac{1}{\sin(1)}\sin(x)\sin(1-z) & \text{for } x < z \\ \frac{1}{\sin(1)}\sin(1-x)\sin(z) & \text{for } x > z \end{cases} \tag{2.17}$$

This is plotted in figure 2.1.

The solution to $\mathcal{L}y = f$ is given by

$$y(x) = \frac{1}{\sin 1}\left(\sin(1-x)\int_0^x \sin(z)f(z)\mathrm{d}z + \sin(x)\int_x^1 \sin(1-z)f(z)\mathrm{d}z\right). \tag{2.18}$$

Watch out that the first integral contains the second definition of G from Eq. (2.17), since $z < x$. Similarly the second integral contains the first definition. Then for instance for $f = 1$ we get

$$\begin{aligned} y(x) &= \frac{1}{\sin 1}\left(\sin(1-x)(-\cos x + 1) + \sin(x)(1 - \cos(1-x))\right) \\ &= \cos(x) + \tan(\tfrac{1}{2})\sin(x) - 1 \end{aligned} \tag{2.19}$$

which could have been obtained much more easily using the particular integral $y_{\mathrm{PI}} = -1$ plus the solution of the homogeneous equation $a\cos x + b\sin x$, together with the boundary conditions! However much more complicated cases can also be handled with the same Green's function.

If the operator is not Sturm-Liouville, but one of the form $\mathcal{L}v \equiv -(p_0 v'' + p_1 v') + qv$, the derivation starts the same way with the form Eq. (2.11) for G, and in fact the result is almost the same with $p \to p_0$. In place of Eq. (2.13) we have

$$\begin{aligned} 1 &= \int_{z-\epsilon}^{z+\epsilon}\left(-p_0(x)G''(x, z) - p_1(x)G'(x, z) + q(x)G(x, z)\right)\mathrm{d}x \\ &= [-p_0(x)G'(x, z)]_{z-\epsilon}^{z+\epsilon} + \int_{z-\epsilon}^{z+\epsilon}\left(p_0'(x)G'(x, z) - p_1(x)G'(x, z) + q(x)G(x, z)\right)\mathrm{d}x \\ &= [-p_0(x)G'(x, z) + \left(p_0'(x) - p_1(x)\right)G(x, z)]_{z-\epsilon}^{z+\epsilon} + \int_{z-\epsilon}^{z+\epsilon}\left(-p_0''(x) + p_1'(x) + q(x)\right)G(x, z)\mathrm{d}x \\ &= [-p_0(x)G'(x, z)]_{z-\epsilon}^{z+\epsilon} \qquad \text{as } \epsilon \to 0. \end{aligned} \tag{2.20}$$

In the $\epsilon \to 0$ limit the continuity of G means that, as in (2.13), only the $p_0(x)G'(x, z)$ term contributes to the integral across the cusp. Then continuing as before we find

$$A(z) = -\frac{1}{p_0(z)W\left(y_1(z), y_2(z)\right)}, \tag{2.21}$$

which resembles Eq. (2.16), but is *not* constant in this case. This expression substituted into (2.11) gives our final result for $G(x, z)$.

Thus for real SL operators, $G(x, z)$ is symmetric under exchange of x and z, whereas for non-SL operators, it is not.

We know that a non-SL operator can be cast in SL form by multiplication by an integrating factor $w(x)$; if $\tilde{G}(x, z)$ is the Green's function of the SL form, then $\tilde{G}(x, z)w(z)$ is the Green's function of the original form.

2.2.2 Eigenfunction expansion

Suppose $\mathcal{L}$ together with the boundary conditions is a Hermitian operator, and hence has a complete set of orthogonal eigenfunctions $\mathcal{L}\phi_n = \lambda_n\phi_n$ (we will come back to the case where there is a weight function). Then the source term can be expanded $f(x) = \sum_n f_n\phi_n(x)$ where $f_n = \langle\phi_n|f\rangle$, and the solution likewise: $y(x) = \sum_n y_n\phi_n(x)$. For the moment we will assume that $\lambda_n \neq 0$. Then we have

$$\mathcal{L}y = f \qquad \Rightarrow \qquad \sum_n y_n\lambda_n\phi_n(x) = \sum_n f_n\phi_n(x) \qquad \Rightarrow \qquad y_n = \frac{f_n}{\lambda_n}. \tag{2.22}$$

It is easily seen that the following expression for the Green's function

$$G(x, z) = \sum_n \frac{\phi_n(x)\phi_n^*(z)}{\lambda_n} \tag{2.23}$$

reproduces this:

$$\int G(x, z)f(z)\mathrm{d}z = \sum_n \frac{f_n}{\lambda_n}\phi_n(x) = y(x). \tag{2.24}$$

This nicely demonstrates what we saw before, namely that for a Hermitian operator, $G(x, z) = G^*(z, x)$. Similarly it illustrates the fact that we run into problems if there is a zero eigenfunction, that is if the homogeneous equation $\mathcal{L}\phi_0 = 0$ has a solution that satisfies both boundary conditions. This time though we see one way out: provided $\langle\phi_0|f\rangle = 0$ we can simply omit the homogeneous solution (or "zero mode") from the sum. If the source does not excite the zero mode, we don't need to include it in the solution, though that solution is then not unique as we can always add in any multiple of the zero mode.

We are reminded of matrix equations $\mathbf{A}\mathbf{y}_n = \mathbf{f}$, which are not invertible if $\det\mathbf{A} = 0$. Again if $\mathbf{f}$ is not orthogonal to the zero eigenvector there is no solution; if it is, there are infinitely many solutions.

A case in point is the electrostatic potential, considered at the start of the problem. Depending on the boundary conditions, extra solutions of $\nabla^2\Phi = 0$ corresponding to external electric fields may be added to the solution. In that physical case, though, the boundary conditions will suffice to make the solution unique.

What about the case with a weight function, $\mathcal{L}\phi_n = \lambda_n\rho(x)\phi_n$? In fact the Green's function has exactly the same form, though the proof that it works is slightly more involved, see the examples. For non-Hermitian operators the integrating factor required to cast the problem in Hermitian form enters though, as discussed at the end of the previous subsection.

For the problem we considered above, $\mathcal{L}y \equiv -y'' - y$, subject to boundary conditions $y(0) = 0$ and $y(1) = 0$, the normalised eigenfunctions are $\sqrt{2}\sin(n\pi x)$ and the eigenvalues are $(n\pi)^2 - 1$. Thus an alternative form for the Green's function is

$$G(x, z) = \sum_{n=1}^{\infty} \frac{\sqrt{2}\sin(n\pi x)\sqrt{2}\sin(n\pi z)}{(n\pi)^2 - 1} \tag{2.25}$$

This is usually much less convenient for finding actual solutions. For the source $f = 1$ considered before a solution is easily found using $\int_0^1 \sin(n\pi z)\mathrm{d}z = 2/n\pi$ for odd n, and equating the two forms gives

$$\cos(x) + \tan(\tfrac{1}{2})\sin(x) - 1 = \sum_{n=1,3\ldots} \frac{4\sin(n\pi x)}{n\pi(n^2\pi^2 - 1)} \tag{2.26}$$

which it can be checked numerically is true!

We chose above an operator and boundary conditions with no zero mode. Had we chosen the more physical case of $\mathcal{L}y \equiv -y'' - k^2 y$, with $y(0) = y(L) = 0$, the eigenvalues would be k_n^2 where $k_n = n\pi/L$ and the Green's function would read

$$G(x,z) = \sum_{n=1}^{\infty} \frac{2}{L} \frac{\sin(k_n x)\sin(k_n z)}{k_n^2 - k^2} \tag{2.27}$$

Such an equation arises for a stretched string driven at a frequency ω/c; we see that as expected, the response becomes very large close to a resonant frequency, unless the spatial form of the driving force cannot excite the relevant mode. An example would be driving at the mid-point, which can't excite modes on even n since they have nodes there.

2.2.3 Initial value boundary conditions

Here we consider the Green's function for the case of boundary conditions fixed only at one point, $x = a$, where we want a solution for $x > a$. We assume $\mathcal{L}$ has no singular points for $x \in [a, \infty)$, and write $\mathcal{L}v \equiv -(p_0 v'' + p_1 v') + q_0 v$.

Homogeneous boundary conditions at a single point can only be of the form $y(a) = 0$, $y'(a) = 0$ and the only solution of the homogeneous equation compatible with these is $y = 0$. Thus $G(x,z) = 0$ for $a \leq x < z$. For $x > z$, though, the Green's function will be proportional to the full, unconstrained solution with two undetermined "constants" (which can depend on z):

$$G(x,z) = \begin{cases} 0 & \text{for } a \leq x < z \\ u_1(z)y_1(x) + u_2(z)y_2(x) & \text{for } x > z. \end{cases} \tag{2.28}$$

Continuity of G gives $G(z,z) = 0$, so

$$\frac{u_1(z)}{u_2(z)} = -\frac{y_2(z)}{y_1(z)}. \tag{2.29}$$

For $x < z$, $G' = 0$ also, so the discontinuity in the slope constrains the slope for $x > z$ via Eq. (2.20):

$$-p_0(z)\Big(u_1(z)y_1'(z) + u_2(z)y_2'(z)\Big) = 1. \tag{2.30}$$

Together, these give

$$u_2(z) = A(z)y_1(z), \qquad u_1(z) = -A(z)y_2(z), \qquad A(z) = \Big(-p_0(z)W(y_1(z), y_2(z))\Big)^{-1}. \tag{2.31}$$

(As before, $A(z)$ will be a constant if $\mathcal{L}$ is Hermitian.) Hence

$$G(x,z) = \Theta(x - z)A(z)\Big(y_1(z)y_2(x) - y_2(z)y_1(x)\Big), \tag{2.32}$$

recalling the definition of the step function $\Theta(x)$ which is zero for negative x and one for positive x.

Because $G(x, z > x) = 0$, only $G(x, z < x)$ contributes to the solution of $\mathcal{L}y = f$, and

$$y(x) = \int_a^{\infty} G(x,z)f(z)\,\mathrm{d}z = y_2(x)\int_a^x A(z)y_1(z)f(z)\,\mathrm{d}z - y_1(x)\int_a^x A(z)y_2(z)f(z)\,\mathrm{d}z. \tag{2.33}$$

This embodies an important point: at a given point, x_0, only the values of $f(x)$ for $x < x_0$ contribute to $y(x_0)$. If the independent variable x is in fact time (as is common in initial value problems) this embodies *causality*. What the source does in the future can't influence the solution at the present time![1]

Consider the case of $\mathcal{L}y(t) \equiv \ddot{y}(t) + w^2 y(t)$, where we do use time as the variable, $t \in (-\infty, \infty)$, and y could be the position of an object subject to an undamped harmonic restoring force as well as an external driving term. The solutions are $y_1 = \sin \omega t$, $y_2 = \cos \omega t$, so $W = -\omega$, $p_0 = -1$ and $A = -1/\omega$, and

$$G(t, t') = \begin{cases} 0 & \text{for } -\infty \leq t < t' \\ -\frac{1}{\omega}\big(\sin \omega t' \cos \omega t - \cos \omega t' \sin \omega t\big) & \text{for } t > t' \end{cases}$$

$$= \Theta(t - t') \frac{\sin\big(\omega(t - t')\big)}{\omega}, \tag{2.34}$$

where in the last line we have used a trig identity. We note that the Green's function only depends on $t - t'$, which makes sense as neither the equation nor the boundary conditions introduce any special time; they are time-translation invariant. Then the response to a driving term $f(t)$ is

$$y(t) = \int_{-\infty}^{t} \frac{\sin\big(\omega(t - t')\big)}{\omega} f(t') \, dt'. \tag{2.35}$$

Typically a driving term will be switched on at some initial time t_i, which will change the lower limit of the integral in (2.35) from $-\infty$ to t_i.

It may be noted that we have seen something close to this before, namely Eq. (1.82). There we considered a lightly damped oscillator, and obtained a Green's function (though we didn't call it that) which reduces to Eq. (2.34) if we take the damping coefficient γ to zero.[2]

2.2.4 "Outgoing wave" boundary conditions

The Helmholtz operator, $\mathcal{L}y \equiv -y'' - k^2 y$, arises from the wave equation if the time-dependence of the source and solution is assumed to be $e^{-i\omega t}$, and $k = \omega/c$. (In form, it is identical to the problem we considered immediately above.) Another form of boundary condition that we can impose is "outgoing waves only": we have a source function confined to some region and its influence can propagate away from the region, but we don't want anything coming in. This corresponds to demanding $y(x \to -\infty) = e^{-ikx}$ and $y(x \to \infty) = e^{ikx}$, which we can see corresponds to out-going waves if we reintroduce the time dependence to give $e^{i(k|x|-\omega t)}$, a wave which is travelling to the right for positive x and to the left for negative x.[3]

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[1]The equations of course are symmetric under time. We could have explored the solutions for $x < a$ and obtained backwards-travelling influence. This is a common feature: we need to set up the problem to obtain physically-sensible solutions.

[2]If we recall the *method* of solution there, which was via contour integration, we required the damping term to keep the poles off-axis; they were at $\pm\sqrt{\omega^2 - \frac{1}{4}\gamma^2} - i\frac{1}{2}\gamma \approx \pm\omega - i\frac{1}{2}\gamma$. We will return to contour integrals as a method of solution, and will again discover that physically-sensible results are obtained by moving poles off-axis by an infinitesimal amount in a way that corresponds to introducing damping, see section 2.3.5.

[3]Had we assumed time dependence of $e^{i\omega t}$ the two solutions $e^{\pm ikx}$ would of course be reversed. For classical problems where the physical solution is real and the use of complex solutions is only for simplicity, we end up taking the real part to get $\cos(k|x| - \omega t)$ either way. In QM though the sign is not arbitrary and our choice corresponds to positive energy.

In constructing the Green's function therefore we have to use these two solutions for $x < z$ and $x > z$ respectively. The Wronskian is $2ik$ and so

$$G(x, z) = \begin{cases} -\frac{1}{2ik} e^{ikz} e^{-ikx} & \text{for } -\infty < x < z \\ -\frac{1}{2ik} e^{-ikz} e^{ikx} & \text{for } z < x < \infty \end{cases} \quad \Rightarrow \quad G(x, z) = -\frac{1}{2ik} e^{ik|x-z|} \quad (2.36)$$

Then for the solution we have

$$y(x) = -\frac{1}{2ik} \left(\int_{-\infty}^{x} e^{ik(x-z)} f(z) \, dz + \int_{x}^{\infty} e^{ik(z-x)} f(z) \, dz \right) \quad (2.37)$$

It is assumed that the restricted spatial extent of the source will avoid diverging integrals.

This deals with sources that oscillate in time; we will postpone more general time dependence to our treatment of the wave equation.

2.2.5 First order equations

We have concentrated on second-order equations since these are the ones we meet most often. For first-order equations there is only one linearly-independent solution of the homogeneous equation, and so we cannot satisfy separated boundary conditions. However the solution can satisfy a periodic boundary condition such as $y(a) = y(b)$ (see the second problem sheet), or an initial condition such as $y(a) = 0$. In the latter case (switching to time), if $y_1(t)$ is a solution of the homogeneous equation, the Green's function itself is discontinuous at $t = t'$ and has the form
$G(t, t') = \Theta(t - t') A(t') y_1(t)$. The discontinuity of G, rather than of its derivative, is given by integrating across $\delta(t - t')$, and that fixes $A(t')$.

For the simple case $\mathcal{L}y \equiv \frac{dy}{dt} + \kappa y$, $y_1 = e^{-\kappa t}$ and

$$\lim_{\epsilon \to 0} \int_{t'-\epsilon}^{t'+\epsilon} \mathcal{L}_t G(t, t') dt = \int_{t'-\epsilon}^{t'+\epsilon} \delta(t - t') = 1$$
$$\Rightarrow A(t') y_1(t') - 0 = 1 \qquad \Rightarrow A(t') = e^{\kappa t'}. \quad (2.38)$$

Thus

$$G(t, t') = \Theta(t - t') e^{-\kappa(t-t')}. \quad (2.39)$$

2.3 Partial differential equations

Arfken 10.3, 20.3
Riley 21.5

In this section we will only be interested in problems in which the spatial derivatives take the form of the Laplacian in one to three dimensions; these include Poisson's equation (no time dependence), the Helmholtz equation $\mathcal{L} \equiv -\nabla^2 - k^2$ which, among other cases, arises from purely periodic time dependence; the diffusion equation, the Schrödinger equation and the wave equation. In this section we will use variables (x, x') rather than (x, z), and in higher dimensions $(\mathbf{r}, \mathbf{r}')$ as in the introduction. Spatial integrals $\int \dots d^n r$, and their momentum-space equivalents, are over all space if not otherwise specified.

2.3.1 Poisson's equation

Poisson's equation is

$$-\nabla^2 \phi(\mathbf{r}) = \rho(\mathbf{r}), \tag{2.40}$$

familiar from electrostatics (setting ϵ_0 to 1).

We are not going to construct the Green's functions; rather we are going to note the results that are required to reproduce the known potentials for an infinite sheet of charge, and line charge and a point charge of (effectively) 1D, 2D and 3D respectively.[4]

In 3D the known potential from a point source $\rho(\mathbf{r}) = q\delta(\mathbf{r} - \mathbf{r}')$ leads immediately to

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|}. \tag{2.41}$$

Similarly in 2D, the $1/|\mathbf{r} - \mathbf{r}'|$ fall-off of the electric field of an infinite line charge leads to a logarithmically-rising potential

$$G(\mathbf{r}, \mathbf{r}') = -\frac{1}{2\pi} \ln |\mathbf{r} - \mathbf{r}'| \tag{2.42}$$

($\mathbf{r}$ being the position vector in the 2D plane perpendicular to the line).

For the 1D case, we recall the case of an infinite sheet of charge in the yz-plane corresponding to $\rho(x) = \sigma\delta(x)$. The potential rises linearly with $|x|$ on either side, and the field is constant and outwards-directed on both sides, $E = \sigma/2\epsilon_0$. This is achieved by

$$G(x, x') = -\tfrac{1}{2}|x - x'|. \tag{2.43}$$

All of these have something in common: they depend only on $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ (only the distance from the source to the field point matters, not the absolute position of each). This comes from the fact that the implicit boundary conditions are the behaviour of the field at infinity, and not at any finite $\mathbf{r}$. Hence there is nothing in the homogeneous equation or boundary conditions to break translational invariance. All the problems in the rest of this section have the same feature, and instead of $G(\mathbf{r}, \mathbf{r}')$ we write $G(\mathbf{r} - \mathbf{r}')$ or $G(\mathbf{R})$.

This might seem rather restrictive—large classes of interesting problems do involve finite boundaries. But in fact we can continue to use the free Green's function to construct the particular integral, and then add solutions of the homogeneous equation to satisfy the boundary condition. So though that is easier said than done in practice, it still means that the following sections are in fact of wider applicability than one might think.

2.3.2 Differential equations in time and space

Examples of these are the diffusion equation, the wave equation and Schrödinger's equation. Generically they are written

$$\mathcal{L}_{\mathbf{r},t} y(\mathbf{r}, t) = f(\mathbf{r}, t), \tag{2.44}$$

with $\mathcal{L}_{\mathbf{r},t}$ being written explicitly to indicated that it is an operator involving partial derivative in time t and space $\mathbf{r}$. The Green's function is the response to a unit impulse at an instant in time and a point in space; we need it to satisfy

$$\mathcal{L}_{\mathbf{r},t} G(\mathbf{r}, \mathbf{r}', t, t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t'). \tag{2.45}$$

---

[4]In 2D and 3D, one can also exploit axial/spherical symmetry of a problem and only use a Green's function to solve the radial equation; this is effectively a 1D problem with solutions involving powers of r and we won't pursue it further here though it features on the problem sheet. More interesting, at least for the development of this section, is the general case without symmetry.

Then the solution for a given space- and time-dependent source f is given by

$$\int_V \int_{-\infty}^{\infty} G(\mathbf{r}, \mathbf{r}', t, t') f(\mathbf{r}', t') \mathrm{d}t' \, \mathrm{d}^3 r'. \tag{2.46}$$

$\int_V$ indicates integration over all space; all of our integrals will be of that form though so we will drop the subscript.

As signalled above, we are going to exploit translational symmetry in the absence of boundary conditions other than at infinity, and assert that G can depend only on $\mathbf{R} = \mathbf{r} - \mathbf{r}'$; furthermore the similar absence of any special time means that it also only depends only on $\tau \equiv t - t'$. Since, from the point view of differentiation wrt $\mathbf{r}$ and t, these are just constant shifts which place the impulse at the origin and at $t = 0$, so we can write Eq. (2.45) as

$$\mathcal{L}_{\mathbf{R}, \tau} G(\mathbf{R}, \tau) = \delta(\mathbf{R}) \delta(\tau). \tag{2.47}$$

(We could just use $\mathbf{r}$ and t now, and many texts do.) We note too that the integral over the source in Eq. (2.46) now has the form of a convolution.

