Mathematical Methods I

Peter S. Riseborough

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1 Mathematics and Physics

Physics is a science which relates measurements and measurable quantities to a few fundamental laws or principles.

It is a quantitative science, and as such the relationships are mathematical. The laws or principles of physics must be able to be formulated as mathematical statements.

If physical laws are to be fundamental they must be few in number and must be able to be stated in ways which are independent of any arbitrary choices. In particular, a physical law must be able to be stated in a way which is independent of the choice of reference frame in which the measurements are made.

The laws or principles of physics are usually formulated as differential equations, as they relate changes. The laws must be invariant under the choice of coordinate system. Therefore, one needs to express the differentials in ways which are invariant under coordinate transformations, or at least have definite and easily calculable transformation properties.

It is useful to start by formulating the laws in fixed Cartesian coordinate systems, and then consider invariance under:-
(i) Translations
(ii) Rotations
(iii) Boosts to Inertial Reference Frames
(iv) Boosts to Accelerating Reference Frames

Quantities such as scalars and vectors have definite transformation properties under translations and rotations.

Scalars are invariant under rotations.

Vectors transform in the same way as a displacement under rotations.

2 Vector Analysis

2.1 Vectors

Consider the displacement vector, in a Cartesian coordinate system it can be expressed as

$$\overrightarrow{r} \ = \ \hat{e}_x \ x \ + \ \hat{e}_y \ y \ + \ \hat{e}_z \ z \tag{1}$$

where $\hat{e}_x$, $\hat{e}_y$ and $\hat{e}_z$, are three orthogonal unit vectors, with fixed directions. The components of the displacement are (x, y, z).

In a different coordinate system, one in which is (passively) rotated through an angle θ with respect to the original coordinate system, the displacement vector is unchanged. However, the components with respect to the new unit vectors $\hat{e}'_x$, $\hat{e}'_y$ and $\hat{e}'_z$, are different (x', y', z').

A specific example is given by the rotation about the z axis

$$\overrightarrow{r} \ = \ \hat{e}'_x \ x' \ + \ \hat{e}'_y \ y' \ + \ \hat{e}'_z \ z' \tag{2}$$

The new components are given in terms of the old components by

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{3}$$

Hence,

$$\overrightarrow{r} \ = \ \hat{e}'_x \ (\ x \ \cos\theta \ + \ y \ \sin\theta \ ) \ + \ \hat{e}'_y \ (\ y \ \cos\theta \ - \ x \ \sin\theta \ ) \ + \ \hat{e}'_z \ z' \tag{4}$$

The inverse transformation is given by the substitution $\theta \ \rightarrow \ - \ \theta$,

$$\overrightarrow{r} \ = \ \hat{e}_x \ (\ x' \ \cos\theta \ - \ y' \ \sin\theta \ ) \ + \ \hat{e}_y \ (\ y' \ \cos\theta \ + \ x' \ \sin\theta \ ) \ + \ \hat{e}_z \ z \tag{5}$$

Any arbitrary vector $\overrightarrow{A}$ can be expressed as

$$\overrightarrow{A} \ = \ \hat{e}_x \ A_x \ + \ \hat{e}_y \ A_y \ + \ \hat{e}_z \ A_z \tag{6}$$

where $\hat{e}_x$, $\hat{e}_y$ and $\hat{e}_z$, are three orthogonal unit vectors, with fixed directions. The components of the displacement are (A_x, A_y, A_z). The arbitrary vector transforms under rotations exactly the same way as the displacement

$$\overrightarrow{A} \ = \ \hat{e}'_x \ (\ A_x \ \cos\theta \ + \ A_y \ \sin\theta \ ) \ + \ \hat{e}'_y \ (\ A_y \ \cos\theta \ - \ A_x \ \sin\theta \ ) \ + \ \hat{e}'_z \ A'_z \tag{7}$$

2.2 Scalar Products

Under rotations the following quantities associated with vectors that are invariant include:-
(i) Lengths of vectors.
(ii) Angles between vectors.
These invariance properties can be formulated in terms of the invariance of a scalar product.

The scalar product of two vectors is defined as

$$\overrightarrow{A} \, . \, \overrightarrow{B} \; = \; A_x \; B_x \; + \; A_y \; B_y \; + \; A_z \; B_z \tag{8}$$

The scalar product transforms exactly the same way as a scalar under rotations, and is thus a scalar or invariant quantity.

$$\begin{aligned} \overrightarrow{A} \, . \, \overrightarrow{B} \; &= \; A_x \; B_x \; + \; A_y \; B_y \; + \; A_z \; B_z \\ &= \; A'_x \; B'_x \; + \; A'_y \; B'_y \; + \; A'_z \; B'_z \end{aligned} \tag{9}$$

2.3 The Gradient

The gradient represents the rate of change of a scalar quantity $\phi(\overrightarrow{r})$. The gradient is a vector quantity which shows the direction and the maximum rate of change of the scalar quantity. The gradient can be introduced through consideration of a Taylor expansion

$$\begin{aligned} \phi(\overrightarrow{r} + \overrightarrow{a}) \; &= \; \phi(\overrightarrow{r}) \; + \; a_x \, \frac{\partial \phi}{\partial x} \; + \; a_y \, \frac{\partial \phi}{\partial y} \; + \; a_z \, \frac{\partial \phi}{\partial z} \; + \; \ldots \\ &= \; \phi(\overrightarrow{r}) \; + \; \overrightarrow{a} \, . \, \overrightarrow{\nabla} \, \phi(\overrightarrow{r}) \; + \; \ldots \end{aligned} \tag{10}$$