The method we will pursue is to take the spatial Fourier transform of the Green's function, denoting (in 3D) the conjugate variable to $\mathbf{R} = (X, Y, Z)$ as $\mathbf{K} = (K_x, K_y, K_z)$, but initially keeping the number of spatial dimensions (n) general:

$$\tilde{G}(\mathbf{K}, \tau) = \int e^{-i\mathbf{K} \cdot \mathbf{R}} G(\mathbf{R}, \tau) \mathrm{d}^n \mathbf{R}, \qquad G(\mathbf{R}) = \frac{1}{(2\pi)^n} \int e^{i\mathbf{K} \cdot \mathbf{R}} \tilde{G}(\mathbf{K}, \tau) \mathrm{d}^n \mathbf{K}. \tag{2.48}$$

The reason that this is useful is that spatial derivatives of G are replaced by factors of $\mathbf{K}$ times $\tilde{G}$, as we saw in 1.5.1: F.T.$[\nabla_{\mathbf{R}} G] = i\mathbf{K}\tilde{G}$ and F.T.$[\nabla_{\mathbf{R}}^2 G] = -K^2 \tilde{G}$, where $K = |\mathbf{K}|$.[5] In particular if $\mathcal{L}_{\mathbf{R}, \tau} \equiv \mathcal{L}_\tau - \nabla^2$, where the first term has only time derivatives, then

$$\mathcal{L}_{\mathbf{R}, \tau} G(\mathbf{R}, \tau) = \frac{1}{(2\pi)^n} \int e^{i\mathbf{K} \cdot \mathbf{R}} (\mathcal{L}_\tau + K^2) \tilde{G}(\mathbf{K}, \tau) \mathrm{d}^n \mathbf{K} = \delta(\tau) \frac{1}{(2\pi)^n} \int e^{i\mathbf{K} \cdot \mathbf{R}} \mathrm{d}^n \mathbf{K}, \tag{2.49}$$

where the extreme RHS is a representation of $\delta(\mathbf{R})$, and we can read off

$$(\mathcal{L}_\tau + K^2) \tilde{G}(\mathbf{K}, \tau) = \delta(\tau). \tag{2.50}$$

Thus we obtain an ODE in τ for $\tilde{G}(\mathbf{K}, \tau)$ in which K just appears as a parameter; we solve this using methods from sections 2.2.3 and 2.2.5 and then take the inverse Fourier transform to recover $G(\mathbf{R}, \tau)$.

2.3.3 Diffusion Equation

The diffusion equation is derived from two considerations. Defining $\psi(\mathbf{r}, t)$ as the density of particles, $\rho(\mathbf{r}, t)$ a source (a rate of injection of particles at a given point in space and time) and $\mathbf{j}(\mathbf{r}, t)$ as the current density of particles, continuity gives

$$\nabla \cdot \mathbf{j} = -\frac{\partial \psi}{\partial t} + \rho(\mathbf{r}, t) \tag{2.51}$$

---

[5]The same is true of time-derivatives under a temporal FT, of course. So why not do both? We can in fact—see section 2.3.6—but the method of this section is easier, particularly in cases incorporating causality.

while the current is related to the density gradient by the diffusion constant by the relation $\mathbf{j} = -D\nabla\psi$ if the density is not too large. Hence we have

$$\frac{\partial\psi}{\partial t} - D\nabla^2\psi \equiv \mathcal{L}\psi = \rho(\mathbf{r}, t)\,. \tag{2.52}$$

It is clear that in this case we want the Green's function to give the concentration of particles at $(\mathbf{r}, t)$ due to an injection of unit strength at position and time $(\mathbf{r}', t')$, with

$$\psi(\mathbf{r}, t) = \int_{t_i}^{\infty} \int G(\mathbf{r} - \mathbf{r}', t - t')\rho(\mathbf{r}', t')\mathrm{d}t'\mathrm{d}^3\mathbf{r}\,. \tag{2.53}$$

The injection of particles has to start at some finite time which we typically take as $t_i = 0$; we will see that the effective upper bound on the t' integral is in fact t.

We define $\tilde{G}(\mathbf{K}, \tau)$ as the spatial Fourier transform, (2.48), and obtain by comparison with Eq. (2.50):

$$\frac{\partial\tilde{G}(\mathbf{K}, \tau)}{\partial\tau} + DK^2\tilde{G}(\mathbf{K}, \tau) = \delta(\tau)\,. \tag{2.54}$$

This is a straightforward one-dimensional Green's function equation in time. By causality, $\tilde{G}(\mathbf{K}, \tau < 0) = 0$; as the operator is first-order, $\tilde{G}$ itself is discontinuous at $\tau = 0$. We have solved this already, see Eq. (2.39):

$$\tilde{G}(\mathbf{K}, \tau) = \Theta(\tau)\mathrm{e}^{-DK^2\tau}. \tag{2.55}$$

Then in 3D,

$$\begin{aligned}
G(\mathbf{R}, \tau) &= \Theta(\tau)\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{e}^{i\mathbf{K}\cdot\mathbf{R}}\mathrm{e}^{-D|\mathbf{K}|^2\tau}\mathrm{d}K_x\mathrm{d}K_y\mathrm{d}K_z \\
&= \Theta(\tau)\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\mathrm{e}^{-D\tau K_x^2 + iK_x X}\mathrm{d}K_x\int_{-\infty}^{\infty}\mathrm{e}^{-D\tau K_y^2 + iK_y Y}\mathrm{d}K_y\int_{-\infty}^{\infty}\mathrm{e}^{-D\tau K_z^2 + iK_z Z}\mathrm{d}K_z \\
&= \Theta(\tau)\left(\tfrac{1}{4\pi D\tau}\right)^{3/2}\mathrm{e}^{-R^2/(4D\tau)}\,. \tag{2.56}
\end{aligned}$$

Equally, we can write down the solution in any other number of dimension, with only the power of $3/2$ changed to $n/2$.

For future reference let us write

$$G(\mathbf{R}, \tau) = \Theta(\tau)U(\mathbf{R}, \tau) \qquad \text{where} \quad U(\mathbf{R}, \tau) = \left(\tfrac{1}{4\pi D\tau}\right)^{n/2}\mathrm{e}^{-R^2/(4D\tau)}\,. \tag{2.57}$$

We note for $\tau > 0$, G and U are the same, and a solution of the homogeneous equation. $U(\mathbf{R}, t)$ is called the propagator, and represents the subsequent spatial distribution of particles in response to an instantaneous source of unit strength.

The spatial distribution $U(\mathbf{R}, t - t')$ is a Gaussian with a time-dependent width that starts as zero at $t = t'$ and grows with $\sqrt{t - t'}$. This $\sqrt{\tau}$ behaviour is of course a well-known result for a random walk. Furthermore the height tends to infinity as $\tau \to 0$. This behaviour suggests that the limit is a spatial delta function, something which is most easily seen if we return to the Fourier transform Eq. (2.55) which is independent of K as $\tau \to 0$, so that the inverse FT is indeed a delta function. Hence the propagator has the properties $U(\mathbf{R}, 0) = \delta(\mathbf{R})$ and $\mathcal{L}U(\mathbf{R}, \tau > 0) = 0$.

A typical diffusion problem, in fact, does not involve a source at all, but an initial distribution $\psi_0(\mathbf{r})$ at time $t = 0$. This is an initial-value problem, and as the evolution is first-order

in time, the initial value is all we need (i.e. not its time derivative). The subsequent solution satisfies the homogeneous equation $\mathcal{L}\psi = 0$. Given the properties of U deduced above, it can be shown (see the problem sheet) that the solution at subsequent times is

$$\psi(\mathbf{r}, t) = \int U(\mathbf{r} - \mathbf{r}', t)\psi_0(\mathbf{r}')\, \mathrm{d}^n\mathbf{r}'\,. \tag{2.58}$$

So for the diffusion equation, a source which injects particles at time zero and an initial distribution at time zero have the same subsequent effect!

A problem with both a source and an initial distribution will have a solution which is the sum of Eqns (2.53) and (2.58).

2.3.4 Wave Equation

Now we consider

$$-\nabla^2\psi + \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} \equiv \mathcal{L}\psi = \rho(\mathbf{r}, t). \tag{2.59}$$

We can proceed as for the diffusion equation, performing a Fourier transform on the spatial variables and obtaining by comparison with Eq. (2.50):

$$\frac{1}{c^2}\frac{\partial^2\tilde{G}(\mathbf{K}, \tau)}{\partial\tau^2} + K^2\tilde{G}(\mathbf{K}, \tau) = \delta(\tau) \tag{2.60}$$

which is a one-dimensional Helmholtz-type equation with homogeneous solutions $Ae^{i\omega\tau} + Be^{-i\omega\tau}$ (setting $cK = \omega$). We solved this above in the "initial values" section, see Eq. (2.34):

$$\tilde{G}(\mathbf{K}, \tau) = c^2\Theta(\tau)\frac{\sin(cK\tau)}{cK}\,, \tag{2.61}$$

whence (in 3D)

$$G(\mathbf{R}, \tau) = \Theta(\tau)\frac{c}{(2\pi)^2}\int e^{iKR\cos\theta_K}\sin(cK\tau)\sin\theta_K\mathrm{d}\theta_K K\mathrm{d}K \tag{2.62}$$

$$= -\Theta(\tau)\frac{c}{2R(2\pi)^2}\int_0^\infty \left(e^{iKR} - e^{-iKR}\right)\left(e^{icK\tau} - e^{-iKc\tau}\right)\mathrm{d}K$$

$$= \Theta(\tau)\frac{c}{4\pi R}\Big(\delta(c\tau - R) - \delta(c\tau + R)\Big)$$

$$= \Theta(\tau)\frac{1}{4\pi R}\delta(\tau - R/c) \tag{2.63}$$

In the penultimate step, we used symmetry to extend the integral to $-\infty$, and in the last step we used the Θ function to kill the second δ function whose argument only vanishes at negative τ. In the final form the $\Theta(\tau)$ is actually redundant.

In 1D we can also do the integral simply; using $X = x - x'$ (which unlike R can be negative

as well as positive) we have

$$
\begin{aligned}
G(X, \tau) &= c^2 \Theta(\tau) \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iKX} \left(e^{icK\tau} - e^{-iKc\tau} \right) \frac{1}{2icK} dK \\
&= \Theta(\tau) \frac{c}{4\pi} \int dX \int_{-\infty}^{\infty} e^{iKX} \left(e^{icK\tau} - e^{-iKc\tau} \right) dK \\
&= \Theta(\tau) \frac{c}{2} \int dX \left(\delta(X + c\tau) - \delta(X - c\tau) \right) \\
&= \Theta(\tau) \frac{c}{2} \left(\Theta(X + c\tau) - \Theta(X - c\tau) \right) \\
&= \tfrac{1}{2} c\, \Theta(\tau) \Theta(\tau - |X|/c).
\end{aligned}
$$
(2.64)

(2.65)

The $\Theta(\tau)$ is again redundant since the second Θ requires $\tau \geq |X|/c \geq 0$.

In 2D the result, which we won't prove, is

$$
G(\mathbf{R}, \tau) = \Theta(\tau) \frac{1}{2\pi} \frac{\Theta(\tau - R/c)}{\sqrt{\tau^2 - R^2/c^2}}.
$$
(2.66)

(It can most readily be obtained by integrating the 3D Green's function over all z.) These results all satisfy causality in the forward time direction, so that no influence of a source is felt at a distance from it until a signal travelling at the speed of light would have time to reach it. The Green's function we have obtained is often called the *retarded* Green's function. The asymmetry in time was built into our initial value problem, but the light-travel time restriction was not, and arises from the form of the equation.

In three dimensions the reaction at a distance r to a briefly pulsed source (at the origin at time zero for definiteness) is felt *only* at $t = r/c$. In one and two dimensions though this is not so; nothing is felt before $t = r/c$, but the effect does not then vanish immediately but lingers: there is an "afterglow". In 2D it fades, in 1D it does not; the displacement of a stretched string, for instance, is changed by a finite amount by the passage of the signal.

In Lorentz gauge, Maxwell's equations can be recast as four separate wave equations for the electric potential and the components of the vector potential, with the charge density and the components of the current density as sources. The solution in two special cases (both 3D) can be obtained simply:

1. For a charge distribution $\rho(\mathbf{r}, t)$, we find for the electric potential

$$
\begin{aligned}
\Phi(\mathbf{r}, t) &= \int \frac{\delta\big(t - t' - |\mathbf{r} - \mathbf{r}'|/c\big)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \rho(\mathbf{r}', t')\, d^3\mathbf{r}'\, dt' \\
&= \int \frac{\rho(\mathbf{r}', t_{\text{ret}})}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}',
\end{aligned}
$$

where the retarded time, $t_{\text{ret}} = t - |\mathbf{r} - \mathbf{r}'|/c$, ensures that it is the charge density at $\mathbf{r}'$ at the appropriate point in the past that influences the field at $(\mathbf{r}, t)$. This should be familiar from electrodynamics. For a static charge distribution this simply gives

$$
\Phi(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}',
$$
(2.67)

a result which should need no explanation!

2. If the source is a single moving charged particle, which is at a position $\mathbf{s}(t')$ at time t', we use $\rho(\mathbf{r}', t') = q\delta\big(\mathbf{r}' - \mathbf{s}(t')\big)$ and we find the potential,

$$
\begin{aligned}
\Phi(\mathbf{r}, t) &= \int \frac{\delta\big(t - t' - |\mathbf{r} - \mathbf{r}'|/c\big)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} q\delta\big(\mathbf{r}' - \mathbf{s}(t')\big)\, \mathrm{d}^3\mathbf{r}'\, \mathrm{d}t' \\
&= \int \frac{q}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{s}(t')|} \delta\big(t - t' - |\mathbf{r} - \mathbf{s}(t')|/c\big)\mathrm{d}t'.
\end{aligned} \tag{2.68}
$$

The radiation that is observed at point $\mathbf{r}$, time t is emitted at the "event" of the particle reaching $(\mathbf{s}(t_{\mathrm{ret}}), t_{\mathrm{ret}})$, where the retarded time is such that this event lies on the past light cone.

In the second problem sheet, you are asked to show that the above expression reduces to the usual formula for the Liénard-Wiechert potential.

As with the diffusion equation the Green's function is related to a propagator $U(\mathbf{R}, \tau)$ with $\Theta(\tau)U(\mathbf{R}, \tau) = G(\mathbf{R}, \tau)$, and the propagator can be used to solve the homogeneous equation with initial conditions, but it is rather more fiddly than in the diffusion case so we won't give details here.

2.3.5 Helmholtz's equation

For a given source, we find the solution to the wave equation by integrating:

$$
\psi(\mathbf{r}, t) = \int \mathrm{d}^3 r' \int_{-\infty}^{t} \mathrm{d}t'\, G_W(\mathbf{r} - \mathbf{r}', t - t')\, \rho(\mathbf{r}', t') \tag{2.69}
$$

(where G_W denotes the GF of the wave equation). However if we have an oscillatory source, $\rho(\mathbf{r})\mathrm{e}^{-i\omega t}$, the steady-state solution will also have the form $\psi(\mathbf{r})\mathrm{e}^{-i\omega t}$, and by imposing this right at the start we would be left with the (time-independent) Helmholtz equation

$$
-\nabla^2 \psi(\mathbf{r}) - k_0^2 \psi(\mathbf{r}) = \rho(\mathbf{r}), \tag{2.70}
$$

where $k_0 = \omega/c$.

It therefore follows that if $G_{k_0}(\mathbf{R})$ is the GF of the Helmholtz equation,

$$
\int_{-\infty}^{t} G_W(\mathbf{R}, t - t')\mathrm{e}^{-i\omega t'}\, \mathrm{d}t' = \mathrm{e}^{-i\omega t}\, G_{\omega/c}(\mathbf{R}) \tag{2.71}
$$

If for definiteness we work in 3D, G_W is given by Eq. (2.63), so

$$
\frac{1}{4\pi R} \int_{-\infty}^{t} \mathrm{d}t'\delta(t - t' - R/c)\mathrm{e}^{-i\omega t'} = \frac{\mathrm{e}^{i\omega(R/c - t)}}{4\pi R} = \mathrm{e}^{-i\omega t}\frac{\mathrm{e}^{i\omega R/c}}{4\pi R}
$$

$$
\Rightarrow G_{k_0}(\mathbf{R}) = \frac{\mathrm{e}^{ik_0 R}}{4\pi R}; \tag{2.72}
$$

(note $\delta(t - t' - R/c) = \delta(t' - (t - R/c))$ so the integral always picks up the δ-function).

We should be able to obtain this Green's function (for the rest of the section, just $G(\mathbf{R})$ without the label) directly from Eq. (2.70); since there is no time dependence it looks easier than the cases we have already considered. We work with the Fourier transform $\tilde{G}(\mathbf{K})$ giving

$$
\mathcal{L}_{\mathbf{R}} G(\mathbf{R}) = \frac{1}{(2\pi)^n} \int \mathrm{e}^{i\mathbf{K}\cdot\mathbf{R}}(K^2 - k_0^2)\tilde{G}(\mathbf{K})\mathrm{d}^n\mathbf{K} = \frac{1}{(2\pi)^n} \int \mathrm{e}^{i\mathbf{K}\cdot\mathbf{R}}\mathrm{d}^n\mathbf{K}, \tag{2.73}
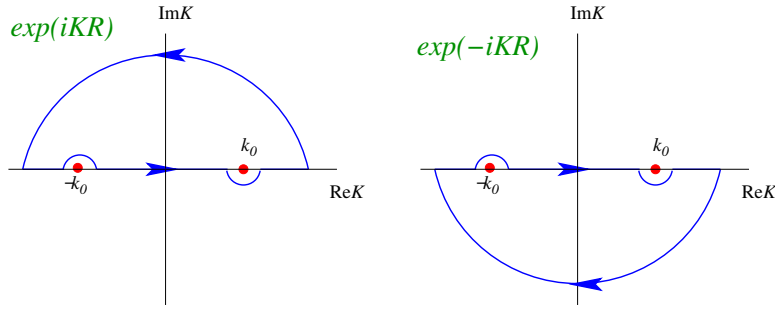$$

Figure 2.2: One possible contour choice for the principal value integration.

where the extreme RHS is a representation of the δ function. Hence we read off

$$\tilde{G}(\mathbf{K}) = \frac{1}{K^2 - k_0^2} \qquad \text{and} \qquad G(\mathbf{R}) = \frac{1}{(2\pi)^n} \int \frac{e^{i\mathbf{K}\cdot\mathbf{R}}}{K^2 - k_0^2} d^n\mathbf{K}. \tag{2.74}$$

In fact we could have written the last expression down directly since it is an eigenfunction expansion, albeit integrated rather than summed because the eigenvalues are continuous. At this point we have to specify n to continue, so we specify 3D.

The trick to evaluating the angular part of the integral is to choose the z-axis for the $\mathbf{K}$ integration along $\mathbf{R}$ ($\mathbf{K}$ is a dummy variable and we can choose it as we wish); then $\mathbf{K} \cdot \mathbf{R} = KR\cos\theta_K$ and so

$$G(\mathbf{R}) = \frac{1}{(2\pi)^2} \int \frac{e^{iKR\cos\theta_K}}{K^2 - k_0^2} K^2 \sin\theta_K d\theta_K dK = \frac{1}{iR(2\pi)^2} \int_0^\infty \frac{e^{iKR} - e^{-iKR}}{K^2 - k_0^2} K dK \tag{2.75}$$

The K-integral is of the kind we learned how to do in Complex Variables (see Fig. 2.2). First we see that the integrand is even in K, so we extend the integration to $-\infty$. We treat each complex exponential separately; we note that as $R > 0$ Jordan's Lemma is satisfied for closure in the upper half plane for the first term and the lower half plane for the second term. The only poles are simple poles on axis at $K = \pm k_0$ and we can either detour above or below, including or excluding the poles from the contour but picking up a contribution from the small semicircle of $\mp i b_1$, b_1 being the residue. Either way the full contribution from the first term

$$\int_{-\infty}^\infty \frac{K e^{iKR}}{(K - k_0)(K + k_0)} dK = i\pi \left. \frac{K e^{iKR}}{(K + k_0)}\right|_{K=k_0} + i\pi \left. \frac{K e^{iKR}}{(K - k_0)}\right|_{K=-k_0} = i\pi \cos k_0 R, \tag{2.76}$$

and from the second, an equal contribution (remember a minus sign for the clockwise integral). Thus the solution is

$$G(\mathbf{R}) = \frac{\cos k_0 R}{4\pi R} = \frac{e^{ik_0 R} + e^{-ik_0 R}}{8\pi R} \qquad \text{warning: not our final result.} \tag{2.77}$$

Let's step back. This is **a** solution. We recognise it, when multiplied by $e^{-i\omega t}$, as a sum of spherical waves, one outgoing and one incoming. But in physical applications, we don't want a wave coming in "from infinity", we want localised sources to generate disturbances that travel outwards, as we discussed in section 2.2.4 above. How can we impose such a boundary condition?
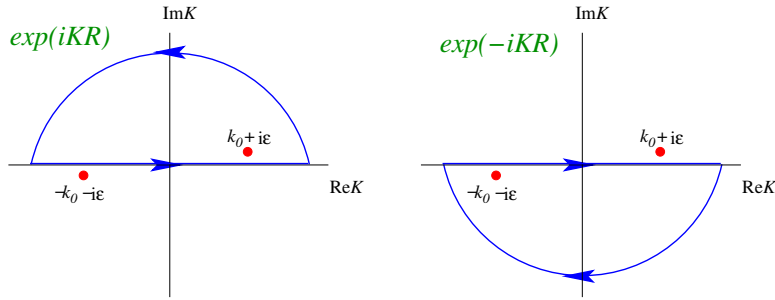
Figure 2.3: Choice of pole position to obtain out-going waves.

The problem came from the type of integral we did: it was a principal-value integral. But that is not the only possible definition of the integral past a pole on the real axis. Other possibilities imagine the poles being shifted infinitesimally off-axis, so that they are fully excluded or included from the contour integration. By looking at the two terms in Eq. (2.76), we see that the pole at $K = k_0$ is the one we want to include; this is achieved by giving k_0 a small positive imaginary part: $k_0 \to k_0 + i\epsilon$ (see Fig. 2.3). Then we have

$$G(\mathbf{R}) = \frac{1}{2iR(2\pi)^2}\left(2\pi i \left.\frac{K\mathrm{e}^{iKR}}{(K+k_0)}\right|_{K=k_0+i\epsilon} - (-2i\pi)\left.\frac{K\mathrm{e}^{-iKR}}{(K-k_0)}\right|_{K=-k_0-i\epsilon}\right)$$

$$\Rightarrow \quad G(\mathbf{r} - \mathbf{r}') = \frac{\mathrm{e}^{ik_0|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}, \tag{2.78}$$

where at the end, but not before, we have taken $\epsilon \to 0$. This is the result we obtained from the wave equation with a periodic source, Eq. (2.72)

This is a very powerful result: we determine the kind of solution we want by our treatment of poles. Had we made the opposite shift $k_0 \to k_0 - i\epsilon$ we would have obtained incoming waves. The principal value condition corresponds to standing waves. This choice is not as arbitrary as it seems: if k_0 did have a small positive imaginary part, the outgoing wave would actually be slightly damped and would continue to obey the boundary conditions at infinity, whereas the incoming wave would grow exponentially with increasing R and so would not.

It should be noted that when this result is required the contour is often drawn with the poles on axis and little circles around them, as in Fig. 2.2. But when that is done, the contributions from the little circles is considered part of the desired integral, not subtracted off. Showing the poles off-axis, as in the RH panel, is clearer but less common.

We could repeat the analysis in 2D but it is not so easy because the angular integral is more involved (no $\sin \theta_K$ in the integrand); we will not do so here. In 1D the result would be the one we obtained previously by other methods, Eq. (2.36).

2.3.6 Wave Equation as $(n+1)$D Fourier transform

The essential symmetry of the wave equation with respect to space and time is obscured by the solution method above. As an alternative we can write

$$\tilde{G}(\mathbf{K},\omega) = \int_{-\infty}^{\infty}\int \mathrm{e}^{-i\mathbf{K}\cdot\mathbf{R}+i\omega\tau}G(\mathbf{R},\tau)\,\mathrm{d}^n\mathbf{R}\,\mathrm{d}\tau, \qquad G(\mathbf{R},\tau) = \frac{1}{(2\pi)^{n+1}}\int \mathrm{e}^{i\mathbf{K}\cdot\mathbf{R}-i\omega\tau}\tilde{G}(\mathbf{K},\omega)\,\mathrm{d}^n\mathbf{K}\,\mathrm{d}\omega. \tag{2.79}$$
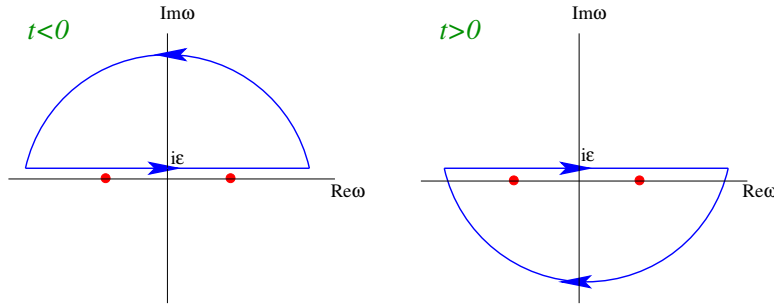
Figure 2.4: Contour for the ω integration, displaced upwards by ϵ.

In a method closely following the Helmholtz case, Eq. (2.74), we get

$$G(\mathbf{R}, \tau) = \frac{1}{(2\pi)^{n+1}} \int \frac{\mathrm{e}^{i(\mathbf{K} \cdot \mathbf{R} - \omega\tau)}}{K^2 - \omega^2/c^2} \, \mathrm{d}^n \mathbf{K} \, \mathrm{d}\omega \,, \tag{2.80}$$

which is the eigenfunction representation; however unlike the Helmholtz case we have an integral over ω as well, rather than a fixed $k_0 = \omega/c$; this allows for non-harmonic sources.

We can perform the K integral first (see Eq. (2.78)) to obtain as before

$$G(\mathbf{R}, \tau) = \frac{1}{8\pi^2 R} \int_{-\infty}^{\infty} \mathrm{e}^{i\omega(R/c - \tau)} \mathrm{d}\omega = \frac{1}{4\pi R} \delta(\tau - R/c) \,. \tag{2.81}$$

It is more conventional though to perform the ω integral first. Comparing Eq. (2.80) with (1.82) and focusing on the ω integral in each, we see that we get the right result if we allow a small damping term which we then take to zero, which is equivalent to assigning a small negative imaginary part to ω. Equivalently we shift the contour to lie just above the real axis (see Fig. 2.4). Then the poles are only included when the contour is closed in the lower-half plane, as required when $\tau > 0$, and causality is respected.

We now have two derivations of the wave equation Green's function. The first imposed forward propagation in time explicitly, via the solution to the 1D Helmholtz equation in time subject to G and its derivative vanishing for $t < t'$, Eq. (2.34). The second shifted poles to pick up only outgoing waves. Hopefully their equivalence will help to convince you of the validity of the latter method!

2.3.7 The free Schrödinger equation and the Born approximation

The time-dependent free Schrödinger equation looks just like the diffusion equation and in spite of the very different physics can be treated in the same way mathematically, with the replacement $D \to i\hbar/2m$. The free propagator was briefly covered in Maths fundamentals of QM (section 3.3.2). Here we are going to look at the time-independent equation, for which the free case,

$$-\frac{\hbar^2}{2m} \nabla^2 \psi - E\psi = 0, \tag{2.82}$$

is just the Helmholtz equation with $k_0^2 = 2mE/\hbar$. We will just call it k from now on; $\hbar k = p$. Here E is not being treated as an eigenvalue but as an externally-determined parameter (the energy of an incident particle in a scattering experiment). One set of solutions of the free homogeneous equation in 3D are just $\mathrm{e}^{i\mathbf{k} \cdot \mathbf{r}}$ where $\mathbf{k}$ can be in any direction; solutions

corresponding to spherical waves can be built out of spherical harmonics and spherical Bessel functions.

Of course the interesting case is not the free one, but with a potential, and for the general case the full GF will be hard to obtain. Consider instead a localised, weak potential $V(\mathbf{r})$, vanishing outside some range $r > a$. Consider too a wave function which consists of a plane wave (ψ) incident on the potential, and a scattered wave (ϕ) which would be absent in the absence of $V(\mathbf{r})$, and which is small compared to the plane wave. The full solution is $\Psi = \psi + \phi$. Hence the full Schrödinger equation can be approximated in first-order perturbation theory as

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

$$\Rightarrow -\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r}) - E\phi(\mathbf{r}) = -V(\mathbf{r})\Psi(\mathbf{r}) \approx -V(\mathbf{r})\psi(\mathbf{r}), \qquad (2.83)$$

where we have used the fact that ψ satisfies the homogeneous equation $\hat{H}^{(0)}\psi = 0$ to drop it from the LHS.

As an equation for the scattered wave ϕ, this is of the form $\hat{H}^{(0)}\phi = \rho$, where the plane wave interacting with the potential acts as a source. And so we can immediately write down the solution using the free Green's function Eq. (2.78),

$$\phi(\mathbf{r}) = -\frac{2m}{\hbar^2}\int G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}' = -\frac{2m}{\hbar^2}\int G(\mathbf{r},\mathbf{r}')\mathrm{e}^{i\mathbf{k}_i\cdot\mathbf{r}'}V(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}'$$

$$= -\frac{2m}{\hbar^2}\int \frac{\mathrm{e}^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}\mathrm{e}^{i\mathbf{k}_i\cdot\mathbf{r}'}V(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}', \qquad (2.84)$$

where $\mathbf{k}_i$ is the wave vector of the incoming plane wave.

We are interested in the solution at the location of our detector, well away from the (localised) potential, so we can Taylor-expand $|\mathbf{r}-\mathbf{r}'| \approx r - \hat{\mathbf{r}}\cdot\mathbf{r}'$ for $r \gg r'$ to obtain

$$\phi(\mathbf{r}) = -\frac{\mathrm{e}^{ikr}}{r}\frac{m}{2\pi\hbar^2}\int \mathrm{e}^{i(\mathbf{k}_i - k\hat{\mathbf{r}})\cdot\mathbf{r}'}V(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}'$$

$$\equiv \frac{\mathrm{e}^{ikr}}{r}f(\theta,\phi) \qquad \text{where } f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}'}V(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}'. \qquad (2.85)$$

If we define $k\hat{\mathbf{r}}$ as $\mathbf{k}_f$, the wave vector of a plane wave travelling from the source to the detector at $\mathbf{r}$, then $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$ is the momentum transfer between the incoming and scattered wave. (θ,ϕ) are the scattering angles, defined by the angle between the beam and the detector position. The scattered wave is an outgoing spherical wave e^{ikr}/r moderated by an angle-dependent scattering amplitude $f(\theta,\phi)$ whose square is the differential cross section. This expression for the scattered wave, valid at first order in perturbation theory, is called the *Born approximation*. For more details on scattering see here.

If we do not replace the full wave function by the free one in the "source" term of Eq. (2.83), we can instead write

$$\Psi(\mathbf{r}) = \psi(\mathbf{r}) - \frac{2m}{\hbar^2}\int G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\Psi(\mathbf{r}')\,\mathrm{d}^3\mathbf{r}'. \qquad (2.86)$$

We see that the unknown Ψ occurs on both sides of the equation, and we need new methods to solve it. It is an example of an *integral equation*, which is the topic of the next section. One method of solution is iterative, akin to perturbation theory, in which ϕ calculated in the Born

approximation is substituted for Ψ in the integral to obtain a second-order correction, and that in turn is used to obtain a third-order correction, and so on. This is called the Neumann series for Ψ, see section 3.4. But if the potential is not weak, or indeed if we seek the bound-state solutions (in which case ψ is absent as there are no free solutions with negative kinetic energy, and E is again an eigenvalue to be determined), then other methods will be needed.

3.   Integral Equations

3.1   Introduction

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In the previous section we solved equations of the form $\mathcal{L}y(x) = f(x)$ with an expression of the form $y(x) = \int_a^b G(x,z)f(z)\mathrm{d}z$. We are used to thinking of $\mathcal{L}$ as a (differential) operator acting on y, but equally $G(x,z)$ is an (integral) operator acting on f. Indeed $\mathcal{L}G(x,z) = \delta(x-z)$ suggests that the operators are in some sense one another's inverses. Though usually f is known, if instead y is known this becomes an integral equation for f: the question becomes "what source will produce this specified effect"?[1]

In this section we will consider integral operators of this form that are not necessarily Green's functions of differential operators. We define a *kernel* to be a function of two variables, $K(x,z)$, and define its operation on a function u as $\mathcal{K}u(x) \equiv \int_a^b K(x,z)u(z)\mathrm{d}z$. Like the differential operators we have considered, $\mathcal{K}$ is a *linear* operator:

$$\mathcal{K}(au(x) + bv(x)) = a\mathcal{K}u(x) + b\mathcal{K}v(x)\,. \tag{3.1}$$

Note we could more carefully write $\mathcal{K}u(x)$ as $(\mathcal{K}u)(x)$, (it is $u(z)$ that enters) but we won't be that pedantic.

We can also consider

$$\langle v|\mathcal{K}u\rangle = \int_a^b v^*(x)\left(\int_a^b K(x,z)u(z)\mathrm{d}z\right)\mathrm{d}x \tag{3.2}$$

and determine if it equals $\langle u|\mathcal{K}v\rangle^*$; if so it is a Hermitian operator. In general

$$\begin{aligned}
\langle v|\mathcal{K}u\rangle &= \int_a^b v^*(x)\left(\int_a^b K(x,z)u(z)\mathrm{d}z\right)\mathrm{d}x \\
&= \int_a^b \int_a^b v^*(x)u(z)K(x,z)\mathrm{d}z\,\mathrm{d}x \\
&= \int_a^b \int_a^b v^*(z)u(x)K(z,x)\mathrm{d}x\,\mathrm{d}z \\
&= \left(\int_a^b u^*(x)\left(\int_a^b K^*(z,x)v(z)\mathrm{d}z\right)\mathrm{d}x\right)^*\,.
\end{aligned} \tag{3.3}$$

where in the third line we simply swapped dummy variables x and z. Thus a sufficient condition for Hermiticity of $\mathcal{K}$ is $K^*(z,x) = K(x,z)$ or, for real functions, simply the symmetry condition

---

[1] When considering integral equations for their own sake though, the roles of y and f will be reversed; the known function will usually be denoted f and may be called the source, while the unknown function to be determined may be called y or u.

$K(z, x) = K(x, z)$. We recall that Hermitian differential operators do have Hermitian Green's functions, as is obvious from the eigenfunction expansion (recall the eigenvalues λ_n are real):

$$G(x, z) = \sum_n \frac{\phi_n(x)\phi_n^*(z)}{\lambda_n} = G^*(z, x). \tag{3.4}$$

Note that there is no extra boundary condition requirement for the Hermiticity of integral operators.

An *integral equation* for the unknown function (solution) $y(x)$ has the form $\mathcal{K}y(x) = f(x)$, or

$$\int_a^b K(x, z)y(z)\mathrm{d}z = f(x). \tag{3.5}$$

This is called a *Fredholm equation of the first kind*.

A general $K(x, z)$ might include an additive term proportional to $\delta(x - z)$ for which the integration is trivial; reserving the term kernel for the non-trivial part gives an equation of the form

$$y(x) = f(x) + \lambda \int_a^b K(x, z)y(z)\mathrm{d}z \tag{3.6}$$

(the point of the explicit λ will become apparent in a moment) and this is called a *Fredholm equation of the second kind*. (Similarly, differential equations may have a $q(x)y(x)$ term in them, as well as derivatives of y.)

Both types of Fredholm equation have fixed limits. Volterra equations of the first and second form replace the upper limit with x:

$$\int_a^x K(x, z)y(z)\mathrm{d}z = f(x) \qquad \text{or} \qquad y(x) = f(x) + \lambda \int_a^x K(x, z)y(z)\mathrm{d}z \tag{3.7}$$

Fredholm equations of the second kind can be homogeneous ($f = 0$). We will be almost exclusively concerned with equations of the second kind in what follows.

Some integral equations are equivalent to differential equation. Consider for instance the following Volterra equation of the second kind

$$y(x) = 1 + x^2 + \int_0^x y(z) \ \mathrm{d}z. \tag{3.8}$$

(unit kernel and $f(x) = 1 + x^2$). Note that we can immediately tell one thing about y: since $\lim_{x \to 0} \int_0^x y(z)\,\mathrm{d}z = 0$, we have $y(0) = 1$. We can differentiate wrt x to give:[2]

$$y'(x) = 2x + y(x) \qquad \Rightarrow \quad y'(x) - y(x) = 2x. \tag{3.9}$$

This can be solved either with the integrating factor e^{-x}, or with the complementary function (solution of the homogeneous equation) $c\mathrm{e}^x$ and a particular integral of the form $ax + b$ which works if $a = b = -2$ (see A.3). Either way we get

$$y = -2 - 2x + 3\mathrm{e}^x \tag{3.10}$$

where $c = 3$ is required to give $y(0) = 1$. We can easily check this solution by substituting back into the original integral equation.

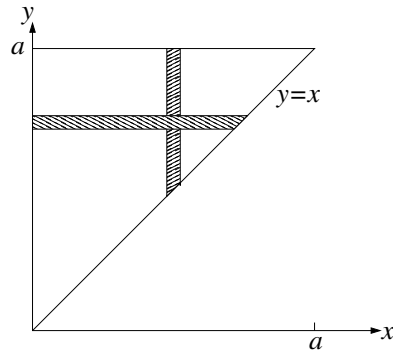[2]If this step isn't obvious to you, check section A.2.

Figure 3.1: integration over a triangular region.

Although not all integral equations can be recast as differential equations, all linear differential equations can be turned into integral equations. For example if we start with $y''(x) + k^2 y(x) = f(x)$ with bcs $y(0) = y'(0) = 0$, we can integrate twice. We will need the identity (obtained by integrating over a triangular region in the xy plane, see figure 3.1)

$$\int_0^a \left(\int_0^y f(x) \mathrm{d}x \right) \mathrm{d}y = \int_0^a \left(\int_x^a \mathrm{d}y \right) f(x) \mathrm{d}x = \int_0^a (a - x) f(x) \mathrm{d}x. \qquad (3.11)$$

Then

$$y''(x) + k^2 y(x) = f(x) \qquad (3.12)$$

$$\Rightarrow y'(x) + \int_0^x \left(k^2 y(z) - f(z) \right) \mathrm{d}z + A = 0$$

$$\Rightarrow y(x) + \int_0^x \left(\int_0^{x'} \left(k^2 y(z) - f(z) \right) \mathrm{d}z \right) \mathrm{d}x' + Ax + B = 0$$

$$\Rightarrow y(x) + k^2 \int_0^x (x - z) y(z) \mathrm{d}z = \int_0^x (x - z) f(z) \mathrm{d}z - Ax - B , \qquad (3.13)$$

but though we have introduced constants A and B we see that the boundary conditions require them both to be zero. Hence we have an integral equation

$$y(x) + k^2 \int_0^x (x - z) y(z) \mathrm{d}z = g(x) \qquad \text{where} \quad g(x) = \int_0^x (x - z) f(z) \mathrm{d}z . \qquad (3.14)$$

Since the source f of the differential equation is known, that of the integral equation, g, is also known.

The form found above should not be a surprise. The Green's function of $\mathcal{L}y \equiv -y''$ subject to $y(0) = y'(0) = 0$ is just $G(x, z) = \Theta(x - z)(z - x)$. So the solution to $-y'' = -f + k^2 y$ is

$$y(x) = \int_0^\infty G(x, z) \left(k^2 y(z) - f(z) \right) \mathrm{d}z = \int_0^x (z - x) \left(k^2 y(z) - f(z) \right) \mathrm{d}z. \qquad (3.15)$$

We chose initial conditions for our explicit demonstration above. Life would have been harder if we'd chosen $y(0) = y(a) = 0$. But the Green's function method gives the solution:[3] given

$$G(x, z) = \frac{1}{a} \left((a - z)x \, \Theta(z - x) + (a - x)z \, \Theta(x - z) \right) , \qquad (3.16)$$

---

[3]See the second examples sheet; qu 1 in 2021.

we obtain the equation

$$y(x) = \int_0^a G(x, z)\big(k^2 y(z) - f(z)\big)\mathrm{d}z\,. \tag{3.17}$$

From the above we see a connection between Volterra integral equations and initial value problems, and between Fredholm integral equations and separated boundary problems (but recall not all integral equations are equivalent to differential equations.)

Just as there are differential eigenfunction problems, so there are integral ones. From the problem considered above, the equivalence of some forms is clear: setting $f = 0$ in Eq. (3.17) and regarding k^2 as the eigenvalue of $\mathcal{L}y = -y''$, we have

$$- y'' = k^2 y \qquad \Rightarrow\; y(x) = k^2 \int_0^a G(x, z) y(z)\mathrm{d}z\,. \tag{3.18}$$

Hence by convention we write integral equation eigenvalue problems as $y = \lambda \mathcal{K}y$ rather than $\mathcal{K}y = \lambda y$. We can always convert to the more natural form by dividing by λ. (Note $\lambda = 0$ implies $y = 0$ which is not considered an eigenfunction, so λ is always non-zero.)

Eigenvalue problems are homogeneous Fredholm equations of the second kind. The equivalent Volterra problem has no solution. Consider

$$y(x) = \lambda \int_0^x K(x, z)\, y(z)\mathrm{d}z\,, \tag{3.19}$$

then we can show (assuming a differentiable kernel and solution) that $y(0) = 0$, $y'(0) = K(0,0)y(0) = 0, \ldots$, ie $y(x) = 0$.

In exactly the same way as for integral operators, we can show that the eigenvalues of a Hermitian integral operator are real[4] and the (non-degenerate) eigenfunctions are orthogonal; furthermore for a real kernel the eigenfunctions can also be taken to be real. We will have more to say about this in section 3.3.

3.2 Special methods of solution

The first solution method is the one we used above: if differentiation once or twice will convert the integral equation to a differential one, it is worth checking if we can solve it that way; we already have a lot of experience in solving differential equations. For this to work, repeated differentiation has to get rid of the integral; this will work either if the kernel is a low-order polynomial in x (as in (3.8)), or if the kernel is unchanged (an exponential or sine or cosine) in which case the original form of the equation can be used to eliminate the integral. The resulting ODE will of course have undetermined constants, but an appropriate number of boundary conditions will be implicit in the integral equation. Of course there are many differential equations that we won't recognise, and in general numerical methods are more stable for the original integral equation: discretisation or expansion in some appropriate basis converts the integral equation to a matrix inversion problem, for which efficient algorithms exist.

A simple example is the Volterra equation

$$y(x) = 1 + \int_0^x \mathrm{e}^{z-x} y(z)\mathrm{d}z. \tag{3.20}$$

---

[4]The form $\mathcal{K}y_n = (1/\lambda_n)y_n$ is the most useful starting point.

We note that $y(0) = 1$. Then differentiating gives

$$y'(x) = e^{z-x}y(z)|_{z=x} - \int_0^x e^{z-x}y(z)\mathrm{d}z = y(x) - (y(x) - 1) = 1. \qquad (3.21)$$

to which the solution that obeys the initial condition is just $y = 1+x$. (If two differentiations are needed, the first will provide an initial condition on $y'(0)$, so the solution is still fully specified.)

3.2.1 Displacement kernels and integral transforms

In some cases, integral equations can be solved via integral transforms. If the kernel is a function only of the difference of the arguments, $K(x, z) = K(x - z)$, $\mathcal{K}y$ has the form of a convolution if the limits on the integration are appropriate. Such a kernel is called a *displacement kernel*. For instance for the Fredholm equation

$$y(x) = f(x) + \lambda \int_{-\infty}^{\infty} K(x - z)y(z)\mathrm{d}z \qquad \Rightarrow \qquad \left(1 - \lambda\tilde{K}(k)\right)\tilde{y}(k) = \tilde{f}(k) \qquad (3.22)$$

where $\tilde{y}(k)$ is the Fourier transform of $y(x)$ etc. (Depending on the distribution of factors of 2π in the transform and inverse transform, λ might change by a factor of 2π in the transformed equation.) If the IFT of $\tilde{f}(k)/(1 - \lambda\tilde{K}(k))$ can be found, the problem is solved. Note that if the kernel and the source terms share a symmetry under $x \to -x$, problems with integration limits 0 and ∞ can be can be rewritten in the form above and hence may also be amenable to solution by this method.

Similarly for the following Volterra equation we can use the Laplace transform:

$$y(t) = f(t) + \lambda \int_0^t K(t - z)y(z)\mathrm{d}z \qquad \Rightarrow \qquad (1 - \lambda\tilde{K}(s))\tilde{y}(s) = \tilde{f}(s) \qquad (3.23)$$

where $\tilde{y}(s)$ is now the Laplace transform of $y(t)$ etc. (The finite limits arise from the fact that Laplace transforms are conducted on functions that are assumed to vanish for $t < 0$.)

For example, consider

$$y(t) = t - k^2 \int_0^t (t - z)y(z)\mathrm{d}z \qquad (3.24)$$

Two differentiations will convert this to a (familiar) differential equation, but instead we can use Laplace transforms and note that the integral is the convolution of t and $y(t)$:

$$\tilde{y}(s) = \frac{1}{s^2} - k^2\frac{1}{s^2}\tilde{y}(s) \qquad \Rightarrow \qquad \tilde{y}(s) = \frac{1}{s^2 + k^2} \qquad \Rightarrow \qquad y(t) = \frac{1}{k}\sin kt. \qquad (3.25)$$

As a bonus we did not have to worry about boundary conditions, though we can quickly check $y(0) = 0$ (and for that matter $y'(0) = 1$).

Integro-differential equations contain derivatives of y as well as $\mathcal{K}y$; if the kernel and limits are appropriate, Laplace transforms can also be used for these (see section 1.6.2 for the L.T. of derivatives).

3.2.2 Separable kernels

In some cases the kernel is a product of functions of x and z only, or a sum of such terms: $K(x, z) = \sum_{i=1}^{N} g_i(x)h_i(z)$; such kernels are called *separable* or *degenerate*. An example would

be xz^2 or, less obviously, $\cos(x - z) = \cos x \cos z + \sin x \sin z$. The advantage of this kind of kernel is that the terms $g_i(x)$ are not affected by the integration, and hence suggest the form of the solution. It turns out that we can reduce the integral equation to a system of algebraic equations, which is a great simplification.

If the kernel of a Fredholm equation of the second kind is separable, we have

$$y(x) = f(x) + \lambda \int_a^b \Big(\sum_{j=1}^N g_j(x) h_j(z) \Big) y(z) \mathrm{d}z$$

$$= f(x) + \lambda \sum_{j=1}^N g_j(x) \int_a^b h_j(z) y(z) \mathrm{d}z$$

$$= f(x) + \lambda \sum_{j=1}^N c_j g_j(x) \tag{3.26}$$

where the numbers c_i are just constants, albeit not yet known.

We can now find an $N \times N$ matrix equation for the vector of coefficients $\mathbf{c} = (c_1, c_2....)$. First, let us define, along with $c_i = \int_a^b h_i(z) y(z) \mathrm{d}z$,

$$f_i = \int_a^b h_i(z) f(z) \mathrm{d}z \qquad \text{and} \qquad K_{ij} = \int_a^b h_i(z) g_j(z) \mathrm{d}z, \tag{3.27}$$

If we now multiply Eq. (3.26) by one of the $h_i(x)$ and integrate, we get

$$\int_a^b h_i(x) y(x) \mathrm{d}x = \int_a^b h_i(x) f(x) \mathrm{d}x + \lambda \sum_{j=1}^N c_j \int_a^b h_i(x) g_j(x) \mathrm{d}x$$

$$\Rightarrow c_i = f_i + \lambda \sum_{j=1}^N K_{ij} c_j. \tag{3.28}$$

There are N such equations, which can be written together in matrix form:

$$\mathbf{c} = \mathbf{f} + \lambda \mathbf{K} \mathbf{c}$$
$$\Rightarrow \mathbf{c} = (\mathbf{I} - \lambda \mathbf{K})^{-1} \mathbf{f}. \tag{3.29}$$

Having found the c_i, we return to Eq. (3.26) to obtain $y(x)$.

If the equation is homogeneous, $f(x) = 0$, we have

$$\mathbf{c} = \lambda \mathbf{K} \mathbf{c} \quad \Rightarrow \quad \mathbf{K} \mathbf{c} = \lambda^{-1} \mathbf{c} \quad \text{or equivalently } \mathbf{K}^{-1} \mathbf{c} = \lambda \mathbf{c}. \tag{3.30}$$

which has a solution if λ is an eigenvalue of the kernel, λ_n. These are the reciprocals of the eigenvalues of $\mathbf{K}$, and the corresponding $\mathbf{c}_n$ are the eigenvectors. (Equivalently, λ_n and $\mathbf{c}_n$ are the eigenvalues and eigenvectors of $\mathbf{K}^{-1}$.)

Even if the equation is inhomogeneous, $f(x) \neq 0$, we will run into trouble if λ is an eigenvalue, $\lambda = \lambda_n$, because in that case the matrix $(\mathbf{I} - \lambda_n \mathbf{K})$ cannot be inverted. Then as usual there will be either no solution or infinitely many solutions depending on whether an expansion of $\mathbf{f}$ in the eigenvectors $\mathbf{c}_m$ has a coefficient of the problematic $\mathbf{c}_n$ or not. For more on linear systems of algebraic equations, and the existence and uniqueness of their solutions, see section A.5.

As an example, consider the integral equation

$$y(x) = 1 - x + \frac{2}{\pi} \int_0^{\pi/2} \cos(x-z)y(z)\mathrm{d}z \tag{3.31}$$

where $K(x,z) = \cos(x-z) = \cos x \cos z + \sin x \sin z$, so $h_1 = g_1 = \cos x$ and $h_2 = g_2 = \sin x$. $f(x) = 1 - x$ and $\lambda = 2/\pi$. We can construct the matrix $\mathbf{K}$:

$$\mathbf{K} = \frac{1}{4} \begin{pmatrix} \pi & 2 \\ 2 & \pi \end{pmatrix}; \tag{3.32}$$

its (conventional) eigenvalues are $(\pi \pm 2)/4$ with eigenvectors $(1, \pm 1)$. The homogeneous equation ($f(x) = 0$) would only have solutions for $\lambda = 4/(\pi \pm 2)$. For the inhomogeneous equation with any other λ, we can solve straightforwardly. In this case $\mathbf{f} = (2 - \pi/2, 0)$, so

$$(\mathbf{I} - \lambda\mathbf{K})^{-1} = \frac{2\pi}{\pi^2 - 4} \begin{pmatrix} \pi & 2 \\ 2 & \pi \end{pmatrix} \qquad \Rightarrow \qquad \mathbf{c} = \frac{\pi(4-\pi)}{\pi^2 - 4} \begin{pmatrix} \pi \\ 2 \end{pmatrix}. \tag{3.33}$$

So finally we have

$$y(x) = (1-x) + \frac{2}{\pi} \int_0^{\pi/2} \cos(x-z)y(z)\mathrm{d}z \qquad \Rightarrow \qquad y(x) = (1-x) + \frac{2(4-\pi)}{\pi^2 - 4}(\pi \cos x + 2 \sin x). \tag{3.34}$$

Returning to the homogeneous equation, we see that we will have as many eigenvalues as there are independent terms in the separable kernel, N. This is very different from differential equations where there are usually infinitely-many eigenvalues. In this case the eigenfunctions are $(1, \pm 1) \cdot (\cos x, \sin x) = \cos x \pm \sin x$ which can also be written (up to a normalisation) as $\sin(x + \frac{\pi}{4})$ and $\cos(x + \frac{\pi}{4})$.

3.3   Hilbert-Schmidt theory

In this section, we consider Fredholm problems on the interval $x \in [a, b]$ with Hermitian kernels $K^*(z, x) = K(x, z)$ which are *bounded*, ie

$$\int_a^b \int_a^b |K(x,z)|^2 \, \mathrm{d}x \, \mathrm{d}z < \infty \tag{3.35}$$

As we have already noted, the eigenvalue equation

$$\phi(x) = \lambda \int_a^b K(x,z)\phi(z)\mathrm{d}z \tag{3.36}$$

will have one or more real eigenvalue λ_n and eigenfunction ϕ_n, and non-degenerate eigenfunctions are orthogonal on $[a, b]$. We have already discussed these for the particular case of N-term separable kernels, for which there were only N eigenfunctions. We will also use the notation $\phi_n(x) = \lambda_n \mathcal{K}\phi_n(x)$.

We need to introduce the concept of *source-resolvable* functions. A function $f(x)$ is source-resolvable relative to a particular kernel if some function $\rho(x)$ exists such that

$$f(x) = \int_a^b K(x,z)\rho(z)\mathrm{d}z. \tag{3.37}$$

This can be a pretty strong constraint. For instance for an N-term symmetric separable kernel $\sum_{i=1}^{N} h_i(x)h_i(z)$, *only* functions $f(x) = \sum_{n=1}^{N} c_n h_n(x)$ are source-resolvable; for the example with $K = \cos(x - z)$, the only source-resolvable functions have the form $A\cos(x + \alpha)$.

A basic result of Hilbert-Schmidt theory is that source-resolvable functions can be expanded in terms of the normalised eigenfunctions ϕ_n:

$$f(x) = \sum_{n=1}^{N} f_n \phi_n(x) \qquad \text{where} \qquad f_n = \langle \phi_n | f \rangle. \tag{3.38}$$

This is a (possibly finite-dimensional) version of completeness. Then we can write

$$K(x, z) = \sum_n \frac{\phi_n(x)\phi_n^*(z)}{\lambda_n} \tag{3.39}$$

which clearly satisfies $\lambda_m \mathcal{K}\phi_m(x) = \phi_m(x)$.

Consider again the example above, $K(x, z) = \cos(x - z) = \cos x \cos z + \sin x \sin z$, with integration limits 0 and $\pi/2$. We showed already that the eigenvalues are $\frac{4}{\pi \mp 2}$ and the normalised eigenfunctions are $\sqrt{\frac{4}{\pi-2}}\cos(x + \frac{\pi}{4})$ and $\sqrt{\frac{4}{\pi+2}}\sin(x + \frac{\pi}{4})$. (Slightly confusingly the squares of the normalisation constants and the eigenvalues are equal!) It takes only a line to verify that the eigenfunction expansion reproduces the original kernel:

$$K(x, z) = \frac{\frac{4}{\pi-2}\cos(x + \frac{\pi}{4})\cos(z + \frac{\pi}{4})}{\frac{4}{\pi-2}} + \frac{\frac{4}{\pi+2}\sin(x + \frac{\pi}{4})\sin(z + \frac{\pi}{4})}{\frac{4}{\pi+2}} = \cos(x - z). \tag{3.40}$$

It should be noted that the discussion above, about the properties of the eigenvalues and eigenfunction, does not help us actually find them. But if we have found them, we can also solve inhomogeneous equations with the same kernel and source $f(x)$. We can write

$$f(x) = \sum_n f_n \phi_n(x) + u(x) \qquad \text{and} \qquad y(x) = \sum_n y_n \phi_n(x) + v(x), \tag{3.41}$$

where $u(x)$ and $v(x)$ are the "remainders", the parts of f and y respectively which are orthogonal to all eigenfunctions (if the number of the latter is finite; otherwise $u = v = 0$). Then the equation reads

$$y(x) = f(x) + \lambda \int_a^b K(x, z)y(z)$$

$$\Rightarrow \quad \sum_n y_n \phi_n(x) + v(x) = \sum_n f_n \phi_n(x) + u(x) + \lambda \int_a^b \sum_n \frac{\phi_n(x)\phi_n^*(z)}{\lambda_n} \left(\sum_m y_m \phi_m(z) + v(z) \right) \mathrm{d}z$$

$$= \sum_n f_n \phi_n(x) + u(x) + \lambda \sum_{n,m} \frac{\phi_n(x)}{\lambda_n} y_m \delta_{nm}$$

$$\Rightarrow \quad y_n = f_n + \frac{\lambda}{\lambda_n} y_n \qquad \text{and} \qquad v(x) = u(x)$$

$$\Rightarrow \quad y_n = \frac{\lambda_n}{\lambda_n - \lambda} f_n = \left(1 + \frac{\lambda}{\lambda_n - \lambda} \right) f_n$$

$$\Rightarrow \quad y(x) = f(x) + \sum_n \frac{\lambda}{\lambda_n - \lambda} \langle \phi_n | f \rangle \, \phi_n(x). \tag{3.42}$$

In line three we used (by definition) $\langle\phi_n|u\rangle = 0$ for all n, then in the last line we added $u(x)(= v(x))$ to both sides to give the full $f(x)$ and $y(x)$. The final line has therefore lost all reference to the remainders, and thus they do not need to be identified separately.[5] Clearly the final expression for $y(x)$ needs some care if λ equals one of the eigenvalues; in fact, in a fashion which should by now be familiar, if $\lambda = \lambda_m$ there is no solution unless $\langle\phi_m|f\rangle = 0$. In that case we can add any multiple of $\phi_m(x)$ to the solution, which is therefore not unique.

We can rewrite the solution as

$$y(x) = f(x) + \lambda \int_a^b \sum_n \frac{\phi_n(x)\phi_n^*(z)}{\lambda_n - \lambda} f(z)\mathrm{d}z \equiv f(x) + \lambda \int_a^b R(x, z; \lambda)f(z)\mathrm{d}z, \qquad (3.43)$$

where this defines the *resolvent kernel* $R(x, z; \lambda)$.[6] This plays a similar role for the operator $\lambda\mathcal{K}$ as the Green's function does for $\mathcal{L}$: given any source, we can construct the solution by integration.

Taking a simpler example than before, let's consider

$$y(x) = f(x) + \lambda \int_0^1 xz\, y(z)\mathrm{d}z, \qquad (3.44)$$

which is has a one-term symmetric separable kernel $K(x, z) = xz$ The only source-resolvable function with this kernel is multiple of x, so we guess x must be an eigenfunction (the only one) and indeed $\int_0^1 xz\, z\mathrm{d}z = \frac{1}{3}x$: the corresponding eigenvalue is $\lambda_1 = 3$. The normalised eigenfunction is $\phi_1(x) = \sqrt{3}x$. Then we can check that $\phi_1(x)\phi_1(z)/\lambda_1 = K(x, z)$, and write the resolvent kernel as

$$R(x, z; \lambda) = \frac{3xz}{3 - \lambda}. \qquad (3.45)$$

The solution for any given source, for $\lambda \neq 3$, can be found easily from this:

$$y(x) = f(x) + \lambda \int_0^1 \frac{3xz}{3 - \lambda} f(z)\mathrm{d}z. \qquad (3.46)$$

For the rather simple case of $f = x$,

$$y(x) = x + \frac{3x\lambda}{3 - \lambda} \int_0^1 z^2\mathrm{d}z = x\left(1 + \frac{\lambda}{3 - \lambda}\right) = \frac{3x}{3 - \lambda}. \qquad (3.47)$$

If we rearrange the equation in which the resolvent kernel was defined, we obtain

$$f(x) = y(x) - \lambda \int_a^b R(x, z; \lambda)f(z)\mathrm{d}z, \qquad (3.48)$$

which is another integral equation, this time for f with a source y, and with kernel $-R(x, z; \lambda)$.

---

[5]It is common to see textbooks which assume that the ϕ_n are infinite in number and hence complete, so that the remainders u and v never enter. Then the first example they do is a 2D one, which miraculously works....

[6]Riley has the same definition for the resolvent kernel as us; in Prof Walet's notes the definition differs by an overall minus sign. Arfken does not use the term. A web search suggests both definitions are in use. The other definition has the advantage that R, not $-R$, is the kernel of the integral equation (3.48) for f in terms of y.

3.4 Neumann series: perturbation theory

It is not usually possible to find exact solutions or resolvent kernels for most integral equations. An interesting case is where λ is a small parameter. In that case we can write our solution as a power series in λ, and calculate it to any desired level of accuracy. To start with we consider Fredholm equations (fixed integration limits).

Obviously a zeroth-order approximation to $y(x)$, denoted $y^{(0)}$, is just the source, $f(x)$, which is what we get if we set $\lambda = 0$. A first-order correction is obtained by replacing $\lambda \mathcal{K} y$ by $\lambda \mathcal{K} y^{(0)} = \lambda \mathcal{K} f$, and so on. We then treat λ as a free parameter and match powers of λ on either side of the equation, as follows:[7]

$$
\begin{aligned}
&y = f + \lambda \mathcal{K} y \\
\Rightarrow\ &y^{(0)} + \lambda y^{(1)} + \lambda^2 y^{(2)} + \ldots = f + \lambda \mathcal{K}(y^{(0)} + \lambda y^{(1)} + \lambda^2 y^{(2)} + \ldots) \\
\Rightarrow\ &y^{(0)} = f, \quad y^{(1)} = \mathcal{K} y^{(0)}, \quad y^{(2)} = \mathcal{K} y^{(1)}, \quad \ldots \\
\Rightarrow\ &y^{(n)} = \mathcal{K} y^{(n-1)} = \mathcal{K}^n f \\
\Rightarrow\ &y = \sum_{n=0}^{\infty} (\lambda \mathcal{K})^n f
\end{aligned}
\tag{3.49}
$$

Thus we also have a neat expression for the resolvent kernel, $R = \sum_{n=1}^{\infty} \lambda^{n-1} \mathcal{K}^n$. To use, though, this needs some unpacking. What do we even mean by $\mathcal{K}^2 f$? It's simple but a little messy:

$$
\begin{aligned}
\mathcal{K} f(x) &= \int_a^b K(x, z) f(z)\, \mathrm{d}z \\
\Rightarrow\quad \mathcal{K}^2 f(x) &= \int_a^b K(x, z') \left(\int_a^b K(z', z) f(z)\, \mathrm{d}z \right) \mathrm{d}z' \\
&= \int_a^b \left(\int_a^b K(x, z') K(z', z) \mathrm{d}z' \right) f(z)\, \mathrm{d}z \quad \equiv \int_a^b K_2(x, z) f(z)\, \mathrm{d}z
\end{aligned}
\tag{3.50}
$$

and by extension,

$$
\mathcal{K}^n f(x) = \int_a^b K_n(x, z) f(z)\, \mathrm{d}z,
\tag{3.51}
$$

where

$$
\begin{aligned}
K_n(x, z) &= \int_a^b \int_a^b \ldots \int_a^b \int_a^b K(x, z_{n-1}) K(z_{n-1}, z_{n-2}) \ldots K(z_2, z_1) K(z_1, z)\, \mathrm{d}z_{n-1}\, \mathrm{d}z_{n-2} \ldots \mathrm{d}z_2\, \mathrm{d}z_1, \\
&= \int_a^b K(x, z') K_{n-1}(z', z) \mathrm{d}z'
\end{aligned}
\tag{3.52}
$$

with n terms and $n-1$ integrals over dummy variables $z_1, z_2 \ldots z_{n-1}$. (This matches the definition of K_2 if we define $K_1 = K$.) Then the solution is written

$$
y(x) = f(x) + \sum_{n=1}^{\infty} \lambda^n \int_a^b K_n(x, z) f(z)\, \mathrm{d}z.
\tag{3.53}
$$

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[7]Prof Walet's notes approach this in a slightly different, but equivalent, fashion. The current approach is closer to Riley and Arfken. Past exams may reflect the previous approach in their wording.

Though we found an exact solution above, let us consider again

$$y(x) = x + \lambda \int_0^1 xz\, y(z)\, \mathrm{d}z\,, \tag{3.54}$$

this time as a perturbation expansion. We can construct

$$K_2(x,z) = \int_0^1 xs\, sz\, \mathrm{d}s = \tfrac{1}{3}xz; \qquad K_3(x,z) = \int_0^1 xs\, K_2(s,z)\mathrm{d}s = \tfrac{1}{9}xz\,, \tag{3.55}$$

and so on, so that $K_n(x,z) = K_1(x,z)/3^{n-1}$ and

$$y(x) = x + \sum_{n=1}^{\infty} \lambda \left(\frac{\lambda}{3}\right)^{n-1} \int_0^1 xz\, z\, \mathrm{d}z = x\left(1 + \sum_{n=1}^{\infty}\left(\frac{\lambda}{3}\right)^n\right) = \frac{x}{1 - \frac{\lambda}{3}} \tag{3.56}$$

which is the same as before. Of course the main purpose of this method is for cases where the solution cannot be found in closed form, but only evaluated up to some chosen order in λ.

We have written the power series as if it exists; in fact so long as K is bounded and λ satisfies

$$|\lambda|^2 \int_a^b \int_a^b |K(x,z)|^2 \mathrm{d}x\, \mathrm{d}z < 1 \tag{3.57}$$

then the series is guaranteed to converge. For this case the series does not converge for $\lambda > 3$, but the resummed series gives the correct answer for any $\lambda \neq 3$.

In fact we already met an example of first-order perturbation theory with the Born approximation to the Schrödinger equation for scattering from a localised potential; a slight difference is that the solution of the homogeneous equation, rather than a source, acted as the zeroth-order approximation.

The analysis above carries over to Volterra equations, with a lot more care in the construction of $K_n(x,z)$. We have

$$y^{(0)}(x) = f(x); \quad y^{(1)}(x) = \int_0^x K(x,z)f(z)\mathrm{d}z; \quad y^{(2)}(x) = \int_0^x K(x,z')\left(\int_0^{z'} K(z',z)f(z)\mathrm{d}z\right)\mathrm{d}z' \tag{3.58}$$

but we can't yet write the last equation in terms of a single integral involving some $K_2(x,z)$. However we can swap the order of integration over the triangle (c.f. (3.11)) giving

$$\begin{aligned}
y^{(2)}(x) &= \int_0^x K(x,z')\left(\int_0^{z'} K(z',z)f(z)\mathrm{d}z\right)\mathrm{d}z' \\
&= \int_0^x \left(\int_z^x K(x,z')K(z',z)\mathrm{d}z'\right) f(z)\,\mathrm{d}z \equiv \int_0^x K_2(x,z)f(z)\,\mathrm{d}z \tag{3.59}
\end{aligned}$$

By the same token, if we assume the existence of a K_n, we can write

$$\begin{aligned}
y^{(n+1)}(x) &= \int_0^x \left(K(x,z')\int_0^{z'} K_n(z',z)f(z)\mathrm{d}z\right)\mathrm{d}z' \\
&= \int_0^x \left(\int_z^x K(x,z')K_n(z',z)\mathrm{d}z'\right) f(z)\,\mathrm{d}z \equiv \int_0^x K_{n+1}(x,z)f(z)\,\mathrm{d}z. \tag{3.60}
\end{aligned}$$

Since this holds for $n = 1$, by induction it holds for any n.

An example, more details of which are on the examples sheet, is the problem

$$y(x) = f(x) + \lambda \int_0^x e^{x-z} y(z) \, dz. \tag{3.61}$$

Now

$$K_2(x, z) = \int_z^x e^{x-z'} e^{z'-z} dz' = (x-z)e^{x-z}, \quad K_3(x, z) = \int_z^x e^{x-z'}(z'-z)e^{z'-z} dz' = \tfrac{1}{2}(x-z)^2 e^{x-z} \tag{3.62}$$

and in fact we can show that

$$K_n(x, z) = \frac{(x-z)^{n-1}}{(n-1)!} e^{x-z} \tag{3.63}$$

and so

$$R(x, z; \lambda) = \sum_{n=1}^\infty \lambda^{n-1} K_n(x, z) = e^{(1+\lambda)(x-z)}. \tag{3.64}$$

Again the existence of a closed form is not typical. This time the series converges for any λ, as will always be the case (with a finite kernel) for Volterra equations. The reason is that each successive integration in the chain that builds up $K_n(x, z)$ is over a smaller and smaller area of the $z_n - z_{n+1}$ plane, causing the magnitude to diminish with n.

4. Calculus of Variations

4.1 Introduction

Arfken 22
Riley 22

A common problem in physics is to find the function $y(x)$ on an interval $x \in [a, b]$ which minimises some physical quantity which depends on y and/or its derivative y' over the whole length.[1] Often the endpoints of y, $y(a)$ and $y(b)$, are specified. A simple example is the length of the line on the xy plane between the points $(0, 0)$ and $(1, 1)$, where the length is given by $\int_0^1 \sqrt{dx^2 + dy^2}$ or equivalently

$$L[y] = \int_0^1 \sqrt{1 + (y')^2} \, dx. \tag{4.1}$$

Allowed paths are all those which pass through the endpoints and are differentiable; in this case we know that the straight line $y = x$ will minimise the length and $L[y_{\min}] = \sqrt{2}$.

The notation $L[y]$, or more generally $I[y]$, with square brackets, denotes a *functional*, a number (in the sense of being independent of x) which depends on an entire function $y(x)$ over some range.

The condition that $I[y]$ be a minimum gives rise to a second-order differential equation in y which, together with the boundary conditions, is solved by the path $y_{\min}(x)$. We find this by assuming the existence of the minimising path $y_{\min}(x)$ and considering paths which deviate from it. Just as the sign of an extremum of a *function* is flatness (vanishing derivative) as a function of x, so an extremum of a *functional* is signalled by the lack of variation of $I[y]$ with the path y (vanishing functional derivative). For instance if we consider the path $y = x + cx(1 - x)$ in the example above, the functional derivative reduces to a normal derivative wrt c, which is indeed zero for $c = 0$.

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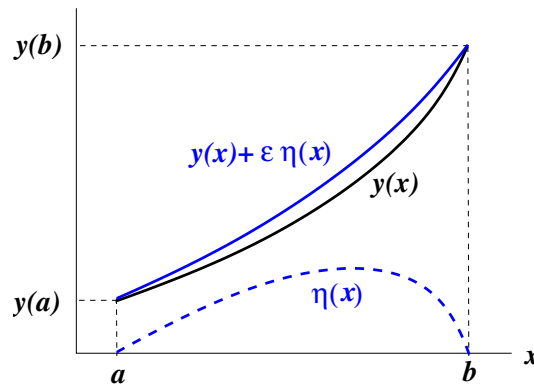
[1]In some texts, and past exam papers, the derivative $\frac{dy}{dx}$ is denoted $y_{,x}$. This is useful for the case of more than one independent variable, where the derivative w.r.t the i-th variable can be written $y_{,i}$, but we will only briefly allude to such cases here.

To find the form of the functional derivative, consider a path $y(x)$ which satisfies the endpoint constraints (boundary conditions) and another, $\eta(x)$ for which $\eta(a) = \eta(b) = 0$; then $y(x)+\epsilon\eta(x)$ is another possible path for any arbitrary $\eta(x)$. We allow the integrand of $I[y]$ to depend explicitly on x, y and the x-derivative of y, y', and denote it $F(y, y', x)$. Then Taylor-expanding in ϵ and dropping higher-order terms gives

$$I[y + \epsilon\eta(x)] = \int_a^b F\left(y + \epsilon\eta, y' + \epsilon\eta', x\right)\mathrm{d}x$$

$$= I[y] + \epsilon \int_a^b \left(\eta(x)\frac{\partial F}{\partial y} + \eta'\frac{\partial F}{\partial y'}\right)\mathrm{d}x$$

$$\Rightarrow \delta I = \epsilon \int_a^b \eta(x)\left(\frac{\partial F}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial F}{\partial y'}\right)\right)\mathrm{d}x + \epsilon\left[\eta\frac{\partial F}{\partial y'}\right]_a^b \tag{4.2}$$

where in the last line we integrated by parts; the boundary term, included explicitly for future reference, vanishes because η is zero at the boundaries.

Now the condition for y to be $y_{\min}$ is that $\mathrm{d}I/\mathrm{d}\epsilon$ must vanish, so integral must vanish. But as η is arbitrary the term it multiplies must vanish and we obtain the *Euler equation*:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial F}{\partial y'}\right) - \frac{\partial F}{\partial y} = 0. \tag{4.3}$$

Since F depends on y and y', this will give a differential equation for y which is satisfied by $y_{\min}(x)$. The solution may not be unique; there may be multiple solutions which are local or global extrema. We always need to check that our solution actually is a global minimum.

We should note that $\frac{\mathrm{d}}{\mathrm{d}x}$, unlike $\frac{\partial}{\partial x}$, picks up implicit dependence on x through y and y', as well as explicit dependence. So

$$\frac{\mathrm{d}}{\mathrm{d}x}F(y, y', x) = \frac{\partial F}{\partial x} + y'\frac{\partial F}{\partial y} + \frac{\mathrm{d}y'}{\mathrm{d}x}\frac{\partial F}{\partial y'}. \tag{4.4}$$

Thus the Euler equation (multiplied by y') can be rewritten

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(F - y'\frac{\partial F}{\partial y'}\right) - \frac{\partial F}{\partial x} = 0. \tag{4.5}$$

which is very useful if F has no *explicit* dependence on x, in which case we get the second form of Euler's equation

$$F - y'\frac{\partial F}{\partial y'} = c. \tag{4.6}$$

For the path-length problem with $F = \sqrt{1 + (y')^2}$, which has no explicit dependence on either x or y, either form may be used; Eq. (4.3) gives

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{y'}{\sqrt{1 + (y')^2}} = 0 \qquad \Rightarrow \qquad \frac{y'}{\sqrt{1 + (y')^2}} = c, \tag{4.7}$$

which with some manipulation yields $y' =$ constant, or $y = Ax + B$. The boundary conditions fix A and B.

Some relatively elementary problems covered in PHYS20401 are:

- Minimisation of the area (and hence surface energy) of soap films, particularly that between two coaxial hoops, for which the area element to be integrated is

$$A[y] = \int_a^b 2\pi y \sqrt{1 + (y')^2} \, \mathrm{d}x; \qquad (4.8)$$

  the solution is a catenary (hyperbolic cosine).

- The brachistochrone problem, whose solution is a cycloid: finding the shape of a wire that minimises the time a frictionless bead takes to slide between two points under gravity, where

$$t[y] = \int_a^b \frac{\sqrt{1 + (y')^2}}{\sqrt{2g(y - y(a))}} \, \mathrm{d}x \qquad (4.9)$$

  (the denominator being the velocity if the bead starts at rest).

- Finding the path light takes though a medium of variable refractive index, by minimising the light travel time with

$$t[y] = \int_a^b \frac{n(x, y)}{c} \sqrt{1 + (y')^2} \, \mathrm{d}x. \qquad (4.10)$$

  For the mirage problem the refractive index varies with height, $n = n(y)$, since the air closest to the hot ground is the least dense. A related problem asks about the light path near a massive star or black hole.

- Finding the shortest path between two points on a curved surface.

- Hamilton's principle says that the evolution of a mechanical system between two times minimises the time integral of the Lagrangian; the resulting equations are usually called the Euler-Lagrange equations in that context.

In the latter problems, we typically have more than one dependent variable, $y_1(x)$, $y_2(x)$, ... (for instance $r(t), \theta(t)$ and $\phi(t)$) and we have one Euler equation for each:

$$\frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial F}{\partial y_i'} - \frac{\partial F}{\partial y_i} = 0. \qquad (4.11)$$

Often "x" is time and the y_i are coordinates of a system $q_i(t)$. If F doesn't depend on one of the coordinates itself, $\partial F/\partial y_i = 0$, then $\partial F/\partial y_i' = 0$ is a "constant of the motion", typically an (angular) momentum in mechanical problems.

It is also possible to have problems with more than one *independent* variable, $x_1, x_2, \ldots$). The functional is obtained by integrating over all these variables, and the resulting Euler equations then read

$$\left(\sum_i \frac{\mathrm{d}}{\mathrm{d}x_i} \frac{\partial F}{\partial y_{j,i}} \right) - \frac{\partial F}{\partial y_j} = 0, \qquad (4.12)$$

where $y_{j,i} = dy_j/dx_i$. When field theories are written in terms of Lagrangian, the fields are functions of position and time and there are four independent variables. For a scalar field corresponding to a particle of mass m, the free field Lagrangian (strictly, Lagrangian density since it has dimensions of energy/volume) is (in units in which $\hbar=c=1$)

$$L = \frac{1}{2} \left(\frac{\partial \Phi}{\partial t} \right)^2 - \nabla\phi \cdot \nabla\phi - \frac{1}{2} m^2 \Phi^2 \qquad (4.13)$$

giving the Klein-Gordon wave equation for the field

$$\frac{\partial^2 \Phi}{\partial t^2} - \nabla^2 \Phi + m^2 \Phi = 0. \tag{4.14}$$

In this course we move on to more involved problems. For example if a heavy chain of mass μ per unit length is suspended under gravity from two end-points, the curve it adopts will minimise the potential energy

$$E[y] = -\int_a^b \mu g y \sqrt{1 + (y')^2} \, \mathrm{d}x; \tag{4.15}$$

This looks just like the soap film problem. But it is not, because the chain has a definite length which the soap-film solution will not in general respect. This problem is an example of *constrained minimisation*. To see how to proceed, we will first look at constrained minimisation for functions rather than functionals.

4.2 Constrained minimisation and Lagrange multipliers

Arfken 22.4
Riley 22.4

We have met problems of minimisation of *functions* subject to a constraint before, in statistical mechanics for instance. There, the method used was that of Lagrange multipliers, and a reminder of the method can be found in A.6. For functionals, the same method can be used.

For the chain of length L_0 we have

$$E[y] = -\int_a^b \mu g y \sqrt{1 + (y')^2} \, \mathrm{d}x \qquad L[y] = \int_a^b \sqrt{1 + (y')^2} \, \mathrm{d}x \,, \tag{4.16}$$

and the constraint on the path $y(x)$ is $L[y] - L_0 = 0$. Hence we will minimise $E[y] + \lambda(L[y] - L_0)$ and impose the constraint as well as the endpoints to find our full solution.[2] Our integrand is

$$F(y, y', x) + \lambda G(y, y', x) = -\mu g(y - h)\sqrt{1 + (y')^2} \tag{4.17}$$

where $\mu g h \equiv \lambda$. The lack of dependence on x suggests the second form of Euler's equation,

$$-(y - h)\sqrt{1 + (y')^2} + \frac{(y - h)y'^2}{\sqrt{1 + (y')^2}} = c \,. \tag{4.18}$$

We can change variables to $z = y - z$, $y' = z'$ to get a replica of the soap-film problem, and the solution before we impose boundary conditions or constraints is

$$y(x) = h + A \cosh\left(\frac{x - B}{A}\right). \tag{4.19}$$

Now in the soap-film problem, y is the radius of the film at any given x, and $y(a)$, $y(b)$ are the radii of the supporting hoops; they have a real influence on the solution. There is no constant h so the endpoints fully specify the constants A and B. But for the chain, the absolute y is

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[2]Since clearly the constant L_0 doesn't enter Euler's equation, it is often in practice dropped so that the new functional is $E[y] + \lambda L[y]$.

irrelevant and can be adjusted by changing h. Only the difference is physical, and that only suffices to fix one combination of A and B. We are left with enough freedom to fix the length, as required. If, for definiteness, we take $b = L/3 = -a$ and $y(a) = y(b)$, then $B = 0$, and $2A \sinh(L/3A) = L$ fixes $A = 0.205L$.

For this problem there is no ambiguity about the interpretation of the solution, which is an absolute minimum and guaranteed to exist so long as the endpoints aren't further apart than the length of the chain. The soap-film problem is actually more complicated; see textbooks.

The classic constrained-variation problem is the isoperimetric problem: what is the maximum area that can be enclosed by a fence of fixed length? The simpler version has fixed endpoints, say $(-a, 0)$ and $(a, 0)$ and a fixed wall running along the x-axis, then the fence follows a curve $y(x)$ between those points to enclose an area with the wall. The area of course is just $A[y] = \int_{-a}^{a} y(x)\mathrm{d}x$, and $L[y]$ has the usual form. Then

$$F(y, y', x) + \lambda G(y, y', x) = y + \lambda \sqrt{1 + (y')^2}. \tag{4.20}$$

The lack of dependence on x suggests the second form of Euler's equation; the two constants of integration are naturally termed y_0 and x_0, and the solution is

$$(x - x_0)^2 + (y - y_0)^2 = \lambda^2. \tag{4.21}$$

The fence is an arc of a circle, radius λ. Symmetry sets $x_0 = 0$, the endpoints give $|y_0| = \sqrt{\lambda^2 - a^2}$ and the centre of the circle is at $(0, -|y_0|)$. The length of the arc is $2\lambda \arcsin(a/\lambda)$, which fixes λ in terms of L, provided $2a < L < \pi a$. The upper limit is required because otherwise the curve $y(x)$ would be double-valued for some x. Physically it would still be an arc of a circle though. There is also a version of the isoperimetric problem for a closed curve, which has a full circle as its solution; this will be covered in lectures if time permits.

These problems are relatively simple because the constraints are integral ones. It is also possible to have a constraint that places restrictions on the path more locally, in the form $G(y, y', x) = 0$ for all $x \in [a, b]$. In that case we need to add to F a term $\lambda(x)G(y, y', x)$; effectively we have a λ for each value of x at which we need to apply the constraint. With more than one dependent variable y_i there can be more constraints, λ_i. Examples of this type of problem arise in Lagrangian mechanics if, rather than finding the minimal set of (perhaps contrived) coordinates, we choose to use more obvious ones and apply a constraint. An advantage is that the approach also yields the constraint forces which, though they do no work, keep the system on the constrained path. Examples can be found in textbooks, but they do not in practice offer a great simplification and I will not pursue them here.

4.3   Endpoints not fixed

Riley 22.3.4

In the above we assumed, as in the chain problem, that $y(a)$ and $y(b)$ are fixed, but this restriction can be lifted. In particular consider $y(a)$ fixed still, but with the other end subject to some more complicated constraint: it might be that b is fixed but $y(b)$ is not, which would be the case if the end of the chain could slide on a vertical rod, or it might be that the endpoint lies somewhere on a line given by the constraint $v(x, y) = 0$, for instance if the rod is not vertical, or is not straight.

The algebra that follows is a bit involved, so it is important to signal at the outset that the Euler equation, and hence the form of the solution, are the same as before. Only the determination of the constants of integration from the endpoints changes.
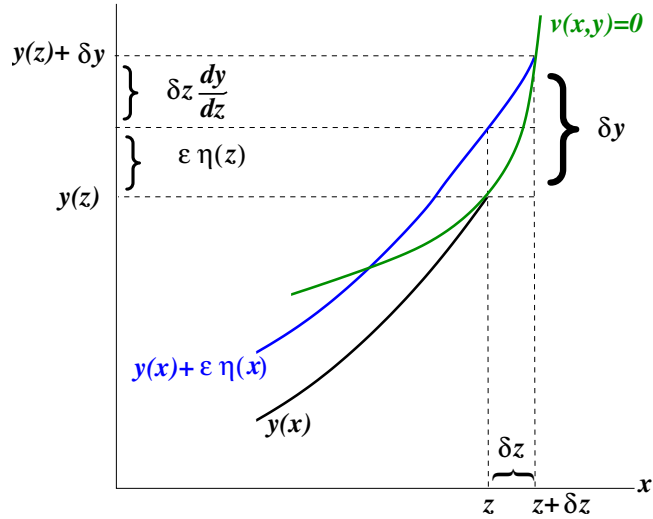
If the problem is well posed, there will be some definite final end-point, which we will denote $(z, y(z))$ (with $v(z, y(z)) = 0$), but we don't know in advance what it is. As before we can define the minimal curve $y_m(x)$ as the one for which the change in $I[y]$ vanishes for small deviations $\epsilon\eta(x)$ and as before $\eta(a) = 0$. The difference is that $\eta(z) \neq 0$ and also the endpoint can move, albeit only on the constraint curve. We denote a change in the endpoint as δz. We will need the corresponding shift in the y value, as illustrated above,

$$\delta y = \epsilon\eta(z) + \delta z\, y'(z), \tag{4.22}$$

and briefly using $F(z)$ as a shorthand for $F(y, y', x)$ evaluated at $x = z$ we have (dropping terms with two small quantities such as $\epsilon\delta z$):

$$I[y + \epsilon\eta(x)] = \int_a^{z+\delta z} F\left(y + \epsilon\eta, y' + \epsilon\eta', x\right)\mathrm{d}x$$

$$= I[y] + \epsilon\int_a^z \left(\eta\frac{\partial F}{\partial y} + \eta'\frac{\partial F}{\partial y'}\right)\mathrm{d}x + F(z)\delta z$$

$$\Rightarrow \delta I = \epsilon\int_a^z \eta(x)\left(\frac{\partial F}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial F}{\partial y'}\right)\right)\mathrm{d}x + \epsilon\left[\eta\frac{\partial F}{\partial y'}\right]_a^z + F(z)\delta z$$

$$= \delta I_{\text{Euler}} + \left(\delta y - \delta z\, y'(z)\right)\left.\frac{\partial F}{\partial y'}\right|_z + F(z)\delta z$$

$$= \delta I_{\text{Euler}} + \delta y\left.\frac{\partial F}{\partial y'}\right|_z + \delta z\left(F(z) - y'(z)\left.\frac{\partial F}{\partial y'}\right|_z\right). \tag{4.23}$$

Compare to last time (the result of which is denoted δI_{Euler}) we have extra terms from the moving of the endpoint. For the minimal path, infinitesimal changes of the path between a and z, and of the endpoint, must separately leave $I[y_m]$ unchanged, so the vanishing of the extra terms forms a new constraint in addition to the Euler equation. We have not yet used the fact that the endpoint is constrained by $v(z, y(z)) = 0$ so

$$\mathrm{d}v = 0 \quad \Rightarrow \quad \frac{\partial v}{\partial z}\delta z + \frac{\partial v}{\partial y}\delta y = 0. \tag{4.24}$$

Using this to write δy in terms of δz in Eq. (4.23) finally gives the the extra constraint which must be satisfied at the endpoint $x = z$ as

$$\frac{\partial v}{\partial z}\left.\frac{\partial F}{\partial y'}\right|_z - \frac{\partial v}{\partial y}\left(F(y, y', z) - y'\left.\frac{\partial F}{\partial y'}\right|_z\right) = 0. \tag{4.25}$$

For the case that z is fixed at b and only $y(z)$ can vary, we have $v(z, y(z)) = z-b$ and $\partial v/\partial y = 0$; then the condition is just

$$\left.\frac{\partial F}{\partial y'}\right|_b = 0. \tag{4.26}$$

For the case of the chain with one end free to slide on a vertical rod, $F \rightarrow F + \lambda G = -\mu g(y - h)\sqrt{1 + (y')^2}$, the constraint yields $(y - h)y' = 0$. Since the overall height of the chain is clearly arbitrary, this requires $y' = 0$, that is the chain is at right-angles to the rod. (In fact if we substitute the form of the solution back in, we see that on the minimal path, $\partial F/\partial y' \propto y'$.) We could have guessed that on physical grounds, since any component of the tension not at right-angles to the rod will cause the end to move up or down. The solution is

$$y(x) = h + A\cosh\left(\frac{x - b}{A}\right), \qquad \text{with} \qquad L = A\sinh\left(\frac{b - a}{A}\right). \tag{4.27}$$

For a tilted rod obeying $mx + c - y = 0$, it can be shown straightforwardly that the boundary constraint gives $y' = -1/m$, so again the rod and chain are at right-angles. (Note that as $F + \lambda G$ does not depend explicitly on x, the term in brackets multiplying $\partial v/\partial y$ is just a constant (second form of Euler's equation), here equal to $-\mu g A$.)

4.4 Rayleigh-Ritz variational technique

Arfken 22.4
Riley 22.6, 22.7

Here we show that Sturm-Liouville and Hilbert-Schmidt problems can be expressed as constrained variational problems. This leads to a useful method for estimating the lowest eigenvalue of such problems, and sometimes certain higher eigenvalues too. This method is traditionally used in quantum mechanics to obtain the approximate ground state energy (actually an upper bound) for systems such as the helium atom which cannot be solved analytically.

Consider the problem of finding an extremum of the functional $I[y]$ subject to the constraint $J[y] = 1$, where

$$I[y] = \int_a^b p(x)y'(x)^2 + q(x)y(x)^2 \, \mathrm{d}x \qquad \text{and} \qquad J[y] = \int_a^b \rho(x)y(x)^2 \, \mathrm{d}x, \tag{4.28}$$

with $y(a)$ and $y(b)$ fixed. We will take $p(x)$ and $\rho(x)$ and $q(x)$ to be positive and bounded.[3]

Setting $\delta(I[y] - \lambda J[y]) = 0$ gives the Euler equation

$$-\frac{\mathrm{d}}{\mathrm{d}x}(p(x)y'(x)) + q(x)y(x) = \lambda\rho(x)y(x). \tag{4.29}$$

This is of course the Sturm Liouville (generalised) eigenfunction equation, where the parameter $-\lambda$ introduced as a Lagrange multiplier now plays the role of the eigenvalue (the sign being chosen to agree with the conventional definition). $J[y]$ is a normalisation condition; without it, if $y(a) = y(b) = 0$, the minimum would just be $y = 0$ which is uninteresting.

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[3]For a general SL equation we only required $q(x)$ to be real, not positive. However we can always add $\Lambda\rho(x)$ to both sides of the eigenvalue equation (4.29), where Λ is a constant chosen large enough that $q(x) + \Lambda\rho(x) > 0$. This defines an equivalent problem with the same eigenfunctions as the original one, and with all eigenvalues simply increased by Λ. This also ensures that all eigenvalues are positive.

As in previous constrained variational problems, the introduction of a Lagrange multiplier allows us to satisfy both the boundary conditions and the constraint. Similarly in SL problems the eigenvalue has to be adjusted so that non-trivial (ie normalisable) solutions can be found which satisfy the boundary conditions.

If, conversely, we start from the SL equation, multiply by $y(x)$ and integrate from a to b, we obtain

$$\int_a^b -y(x)\Big(p(x)y'(x)\Big)' + \Big(q(x) - \lambda\rho(x)\Big)y(x)^2 \, \mathrm{d}x = I[y] - \lambda J[y] - [p(x)y'(x)y(x)]_a^b. \quad (4.30)$$

Boundary conditions on $y(x)$ such that the boundary term vanishes (for example $y(a) = y(b) = 0$) are also sufficient to make the SL operator Hermitian.[4] Assuming such conditions, for $y_n(x)$ which is a solution of the SL equation for some λ_n, the integrand on the LHS will vanish and so $I[y_n] = \lambda_n J[y_n]$.

Thus the extremal value of $I[y] - \lambda J[y]$ is zero, and the constraint $J[y] = 1$ avoids the uninteresting solution $y = 0$ and requires $\lambda = \lambda_n$, an eigenvalue. This extremum is obtained if $y = y_n$.

Now it turns out that we can cast this as an unconstrained extremisation problem of a new kind. If we define $\lambda[y] = I[y]/J[y]$, then $\lambda[y_n] = \lambda_n$. But

$$\delta\lambda[y] = \frac{\delta I}{J} - \frac{I\delta J}{J^2} = \frac{\delta I - \lambda[y]\delta J}{J} \qquad (4.31)$$

so finding the stationary points of $\lambda[y]$ is equivalent to the original constrained extremisation problem: if a solution y_n is found such that $\delta\lambda[y_n] = 0$, then $\delta(I[y_n] - \lambda_n J[y_n]) = 0$ where λ_n is an eigenvalue of the equivalent SL equation.

Now since $p(x), q(x)$ and $\rho(x)$ are all positive, $\lambda[y] > 0$; it is bounded from below. So there must be an absolute minimum λ_1, which is obtained for the true ground-state solution y_1. All the other extrema will be saddle-points in general.

Why is this interesting? Well first of all, we have shown that there *is* a minimum of $\lambda[y]$, and hence there *is* a minimum eigenvalue, something which we made plausible but did not prove previously. Furthermore it follows that if we calculate $\lambda[u]$ for an arbitrary function u, $\lambda[u] \geq \lambda_1$, and equality implies that $u = y_1$. If we do not know λ_1, we can find an upper bound by trying plausible functions *which must however obey the boundary conditions*. This is known as the *Rayleigh-Ritz* variational method of estimating eigenvalues, and is particularly widely used in quantum mechanics (see below).

Conversely, we can use of knowledge of the properties of the eigenfunctions and eigenvalues of regular Hermitian SL problems to discuss the extrema of $\lambda[y]$. The (real, of course) eigenvalues λ_n are non-degenerate and increase without bound; the corresponding eigenfunctions y_n are orthogonal. Hence if we look for extrema in the space of functions u which are orthogonal to y_1, they exist at $\lambda_2, \lambda_3, \ldots$. Hence in this space λ_2 is an absolute minimum and $\lambda[y] \geq \lambda_2$. In general, in the space of functions orthogonal to the first N eigenfunctions, $\lambda[y] \geq \lambda_{N+1}$. Note that one property of the eigenfunctions that we have *not* assumed is completeness. We will in fact use this to *prove* completeness later.

---

[4]In deriving Eq. (4.29) we assumed fixed boundary conditions so that $\left[\eta\frac{\partial F}{\partial y'}\right]_a^b = 0$ because $\eta(a) = \eta(b) = 0$. This term also vanishes for periodic boundary conditions and for $y'(a) = y'(b) = 0$. It does not vanish for general homogeneous boundary conditions $\alpha y = \beta y'$ though, and in that case the functional $I[y]$ has to be slightly modified though the final conclusions still hold.

4.4.1 Estimation of lowest eigenvalue and adjustment of parameters

As a very simple example, consider the SL equation $-y''(x) = \lambda y(x)$ with bc $y(0) = 0 = y(a)$ (the physical problem could be an infinite square well with $V = 0$ for $x \in (0, a)$ and $V = \infty$ otherwise, or waves on a string). As a trial function, we use $u(x) = x(a - x)$, $0 < x < a$, which obeys the boundary conditions. Then we calculate

$$\lambda_1 \leq \frac{\int_0^a y\mathcal{L}y \, dx}{\int_0^a y^2 \, dx} = \frac{10}{a^2} = 1.013\frac{\pi^2}{a^2} \tag{4.32}$$

This is spectacularly good! Obviously it helped that our trial function looked a lot like what we'd expect of the true solution—symmetric about the midpoint, no nodes....

Note that we wrote the numerator as $\int_0^a u\mathcal{L}u \, dx$, However since it is an SL problem (with appropriate bcs), we have shown that the integral could equally have been written $\int_0^a p(u')^2 \, dx$ (with $p(x) = 1$ here) and the avoidance of the second differentiation is often a saving in effort. Note also that we had $\rho = 1$ in this case, but that is not general either.

Though we've said it already, we reiterate that it is of course imperative that trial functions obey the boundary conditions of the problem. Without that constraint, it is easy to evade the bounds: had we chosen $u(x) = C$ above we would have obtained, erroneously, $\lambda_1 \leq 0$!

In general, we will do better if we have an adjustable parameter, because then we can find the value which minimises our upper bound. So in the example above we could try $u(x) = x(a - x) + bx^2(a - x)^2$ (with our previous guess corresponding to $b = 0$). Letting Mathematica do the dirty work, we get an energy bound which is a function of b, which takes its minimum value of $1.00001E_0$ at $b = 1.133/a^2$. Not much room for further improvement here!
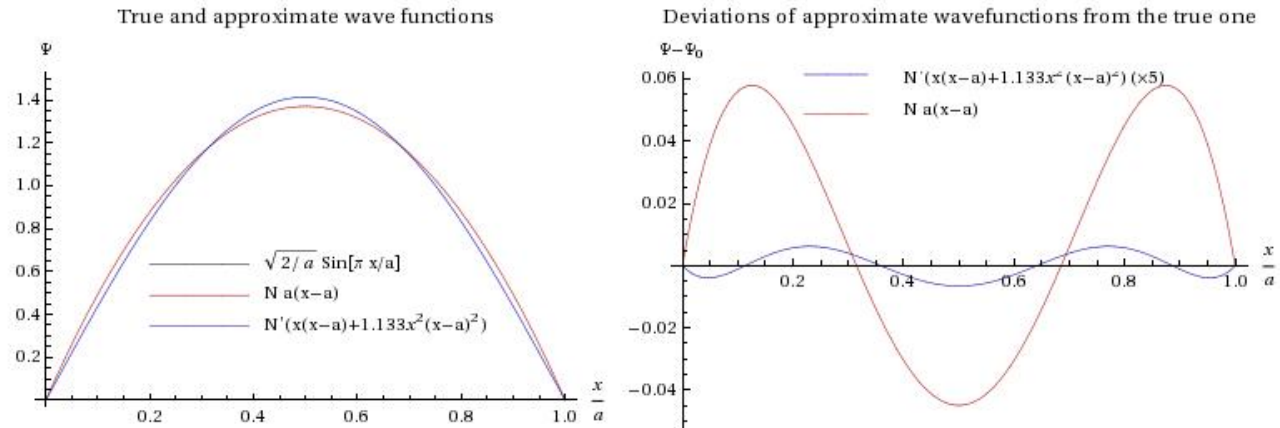
Above we have plotted, on the left, the true and approximate solutions (except that the true one is hidden under the second approximation, given in blue) and on the right, the deviations of the approximate wave functions from the true one (except that for the second approximation the deviation has been multiplied by 5 to render it visible!) This illustrates a general principle though: the best trial solution does have deviations from the true one on the part-per-mil scale, while the eigenvalue is good to 1 part in 10^5. This is explained further below.

4.4.2 Alternative derivation of Rayleigh-Ritz principle

If we *assume* that eigenfunctions y_i of an SL operator form a complete set, we can derive the variational principle more simply; this is the method typically used in quantum mechanics texts.

Completeness implies that any trial solution can be written

$$u(x) \equiv \sum_{n=1}^{\infty} c_n y_n(x) \tag{4.33}$$

and so

$$\mathcal{L}u(x) = \sum_{n=1}^{\infty} c_n \lambda_n \rho(x) y_n(x). \tag{4.34}$$

We also define $d_m = c_m / \sqrt{\sum_n c_n^2}$, the coefficients of u normalised to 1. Then

$$
\begin{aligned}
\lambda[u] = \frac{\int_a^b u \mathcal{L} u \, \mathrm{d}x}{\int_a^b \rho u^2 \, \mathrm{d}x} &= \frac{\sum_{n,m} c_m c_n \lambda_n \int_a^b \rho(x) y_m(x) y_n(x) \, \mathrm{d}x}{\sum_{n,m} c_m c_n \int_a^b \rho(x) y_m(x) y_n(x) \, \mathrm{d}x} \\
&= \frac{\sum_n c_n^2 \lambda_n}{\sum_n c_n^2} = \sum_n d_n^2 \lambda_n \\
&\geq \lambda_1 \sum_n d_n^2 = \lambda_1
\end{aligned}
\tag{4.35}
$$

where we have used the fact that by definition $\lambda_n > \lambda_1$ for $n \geq 2$. In other words the trial wave function has admixtures of higher eigenfunctions, which raise the value of $\lambda[y]$ above its minimum.

This allows us to understand why variational approaches tend to lead to a better result for λ_1 than for $y_1(x)$. This is because the error in the eigenvalue is proportional to the coefficients squared of the admixture of "wrong" states, whereas the error in the wave function is linear in them.

Furthermore, looking again at the expression $\lambda[u] = \sum_n d_n^2 \lambda_n$, and recalling that the d_n are the overlaps between the trial function and the actual eigenstates of the system, we see that if we can arrange for the trial wave function to be orthogonal to the first N states, we obtain a bound on λ_{N+1}. In practice we may only be able to arrange orthogonality to our best ground-state trial function, in which case the bound will not be rigorous (but see the next section).

The fact that we can obtain these bounds by assuming completeness suggests a close link between the variational approach and completeness. This we will formalise in the last section.

4.4.3 Use in Quantum Mechanics

Since the method is used so often in QM to find the ground state energy, we restate it as follows: the variational principle states that if we simply guess the wave function, the expectation value of the Hamiltonian in that wave function will be greater than the true ground-state energy E_0:

$$\frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0. \tag{4.36}$$

We note that

$$\langle \Psi | \hat{H} | \Psi \rangle = \frac{1}{2m} \langle \hat{\mathbf{p}} \Psi | \hat{\mathbf{p}} \Psi \rangle + \langle \Psi | \hat{V} | \Psi \rangle, \tag{4.37}$$

and also if we choose an already-normalised trial function Ψ we can ignore the denominator, $\langle\Psi|\Psi\rangle = 1$. Note too that we are not restricted to one-dimensional problems.

In principle we can also exploit the existence of bounds on higher eigenvalues, but usually this is not possible, because we don't know the states to which we need the trial function to be orthogonal. However an exception occurs where the states of the system can be separated into sets with different symmetry properties or other quantum numbers. Examples include parity and (in 3 dimensions) angular momentum. For example the lowest state with odd parity will automatically have zero overlap with the (even-parity) ground state, and so an upper bound can be found for it as well.

Further examples may be found in the MFQM notes.

4.5 Completeness of the eigenfunctions of a Sturm-Liouville problem

Not examinable!

We can use the variational principle to show that the eigenfunctions $\{\phi_n(x)\}$ of a Hermitian Sturm-Liouville problem are *complete*, in the following sense. For any continuous, piecewise-differentiable function $f(x)$ satisfying the same boundary conditions as the $\phi_n(x)$ (assumed to be real and normalised) we define $c_n = \int_a^b f(x)\phi_n(x)\rho(x)\mathrm{d}x$. If we consider the difference between $f(x)$ and the N-term finite sum

$$g_N(x) = f(x) - \sum_{n=1}^{N} c_n\phi_n(x), \tag{4.38}$$

we note that $g_N(x)$ is orthogonal to all $\phi_n(x)$ for $n \leq N$.

We define the mean-square deviation

$$\delta_N = \int |g_N(x)|^2 \rho(x)\mathrm{d}x \tag{4.39}$$

and we demonstrate completeness by showing that $\lim_{N\to\infty} \delta_N = 0$.

The crucial assumption is that the eigenvalues λ_n are all positive and increase without bound. The method is to consider $\lambda[g_N]$, which we know is not less than the eigenvalue λ_{N+1} since g_N is orthogonal to all eigenfunctions with lower eigenvalues. Explicit evaluation and rearrangement gives

$$\delta_N \leq \frac{\lambda[f] \int_a^b f^2(x)\rho(x)\mathrm{d}x}{\lambda_{N+1}}. \tag{4.40}$$

The numerator is fixed and depends only on f, not N. Since the eigenvalues increase without bound we see that the large-N limit of the deviation is zero, and we write

$$f(x) = \sum_{n=1}^{\infty} c_n\phi_n(x). \tag{4.41}$$

Some further details of the algebra are given here, adapted from Fetter & Walecka, *Theoretical Mechanics of Particles and Continua*.

A. Background

A.1 Linear and Hermitian Operators

It is assumed that the reader has a familiarity with the ideas of vector spaces, both finite and infinite dimensional. For the current course, we will almost exclusively be concerned with the fact that sets of functions obeying homogeneous boundary conditions on an interval form vector spaces, and we will not make a distinction between the vector $|f\rangle$ and its representation $f(x)$. In the context of MFQM many results pertaining to Hermitian operators in finite spaces were carried over without proof into infinite dimensional spaces; by the end of the current course the basis for these should be clearer.

Operators act on vectors to generate new vectors, which may or may not be in the original space. (For instance 2×3 matrices act on vectors in $\mathbb{C}^3$ to generate vectors in $\mathbb{C}^2$, and derivatives of functions such as $\sin(\pi x)$ which vanish at the boundaries of $[0, 1]$ will not generally satisfy the same boundary conditions.) *Linear operators* are those which act term-by-term on a sum of vectors, so that $\hat{Q}(a|f\rangle + b|g\rangle) = a\hat{Q}|f\rangle + b\hat{Q}|g\rangle$. In terms of functions, multiplication by another function, and differentiation, are both linear operators. Less obviously, if $K(x, y)$ is a function of two variables, the operation $\int_a^b K(x, y)f(y)\mathrm{d}y$ is also a linear operator on f. (The limits a and b can be constants or functions of x, but not of y).

The definition of a Hermitian operator in a vector space is one that, for any pair of vectors $|f\rangle$ and $|g\rangle$ in the space, $\langle g|\hat{H}|f\rangle = \langle f|\hat{H}|g\rangle^*$. It is clear that a 2×3 matrix cannot be Hermitian, because the existence of the LHS requires $|f\rangle \in \mathbb{C}^3$ and $|g\rangle \in \mathbb{C}^2$, but then the RHS does not exist. More generally, if we are to consider $\hat{H}$ to be Hermitian (or self-adjoint) when acting in some space, we require that $\hat{H}|f\rangle$ is another vector in the same space as $|f\rangle$. This turns out to be quite a strong condition. It means that, for instance, the momentum operator is not in fact Hermitian in the space of energy eigenstates of the infinite square well (as indeed we might have guessed from the fact that it has no eigenstates in that space) whereas it IS Hermitian in the closely related space of energy eigenstates for a particle moving freely on a circle which satisfy periodic boundary conditions.

In a finite dimensional space it is easy to show that for a Hermitian operator the eigenvalues are real and the eigenvectors are orthogonal. (To be precise, it is easy to show the latter if the eigenvectors are non-degenerate, but the proof can be extended to show that even for degenerate eigenvectors, a choice of orthogonal vectors may be made.) It is also easy to show that the number of eigenvectors is the same as the dimension of the space, and so the set of eigenvectors is complete, *i.e.* it forms a basis in the space. The first two points can be demonstrated equally easily for infinite-dimensional spaces, but completeness is a different matter. At this stage I will only point out that it could not be true if the domain were not restricted to vectors for which $\hat{H}|f\rangle$ is in the same space as $|f\rangle$, since $\hat{H}$ acting on any sum of its own eigenvectors by definition returns a new sum of the eigenvectors, which IS in the same space. So any $|g\rangle$ for which $\hat{H}|g\rangle$ was not in the space could not be so represented.

A.2 Integration and differentiation

If $F(x)$ is the integral of $f(x)$, then $f(x)$ is the derivative of $F(x)$. So much is learned at A-level, but experience shows that students are a little hesitant in actual applications. So let's be more specific. In particular we want to justify

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\int_0^x f(u)\mathrm{d}u\right) = f(x). \tag{A.1}$$

If we define $F_a(x) = \int_a^x f(u)\,\mathrm{d}u$, where a is an arbitrary real number (and u in an integration variable, we could use x'—but to use x would be misleading), then $F_a(b)$ is the net area between the curve $f(x)$ and the x-axis, with limits $x = a$ and $x = b$. The integral is additive: if $a < b < c$, $F_a(c) = F_a(b) + F_b(c)$. We assume $f(x)$ is smooth over some interval (no discontinuities or poles). Then for a and x in that interval,

$$\frac{\mathrm{d}F_a(x)}{\mathrm{d}x} = \lim_{\epsilon\to 0}\frac{F_a(x+\epsilon)-F_a(x)}{\epsilon} = \lim_{\epsilon\to 0}\frac{F_a(x)+F_x(x+\epsilon)-F_a(x)}{\epsilon}$$

$$= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_x^{x+\epsilon} f(u)\,\mathrm{d}u = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\,\epsilon f(x) = f(x). \tag{A.2}$$

In the last step, we have used that the fact that the area corresponding to the integral over a sufficiently short interval is well approximated by the product of the interval and the value of the function at any point in the interval.

This is very pedantic. A similar construction is used in the theory of complex variables where its consequences are more far-reaching (the path-independence of the integral of an analytic function). But it demonstrates what is necessary here, namely that *the lower limit of the integral doesn't matter*. We called our integrated function $F_a(x)$, but a is irrelevant. If we don't specify it, $F(x)$ is only defined up to an additive constant, but that constant vanishes when we differentiate to get the unique original function $f(x)$.

Note if x is the lower limit of the integration, the derivative is $-f(x)$.

We may also encounter cases where one or both limits is a function of x, for instance: $H(x) = \int_0^{g(x)} f(u)\,\mathrm{d}u$. What is the derivative w.r.t. x? This probably wasn't in A-level... Starting as before, we reach

$$\frac{\mathrm{d}H(x)}{\mathrm{d}x} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_{g(x)}^{g(x+\epsilon)} f(u)\,\mathrm{d}u$$

$$= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_{g(x)}^{g(x)+g'(x)\epsilon} f(u)\,\mathrm{d}u = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\,g'(x)\epsilon f\big(g(x)\big) = g'(x)f\big(g(x)\big).$$

But actually it's just a consequence of the chain rule. From the definition, $H(x) = F_0\big(g(x)\big)$, and so

$$\frac{\mathrm{d}H}{\mathrm{d}x} = \frac{\mathrm{d}F}{\mathrm{d}g}\frac{\mathrm{d}g}{\mathrm{d}x} = g'(x)f\big(g(x)\big). \tag{A.3}$$

And for completeness:

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_{p(x)}^{q(x)} f(u)\,\mathrm{d}u = q'(x)f\big(q(x)\big) - p'(x)f\big(p(x)\big). \tag{A.4}$$

A.3   First-order differential equations

Arfken 7.2
Riley 14.2

Most of the differential equations we will be concerned with for their own sake in this course are second-order differential equations. They arise naturally in dynamics and non-relativistic QM. But we will also encounter first-order differential equations, and this is a quick reminder of the main tools we use to solve them.

i) **Constant coefficients**
For linear equations of the kind

$$ay'(x) + by(x) = f(x) \tag{A.5}$$

where a and b are constants and $f(x)$ is simple, we can use the same method as for second-order equations of the same kind, writing y as a sum of the "complementary function" (a solution of the homogeneous equation, $f = 0$) and a "particular integral" (any, guessed, solution of the overall equation): $y = y_{\mathrm{CF}} + y_{\mathrm{PI}}$. Then

$$y_{\mathrm{CF}} = A\mathrm{e}^{mx} \quad \text{where } m = -b/a. \tag{A.6}$$

For $f(x)$ a polynomial, the appropriate trial particular integral is also a polynomial of the same order; for an exponential, the same exponential (with a coefficient to be fixed)—unless the exponent is $-b/a$, in which case multiply by x. For a sum of terms in f, a sum of particular integrals can be used. Note that the particular integral will have no undetermined coefficients unless a term proportional to y_{CF} has been included in error. The full solution will have A undetermined, till a single boundary condition is imposed on the full solution.

ii) **Integrating factor**
For linear equations of the kind

$$p(x)y'(x) + q(x)y(x) = f(x) \tag{A.7}$$

we want to find an integrating factor $w(x)$ such that $\big(w(x)p(x)\big)' = w(x)q(x)$, so that the equation can be written

$$\big(w(x)p(x)y(x)\big)' = w(x)f(x) \quad \Rightarrow \quad y(x) = \frac{\int^x w(x')f(x')\mathrm{d}x'}{w(x)p(x)}. \tag{A.8}$$

It can easily be checked that

$$w(x) = \frac{1}{p(x)} \exp\left(\int^x \frac{q(x')}{p(x')}\mathrm{d}x'\right) \tag{A.9}$$

does what is required.[1] We can ignore the constant of integration in w as it will cancel in the final solution. The indefinite integration in Eq. (A.8) introduces a constant of integration

---

[1] The derivation is simpler if we divide throughout by p; then we set $p = 1$. The expression can be derived, rather than simply verified, by applying the "variables separable" method to the differential equation for w. We will meet integrating factors again when we learn how to cast general linear second-order differential equations in so-called "Sturm-Liouville form", 1.2.3; the expression is identical except that the two functions are then the coefficient of y'' and y'.

which is the one undetermined constant in the final solution (to be fixed via the boundary conditions). Of course for this method to work, we need to be able to perform the two integrations. But in a wide variety of cases, we can.

Note that since Eq. (A.5) is a special case of Eq. (A.7) with $w = \mathrm{e}^{-bx/a}$, this provides us with an alternative method of solution which does not involve guessing the particular integral.

iii) **Variables separable**

Unlike the other two methods, this method can work for non-linear equations. If the method is applicable, it must be possible to rearrange the equation to read

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x)g(y) \qquad \Rightarrow \int \frac{\mathrm{d}y}{g(y)} = \int f(x)\mathrm{d}x. \tag{A.10}$$

Then provided the integrals can be done, the equation is solved.

A.4   Recap of common differential equations in Physics

By this stage of your course you have met a large number of differential equations and their solutions. The ones we refer to in this course are listed below. In this context we particularly stress the role and differences between parameters and eigenvalues, as discussed below.

Many of the equations below arise from PDEs after separation of variables. In particular what we are calling "the wave equation" (or Schrödinger equation) is actually the equation for the spatial part. The full solution takes the form $f(\mathbf{r})\,\mathrm{e}^{-i\omega t}$, where $f(\mathbf{r})$ satisfies

$$\nabla^2 f(\mathbf{r}) + k^2 f(\mathbf{r}) = 0, \tag{A.11}$$

and k^2 is related to ω by the dispersion relation. Working in spherical- (or plane-) polar coordinates, we use separable trial functions and use the method of separation of variables to obtain three (two) ordinary differential equations, one in each variable. This process introduces constant(s) of separation: typically each of these is fixed by the boundary conditions as an *eigenvalue* in one equation, and then functions as a *parameter* in the other equation(s). That parameter then determines the subclass (or *order*) of solutions possible. For example in 2D,

$$f(\mathbf{r}) = R(r)\,\mathrm{e}^{im\phi}; \tag{A.12}$$

in the ϕ-equation the eigenvalue m is constrained to be an integer by the "boundary condition" of single-valuedness, then $R(r) = J_m(kr)$ satisfies Bessel's equation of order m. In 3D we obtain

$$f(\mathbf{r}) = R(r)P_l^m(\cos\theta)\,\mathrm{e}^{im\phi} \propto R(r)Y_l^m(\theta,\phi) \tag{A.13}$$

where $P_l^m(z)$ satisfies the associated Legendre equation, in which m is a parameter but $l(l+1)$ an eigenvalue determined by the requirement of finite solutions. Then $R(r) = j_l(kr)$ satisfies an equation related to Bessel's equation of order $(l + \frac{1}{2})$. (In QM of course m and l are related to the angular momentum; in classical applications they are related to the multipole moments of the solution.)

Equations (Bessel's, associated Legendre's, associated Laguerre's) with different values of the parameter (*i.e.* different orders) are really different equations. For a given parameter value there is a set of eigenfunctions that have the properties we meet in section 1.2.2 including generalised orthogonality. But that doesn't tells us anything about eigenfunctions of different

orders. For instance any two spherical harmonics are orthogonal, but that might be due to the ϕ integration; in general the θ-dependent parts (associated Legendre polynomials) for different m are not orthogonal:

$$\int Y_l^m(\theta,\phi)^* Y_{l'}^{m'}(\theta,\phi)\mathrm{d}\Omega = \delta_{ll'}\delta_{mm'} \qquad \text{but} \quad \int_0^\pi P_l^m(\cos\theta)P_{l'}^{m'}(\cos\theta)\sin\theta\,\mathrm{d}\theta \not\propto \delta_{ll'} \quad \text{(A.14)}$$

unless $m = m'$.

Some of these equations, particularly those based on the Laplacian, are *scale invariant* so they have the same form under $x \to x_0 z$. Others, such Bessel's equation, are not scale invariant but have only a single scale k, so that if written in terms of $z = kx$ there are no dimensioned constants in the equation. (Both scaled and unscaled versions will be given below.) In these the scale k is usually treated as an eigenvalue that allows us to satisfy separated boundary condition, giving rise to discrete vibrational modes or energy levels.

For $k^2 = 0$ we just have the Laplace equation; the angular equations are exactly as above but the radial equations are simpler and have solutions which are just powers of r.

The wave equations all have versions with an eigenvalue of the opposite sign, $k^2 \to -\kappa^2$, as for instance arises in the diffusion equation. In 1D the solutions are decaying and growing exponentials. In 2D they are termed modified (spherical) Bessel functions $I_n(\kappa r)$ and $K_n(\kappa r)$ and also decay or grow exponentially at large values of r; there are spherical analogues with similar properties for the 3D problem.

Below, where the second solution is rarely encountered and has no standard name, it is simply represented by dots.

Laplace's equation in 1D; scale invariant;

$$y''(x) = 0 \qquad \Rightarrow \ y(x) = A + Bx. \tag{A.15}$$

Classical oscillator or wave equation in 1D; eigenvalue k^2 where k is the wave number or frequency

$$y''(z) + y(z) = 0 \qquad \Rightarrow \ y(z) = A\sin(z) + B\cos(z) \qquad \text{or}$$
$$f''(x) + k^2 f(x) = 0 \qquad \Rightarrow \ f(x) = A\sin(kx) + B\cos(kx). \tag{A.16}$$

Radial part of **Laplace's equation in 2D**; parameter n (or often m) a constant of separation; scale invariant:

$$r^2 R''(r) + r R'(r) - n^2 R(r) = 0 \qquad \Rightarrow \ R(r) = Ar^n + Br^{-n}. \tag{A.17}$$

(or $A + B\log r$ for $n = 0$)

Bessel's equation, radial part of **wave equation in 2D**; parameter n (or often m) a constant of separation, eigenvalue k^2 where k is the wave number; solutions regular and irregular Bessel functions:

$$z^2 y''(z) + z y'(z) + (z^2 - n^2)y(z) = 0 \qquad \Rightarrow \ y(z) = AJ_n(z) + BN_n(z) \qquad \text{or}$$
$$r^2 R''(r) + r R'(r) + (k^2 r^2 - n^2)R(r) = 0 \qquad \Rightarrow \ R(r) = AJ_n(kr) + BN_n(kr). \tag{A.18}$$

Radial part of **Laplace's equation in 3D**; l a constant of separation; scale invariant:

$$r^2 R''(r) + 2r R'(r) - l(l+1)R(r) = 0 \qquad \Rightarrow \ R(r) = Ar^l + Br^{-(l+1)}. \tag{A.19}$$

Radial part of **wave equation in 3D**; l a constant of separation; eigenvalue k^2; solutions regular and irregular spherical Bessel functions:

$$z^2 y''(z) + 2z y'(z) + (z^2 - l(l+1))y(z) = 0 \qquad \Rightarrow \ y(z) = Aj_l(z) + Bn_l(z) \qquad \text{or}$$
$$r^2 R''(r) + 2r R'(r) + (k^2 r^2 - l(l+1))R(r) = 0 \qquad \Rightarrow \ R(r) = Aj_l(kr) + Bn_l(kr). \tag{A.20}$$

Legendre equation, arises in spherical problems with axially symmetric solutions; eigenvalue $l(l+1)$, solutions Legendre polynomials and irregular solutions.

$$(1 - z^2)y'' - 2zy' + l(l+1)y = 0 \qquad \Rightarrow \ y(z) = AP_l(z) + BQ_l(z). \tag{A.21}$$

Associated Legendre equation; parameter m; eigenvalue $l(l+1)$:

$$(1 - z^2)y'' - 2zy' + \left(l(l+1) - \frac{m^2}{1 - z^2}\right)y = 0 \qquad \Rightarrow \ y(z) = AP_l^m(z) + \dots \tag{A.22}$$

Hermite's equation; eigenvalue n related to energy in quantum oscillator (quadratic potential); solutions Hermite polynomials; here the second solution is rarely encountered but is technically a confluent hypergeometric function of the first kind.

$$y''(z) - 2zy'(z) + 2ny(z) = 0 \qquad \Rightarrow \ y(z) = AH_n(z) + \dots \tag{A.23}$$

Laguerre equation; eigenvalue N: solutions Laguerre polynomials and irregular solutions

$$zy''(z) + (1 - z)y'(z) + Ny(z) = 0 \qquad \Rightarrow \ y(z) = AL_N(z) + \dots \tag{A.24}$$

Associated Laguerre equation, obtained after scaling and extracting the exponential decay from the radial wave equation for a Coulomb potential, parameter $\nu = 2l+1$ related to angular momentum, eigenvalue $N = n - l - 1$ related to energy.

$$zy''(z) + (\nu + 1 - z)y'(z) + Ny(z) = 0 \qquad \Rightarrow \ y(z) = AL_N^\nu(z) + \dots \tag{A.25}$$

A.5 Systems of algebraic equations

Arfken 2.1
Riley 8.9, 8.18

A.5.1 Determinants and zero-modes

The vanishing of the determinant of an $N \times N$ matrix means that its rows do not form a linearly independent set of N vectors in $\mathbb{C}^N$. Note that the size of the space that is spanned by the rows of $\mathbf{A}$ is called its *rank*. If there are n separate conditions of the form $\sum_{n=1}^{N} c_n a_{ni} = 0$, the rank of $\mathbf{A}$ is $N - n$. For instance if three rows are identical, or if two sets of two rows are identical, $n = 2$.

Since the determinant of a matrix is the product of its eigenvalues, such a matrix must have at least one zero eigenvalue.

An eigenvector $\mathbf{x}$ for which $\mathbf{Ax} = 0$ is sometimes called a *zero mode*. Generally, if the rank is $N - n$, then there will be n zero modes. A matrix of determinant zero is *projective*: whatever vector it acts on, the resulting vector will be in the $(N - n)$-dimensional subspace of non-zero modes. This is easily seen (at least in the common case of the eigenvectors forming a basis) by writing the vector $\mathbf{x}$ as a sum of the eigenvectors; then $\mathbf{Ax}$ will not contain any of the zero modes.

A.5.2 Uniqueness of solutions

A system of N linear equations in N unknowns $x_1, x_2 \ldots, x_N$, is of the form

$$a_{11}x_1 + a_{12}x_2 + \ldots + a_{1N}x_N = y_1$$
$$a_{21}x_1 + a_{22}x_2 + \ldots + a_{2N}x_N = y_2$$
$$\vdots$$
$$a_{N1}x_1 + a_{N2}x_2 + \ldots + a_{NN}x_N = y_N,$$

which can also be written in the form of a matrix equation $\mathbf{Ax} = \mathbf{y}$, may have a unique solution, no solution or infinitely-many solutions, depending on the properties of $\mathbf{A}$.

If $\det \mathbf{A} \neq 0$ then the inverse $\mathbf{A}^{-1}$ exists and the unique solution is $\mathbf{x} = \mathbf{A}^{-1}\mathbf{y}$. The non-vanishing of the determinant means that the rows of $\mathbf{A}$ are linearly independent. Hence each of the y_i can be specified independently and a solution will exist.

However if $\det \mathbf{A} = 0$, the system of equations, in spite of appearances, does not in fact give N conditions on N unknowns. (That would be most obvious if two of the equations have the same LHS, so that two of the rows of $\mathbf{A}$ were identical, but it is more general.) If the left-hand sides are not independent, however, there are two possibilities. One is that the y_i are compatible—for instance if the first two rows were identical, we would also have $y_1 = y_2$. Or more generally if $\sum_{n=1}^{N} c_n a_{ni} = 0$, then $\sum_{n=1}^{N} c_n y_n = 0$ also. Then the system is under-determined; we have at most $N - 1$ independent conditions for N unknowns. The solution is not unique: given one solution, we can add to it multiples of the zero modes and it will still satisfy the original equation.

The other possibility if $\det \mathbf{A} = 0$ is that the y_i are not compatible but contradictory. In this case there are no solutions.

If the y_i are compatible, the expansion of $\mathbf{y}$ in terms of the eigenvectors of $\mathbf{A}$ cannot contain any of the zero modes, since $\mathbf{A}\mathbf{x}$ cannot contain the zero modes for any $\mathbf{x}$. (If the eigenvectors of $\mathbf{A}$ are orthogonal this means $\mathbf{y}$ is orthogonal to the zero modes, and this is easy to test for.)

Consider the matrix

$$\mathbf{A} = \begin{pmatrix} 2 & -\sqrt{2} & \sqrt{2} \\ -2\sqrt{2} & 4 & 0 \\ 2\sqrt{2} & 0 & 4 \end{pmatrix} \tag{A.26}$$

whose eigenvalues are 0, 4 and 6. It is easy to check that row 3 minus row 2 equals $2\sqrt{2}$ times row 1, and hence the three rows—and three simultaneous equations with left hand sides $\mathbf{A}\mathbf{x}$—are not independent. Thus with a source term $\mathbf{y}$, unless $y_3 - y_2 - 2\sqrt{2}y_1 = 0$, there will be no solution. $\mathbf{y} = (1,1,1)^\top$ has no solution for instance. However $\mathbf{y} = (0,1,1)^\top$ and $\mathbf{y} = (\sqrt{2}, -1, 3)^\top$ do have solutions. These are not unique though, and if you try to solve the equations by hand—or with Mathematica—you will just find two of the x_i in terms of the third, eg for $\mathbf{y} = (0,1,1)^\top$, the solution can be written $x_2 = 1 + x_1/\sqrt{2}$, $x_3 = 1 - x_1/\sqrt{2}$, or

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} + c \begin{pmatrix} \sqrt{2} \\ 1 \\ -1 \end{pmatrix} \tag{A.27}$$

where c is an arbitrary constant. Note this form itself is not unique, since if we replace the arbitrary c by the equally arbitrary $d+1$ the first term would change to $(\sqrt{2}, 2, 0)^\top$.

It is easily checked that $(\sqrt{2}, 1, -1)^\top$ is the eigenvector of $\mathbf{A}$ with zero eigenvalue, *i.e.* the zero mode. It can also be shown that the other eigenvectors are $(0,1,1)^\top$ and $(1, -\sqrt{2}, \sqrt{2})^\top$, and so our chosen $\mathbf{y}$ (which is actually one of the eigenvectors) has no admixture of the zero mode in its eigenvector expansion. Nor has the other source for which we said solutions existed:

$$\begin{pmatrix} \sqrt{2} \\ -1 \\ 3 \end{pmatrix} = \sqrt{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ \sqrt{2} \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}. \tag{A.28}$$

But

$$\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 1 \\ -\sqrt{2} \\ \sqrt{2} \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} + \frac{\sqrt{2}}{3} \begin{pmatrix} \sqrt{2} \\ 1 \\ -1 \end{pmatrix} \tag{A.29}$$

which does involve the zero mode, and so for $\mathbf{y} = (1,1,1)^\top$ there are no solutions.

Note that we have chosen a non-symmetric $\mathbf{A}$ here. Its eigenvectors are not orthogonal, but they *are* linearly independent (as they must be since the eigenvalues are distinct). So any source $\mathbf{y}$ can be written as a sum of the eigenvectors, but we can't check for the presence or absence of the zero mode by taking the scalar product; it is non-zero in both the last two cases above.

For a system of three equations the discussion of zero modes is illuminating but not necessary for deciding whether there is a solution; brute force suffices. For anyone wondering what the systematic method is for cases like this where $\mathbf{A}$ is non-symmetric (but still with a complete set of eigenvectors), though, the answer is that $\mathbf{A}^\top$ has the same eigenvalues as $\mathbf{A}$, and any two eigenvectors of $\mathbf{A}^\top$ and $\mathbf{A}$ corresponding to different eigenvalues are orthogonal.[2] So for solutions to exist, $\mathbf{y}$ has to be orthogonal to the zero-mode of $\mathbf{A}^\top$, which is $(2\sqrt{2}, 1, -1)^\top$. That is, $2\sqrt{2}y_1 + y_2 - y_3 = 0$, exactly the condition we found at the start of this example.

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[2]The eigenvectors of $\mathbf{A}^\top$ are also known as the left-eigenvectors of $\mathbf{A}$ since they satisfy $\mathbf{y}^\top \mathbf{A} = \lambda \mathbf{y}^\top$.

A.6 Lagrange multipliers

Consider a hill with height $h(x, y)$ (atypically, here, we use y as an independent variable). To find the highest point, we want to simultaneously satisfy

$$\frac{\partial h}{\partial x} = 0 \qquad \text{and} \qquad \frac{\partial h}{\partial y} = 0 \tag{A.30}$$

(checking that it really is a maximum that we've found). But consider a different problem: on a particular path across the hill (which does not necessarily reach the summit) what is the highest point reached? The path may be specified as $y = g(x)$ or more symmetrically as $u(x, y) = 0$. This is *constrained maximisation*: we are constrained to stay on the path.
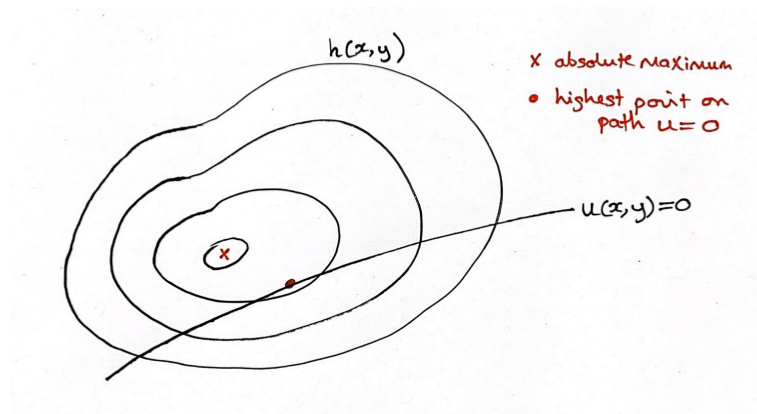
The trick is to extremize $h(x, y) + \lambda u(x, y)$ with respect to x and y; these two equations together with the constraint $u(x, y) = 0$ are enough to fix the three unknowns x_m, y_m and λ (though the value of the last is uninteresting and not usually found explicitly; this is also called the method of "undetermined multipliers".) So for example with a hemispherical hill $h = h_0(1 - x^2 - y^2)$ and a straight-line path $u(x, y) = y - mx - c = 0$ we have[3]

$$\frac{\partial(h + \lambda u)}{\partial x} = 0 \quad \Rightarrow -2h_0 x - \lambda m = 0 \quad \Rightarrow x = -\lambda m/2h_0$$

$$\frac{\partial(h + \lambda u)}{\partial y} = 0 \quad \Rightarrow -2h_0 y + \lambda = 0 \quad \Rightarrow y = \lambda/2h_0 = -x/m. \tag{A.31}$$

Combining the constraint $y - mx - c = 0$ with $y = -x/m$ gives $x = -c/(m^{-1} + m)$, so the maximum is reached at

$$(x_m, y_m) = \frac{c}{1 + m^2}(-m, 1), \qquad h_m = h_0 \frac{1 + m^2 - c^2}{1 + m^2}. \tag{A.32}$$

As promised we didn't find λ, though we could. In this case we could simply have substituted $y = mx + c$ into $h(x, y)$ and minimised with respect to x alone, which would have been easier (check!), but for a more complicated hill and/or path Lagrange's method is simpler.

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[3]Some presentations of this subject add the equation $\frac{\partial(h + \lambda u)}{\partial \lambda} = 0$ to the list, but from that we just recover the imposed constraint $u = 0$.

A.7 Contour Integration for real integrals

Arfken 11.7,11.8
Riley 24.13
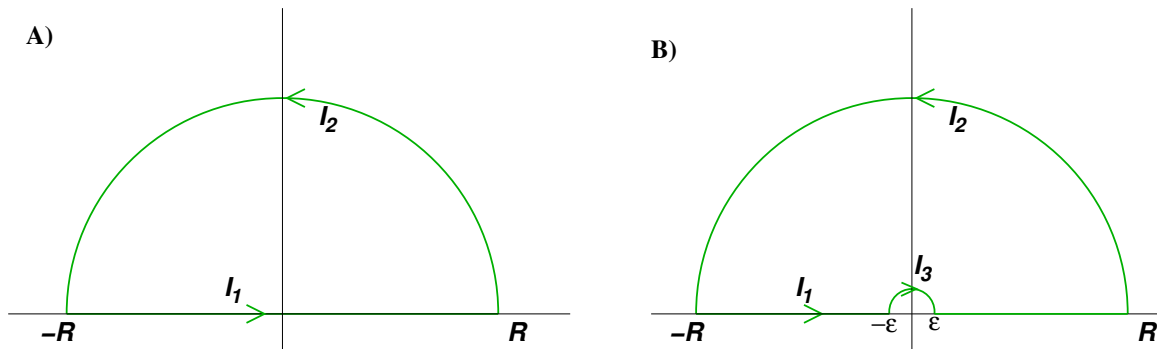
I shall assume that the following result is known: if $f(z)$ is a meromorphic function of the complex variable z, (that is it is analytic everywhere except at a finite number of points z_i which are poles of f), then

$$\oint_C f(z)\mathrm{d}z = 2\pi i \sum_i b_1^{(i)} \tag{A.33}$$

where $b_1^{(i)}$ is the residue at the ith pole, and the sum is over all the poles which lie within the contour C (which is traversed in an anticlockwise fashion; a clockwise contour would change the overall sign). This is called the residue theorem. The residue at z_i is defined as

$$b_1 = \lim_{z \to z_i} \frac{1}{(n-1)!} \frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}} \left((z - z_i)^n f(z) \right) \tag{A.34}$$

where n is equal to or greater than the order of the pole. However it is rarely necessary to use the formula; in particular if by inspection $f(z) = \frac{1}{z-a} \times g(z)$, and $g(z)$ is finite and analytic at $z = a$ (though it may contain factors such as $\frac{1}{z-b}$), then a is a simple pole of f with residue $g(a)$.

Now suppose we have a real integral of the form $I = \int_{-\infty}^{\infty} f(x)\mathrm{d}x$ to perform. If we consider a closed contour consisting of the real axis and a semicircle at infinity in the upper half plane (see (A) in the figure above), then the we can use the residue theorem to calculate $\oint_C f(z)\mathrm{d}z$. We can furthermore argue that this is the integral we want, I, plus the integral over the semicircle. IF we can show that the latter vanishes, then $2\pi i \times$ (the sum of residues in the upper half plane) will equal I.

There are two common cases where this is valid: one is if $\lim_{R\to\infty} Rf(Re^{i\theta}) = 0$. This is satisfied for example by $f(z) = \frac{1}{z^2+1}$, and in this case the only pole in the UHP is at $z = i$, with residue $1/2i$, hence $I = \pi$. (We can equally well close the contour in the LHP; in this case the pole is at $z = -i$ with residue $-1/2i$, but the clockwise contour contributes another minus sign so that the result is unchanged.)

The other is where the integrand can be written $f(x) = e^{ikx}g(x)$, and the less stringent condition $\lim_{R\to\infty} g(Re^{i\theta}) = 0$ holds. Then Jordan's Lemma says that if $k > 0$ the integral over the semicircle at infinity in the UHP will still vanish (crudely, since $z = x + iy$ and $y > 0$, $e^{ikz} = e^{ikx}e^{-ky}$ and the damped exponential improves the convergence). Conversely, if $k < 0$, the integral over the semicircle at infinity in the LHP will vanish. This allows the calculations of integrals such as $\int_{-\infty}^{\infty} \frac{e^{ikx}}{x-i}\mathrm{d}x$ which is $2\pi i e^{-k}$ for $k > 0$ and 0 for $k < 0$.

All of this assumes that the integrand does not have poles on the real axis. If it has a simple pole at x_0, the *principal value* prescription defines

$$\int_a^b f(x)\mathrm{d}x = \lim_{\epsilon \to 0} \left(\int_a^{x_0-\epsilon} f(x)\mathrm{d}x + \int_{x_0+\epsilon}^b f(x)\mathrm{d}x \right), \tag{A.35}$$

Effectively, we allow the diverging areas on either side the pole above and below the axis to cancel. We use this when we write $\int_a^b \frac{1}{x}\mathrm{d}x = \ln|b| - \ln|a|$ whether or not the interval $a \to b$ spans the origin. Then as well as the integral along (almost) the full real axis and the semicircle at infinity, we need to add a semicircle radius ϵ centred on x_0 to complete the contour (see (B) in the figure above, where $x_0 = 0$). Its contribution will not vanish, and so needs to be subtracted from the closed integral to leave the desired integral I. For a simple pole, the contribution of a semicircle in the UHP is just $-i\pi \times$(residue at the pole). As an example, taking $k > 0$,

$$\int_{-\infty}^\infty \frac{\mathrm{e}^{ikx}}{x}\mathrm{d}x = 0 - (-i\pi \mathrm{e}^0) = i\pi. \tag{A.36}$$

(Since the only pole is on the axis and hence not in the closed contour, the full integral vanishes.) If we take the imaginary parts of both sides we get $\int_{-\infty}^\infty k\mathrm{sinc}(kx)\mathrm{d}x = \pi$ for $k > 0$, a useful result. (If $k < 0$ we need to close in the lower half plane and the result above would be $-i\pi$, so the general expression is $\int_{-\infty}^\infty k\mathrm{sinc}(kx)\mathrm{d}x = \pi\mathrm{sign}(k)$, where $\mathrm{sign}(k) = k/|k|$.)

However it must be stressed that the extraction of the principal value is a choice, appropriate in cases like this for finding areas and real integrals, but less so in other cases.

A.8 Delta functions

Arfken 1.11
Riley 13.1.3

A δ-function (or more properly "distribution") is defined by the sifting property:

$$\int_a^b \delta(x - x_0)f(x)\mathrm{d}x = f(x_0) \qquad \text{if } a < x_0 < b, \text{ and zero otherwise.} \tag{A.37}$$

It follows that

$$\int_a^b \delta(x - x_0)f(x)\mathrm{d}x = \int_{x_0-\epsilon}^{x_0+\epsilon} \delta(x - x_0)f(x)\mathrm{d}x \qquad \text{if } a < x_0 < b, \tag{A.38}$$

i.e. that is there is only support for the integral in the immediate vicinity of x_0. Also,

$$\int_{-\infty}^x \delta(y - x_0)f(y)\mathrm{d}x = f(x_0)\Theta(x - x_0) \tag{A.39}$$

where the step function $\Theta(x)$ is 0 for $x < 0$ and 1 for $x > 0$. Though we think of a δ-function as an infinitely tall, infinitesimally narrow spike, it is usually defined as the limit as some parameter goes to infinity of a well-behaved function such as a normalised Gaussian, or top-hat or triangle function, or even $\frac{\kappa}{\pi}\mathrm{sinc}(\kappa x)$ or $\frac{\kappa}{\pi}\mathrm{sinc}^2(\kappa x)$. The sifting property can be demonstrated by doing the integral with the parameter finite and then letting it go to infinity.

One may meet the δ-function with a more complicated argument, such as $\delta(ax - b)$. We can see that the sifting property will pick out the value of $f(b/a)$, but what about the normalisation? In fact $\delta(ax - b) = \frac{1}{|a|}\delta(x - b/a)$, as shown here:

$$\int_{-\infty}^{\infty} \delta(ax - b)f(x)\mathrm{d}x = \int_{-\infty}^{\infty} \delta(y)f\left(\frac{y + b}{a}\right)\frac{1}{|a|}\mathrm{d}y = \frac{1}{|a|}f\left(\frac{b}{a}\right) = \int_{-\infty}^{\infty} \frac{1}{|a|}\delta(x - b/a)f(x)\mathrm{d}x$$

(A.40)

The $|a|$ arises as follows. If $a > 0$, then $x = \pm\infty \Rightarrow y = \pm\infty$ and the order of the limits is unchanged. $\frac{1}{a}$ and $\frac{1}{|a|}$ are the same thing. But if $a < 0$, then $x = \pm\infty \Rightarrow y = \mp\infty$ and the order of the limits is swapped. Then we pick up a minus sign as $\int_{\infty}^{-\infty} \to -\int_{-\infty}^{\infty}$. And in this case, $-\frac{1}{a} = \frac{1}{|a|}$. So writing $\frac{1}{|a|}$ covers both cases.

What about $\delta(g(x))$ where $g(x)$ is some more complicated function? There will be no contribution to the integral wherever $g(x)$ is non-zero, but there may be several points x_i at which $g(x_i) = 0$ and all can contribute to the integral. We will assume $g(x)$ has only simple zeros at real values $x_1, x_2 \ldots, x_n$. Sufficiently close to any one of them, we can write $g(x) \approx (x - x_i)g'(x_i)$. If we integrate over a region spanning only one zero, the integral is equivalent to

$$\int_a^b \delta\big(g(x)\big)f(x)\mathrm{d}x = \int_{x_i-\epsilon}^{x_i+\epsilon} \delta\big((x - x_i)g'(x_i)\big)f(x)\mathrm{d}x = \frac{1}{|g'(x_i)|}f(x_i).$$

For an integration interval that spans more than one zero of $g(x)$ we get more than one contribution, so

$$\delta\big(g(x)\big) = \sum_{i=1}^{n} \frac{1}{|g'(x_i)|}\delta(x - x_i) \qquad \text{where } x_i \text{ are the real simple roots of } g(x). \qquad (A.41)$$

Worked examples on δ-functions and Fourier transforms, including proof of some results quoted in this section and the next, can be found here.

A.9 Fourier Transforms

The Fourier transform of $f(x)$ is

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x)\,\mathrm{d}x. \qquad (A.42)$$

The inverse of the transformation is

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{ikx} F(k)\,\mathrm{d}k. \qquad (A.43)$$

The normalisation, and the sign of i in the exponential are conventions, and should always be checked when other texts are used. In fact in this course we will often use the alternative normalisation that drops the $1/\sqrt{2\pi}$ in the transform and uses $1/2\pi$ in the inverse transform, but here the symmetry is useful. In physics x usually represents space and k, wave number. Where the initial variable is time t, the conjugate variable is angular frequency ω, and the kernel $\mathrm{e}^{i\omega t}$ is often used.

With the normalisation above, Parceval's theorem says that

$$\int_{-\infty}^{\infty} f^*(x)g(x)\mathrm{d}x = \int_{-\infty}^{\infty} F^*(k)G(k)\mathrm{d}k \tag{A.44}$$

In other words the normalisation is preserved. With the alternative normalisation there would be a factor of $1/2\pi$ on the RHS.

The following results can be useful:

a) If $f(x)$ is symmetric (or antisymmetric), so is $F(k)$:
   i.e. if $f(x) = \pm f(-x)$ then $F(k) = \pm F(-k)$.

b) If $f(x)$ is real, $F^*(k) = F(-k)$.

c) If $f(x)$ is real and symmetric (antisymmetric), $F(k)$ is real and symmetric (imaginary and antisymmetric).

d) F.T. $[f(\kappa x)] = \dfrac{1}{|\kappa|} F\left(\dfrac{k}{\kappa}\right)$.

e) F.T. $[f(x + a)] = e^{ika} F(k)$.

f) F.T. $[e^{\alpha x} f(x)] = F(k + i\alpha)$ (for real or complex α.)

g) F.T. $[F(x)] = f(-k)$.

h) F.T. $[\delta(x - x_0)] = \dfrac{1}{\sqrt{2\pi}} e^{-ikx_0}$

i) F.T. $[e^{ik_0 x}] = \sqrt{2\pi}\delta(k - k_0)$

The results from (e) and (f) are called the shift theorems.

Below we show a table Fourier transforms; note that the results above allow us see in addition that the F.T. of a sinc function is a top-hat function. In the last three lines a is a real number.

$f(x)$	$F(k)$	
$\Theta(x)e^{-\alpha x}$, $\mathrm{Re}\,[\alpha] > 0$	$\dfrac{1}{\sqrt{2\pi}} \dfrac{1}{\alpha + ik}$	decaying exponential and Lorentzian
$\frac{1}{a}e^{-x^2/(2a^2)}$	$e^{-k^2 a^2/2}$	both Gaussians
$\frac{1}{a}\Theta(\frac{1}{2}a + x)\Theta(\frac{1}{2}a - x)$	$\dfrac{1}{\sqrt{2\pi}}\mathrm{sinc}(\frac{1}{2}ka)$	Top hat or slit function and sinc function
$\frac{1}{a^2}\Theta(a + x)\Theta(a - x)(a - |x|)$	$\dfrac{1}{\sqrt{2\pi}}\mathrm{sinc}^2(\frac{1}{2}ka)$	Triangle function and sinc-squared

Note that in addition that the F.T. of a sinc function is a top-hat function, and of a sinc-squared function is a triangle function.

All of these F.T.s can be shown with standard integration techniques, but with the exception of the Gaussian, contour integration in the complex k plane, invoking Jordan's lemma, is the easiest way to do the inverse transforms. Confusingly, in the I.F.T. x plays the role of the parameter that we called k in the section on Jordan's Lemma, so we need to close our contour

in the upper or lower half plane according to whether x is positive or negative. Hence the appearance of $\Theta(x)$ and similar terms.

In all of these functions, we can identify a width parameter for the original function (typically a) and see that the typical width of the transform is proportional to its inverse. In the last three lines the functions become $\delta(x)$ in the limit $a \to 0$ (or $\sqrt{2\pi}\delta(x)$ for the Gaussian) and the transforms become constants, in accord with result (h) above. Multiplying the sincs by $a/(2\pi)$ converts them into functions which become $\delta(k)$ as $a \to \infty$ as well.
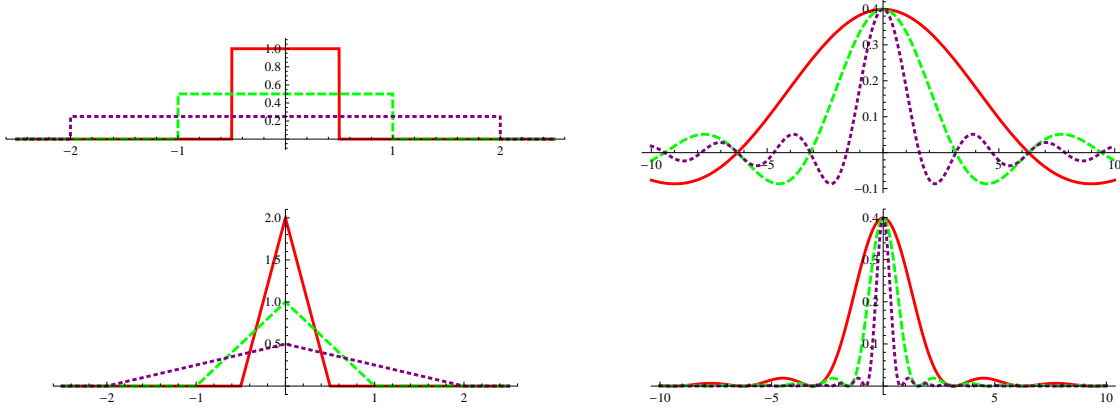
Above we plot the top hat and triangle functions and their Fourier transforms for three values of the width parameter. We see that the wider the original function, the narrower the F.T.

The convolution theorem for Fourier transforms is as follows. We define the convolution $h(x)$ of $f(x)$ and $g(x)$ as

$$h(x) = f(x) * g(x) \equiv \int_{-\infty}^{\infty} f(y) * g(x - y)\mathrm{d}y. \tag{A.45}$$

Then

$$H(k) = \sqrt{2\pi}F(k)G(k). \tag{A.46}$$

With the alternative normalisation, the $\sqrt{2\pi}$ is absent. It can be shown that the triangle function is the convolution of two top-hat functions of half the width. This leads to the bottom line of the table above.