This is written in the form of a scalar product of the vector displacement $\overrightarrow{a}$ given by

$$\overrightarrow{a} \; = \; \hat{e}_x \; a_x \; + \; \hat{e}_y \; a_y \; + \; \hat{e}_z \; a_z \tag{11}$$

and another quantity defined by

$$\overrightarrow{\nabla} \phi \; = \; \hat{e}_x \, \frac{\partial \phi}{\partial x} \; + \; \hat{e}_y \, \frac{\partial \phi}{\partial y} \; + \; \hat{e}_z \, \frac{\partial \phi}{\partial z} \tag{12}$$

The latter quantity is a vector quantity, as follows from the scalar quantities $\phi(\overrightarrow{r})$ and $\phi(\overrightarrow{r} + \overrightarrow{a})$ being invariant. Thus, the dot product in the Taylor expansion must behave like a scalar. This is the case if $\overrightarrow{\nabla} \phi$ is a vector, since the scalar product of the two vectors is a scalar.

The gradient operator is defined as

$$\overrightarrow{\nabla} \; = \; \hat{e}_x \, \frac{\partial}{\partial x} \; + \; \hat{e}_y \, \frac{\partial}{\partial y} \; + \; \hat{e}_z \, \frac{\partial}{\partial z} \tag{13}$$

The gradient operator is an abstraction, and only makes good sense when the operator acts on a differentiable function.

The gradient specifies the rate of change of a scalar field, and the direction of the gradient is in the direction of largest change.

An example of the gradient that occur in physical applications include, is the relationship between electric field and the scalar potential

$$\vec{E} \; = \; - \; \vec{\nabla} \; \phi \tag{14}$$

in electro-statics. This has the physical meaning that a particle will move (accelerate) from regions of high potential to low potential, always in the direction of the maximum decrease in potential.

For a point charge of magnitude q the potential is given by

$$\phi \; = \; \frac{q}{r} \tag{15}$$

and the electric field is given by

$$\vec{E} \; = \; + \; \frac{q \; \vec{r}}{r^3} \tag{16}$$

2.4 The Divergence

The gradient operator, since it looks like a vector, could possibly be used in a scalar product with a differentiable vector field. This can be used to define the divergence of the vector as the scalar product

$$\vec{\nabla} \; . \; \vec{A} \tag{17}$$

The divergence is a scalar.

In Cartesian coordinates, the divergence is evaluated from the scalar product as

$$\vec{\nabla} \; . \; \vec{A} \; = \; \frac{\partial A_x}{\partial x} \; + \; \frac{\partial A_y}{\partial y} \; + \; \frac{\partial A_z}{\partial z} \tag{18}$$

Consider a vector quantity $\vec{A}$ of the form

$$\vec{A} \; = \; \vec{r} \; f(r) \tag{19}$$

which is spherically symmetric and directed radially from the origin. The divergence of $\vec{A}$ is given by

$$\frac{\partial \, x \, f(r)}{\partial x} \; + \; \frac{\partial \, y \, f(r)}{\partial y} \; + \; \frac{\partial \, z \, f(r)}{\partial z} \; = \; 3 \, f(r) \; + \; \frac{x^2 \; + \; y^2 \; + \; z^2}{r} \, \frac{\partial f(r)}{\partial r}$$

$$= \; 3 \, f(r) \; + \; r \, \frac{\partial f(r)}{\partial r} \tag{20}$$

It is readily seen that the above quantity is invariant under rotations around the origin, as is expected if the divergence of a vector is a scalar.

Another example is given by the vector $\vec{t}$ in the $x - y$ plane which is perpendicular to the radial vector $\vec{\rho}$. The radial vector is given by

$$\vec{\rho} \; = \; \hat{e}_x \, x \; + \; \hat{e}_y \, y \tag{21}$$

then tangential vector is founds as

$$\vec{t} \; = \; - \, \hat{e}_x \, y \; + \; \hat{e}_y \, x \tag{22}$$

since it satisfies

$$\vec{t} \, . \, \vec{\rho} \; = \; 0 \tag{23}$$

Then, the divergence of the tangential vector field is zero

$$\vec{\nabla} \, . \, \vec{t} \; = \; 0 \tag{24}$$

In this example, the vector field $\vec{t}$ is flowing in closed circles, and the divergence is zero.

Given a differentiable vector field $\vec{A}$, which represents a flow of a quantity, then the divergence represents the net inflow of the quantity to a volume, and as such is a scalar.

A physical example of the divergence is provided by the continuity equation

$$\frac{\partial \rho}{\partial t} \; + \; \vec{\nabla} \, . \, \vec{j} \; = \; 0 \tag{25}$$

where ρ is the density and $\vec{j}$ is the current density. The continuity equation just states that the accumulation of matter in a volume (the increase in density) is equal to the matter that flows into the volume.

The presence of a non-zero divergence represents a source or sink for the flowing quantity. In electro-magnetics, electric charge acts as a source for the electric field

$$\vec{\nabla} \, . \, \vec{E} \; = \; 4 \, \pi \, \rho \tag{26}$$

For the example of a point charge at the origin

$$\overrightarrow{E} \; = \; \frac{q \; \overrightarrow{r}}{r^3} \tag{27}$$

For $r \; \neq \; 0$, the divergence is given by

$$\begin{aligned} \overrightarrow{\nabla} \; . \; \overrightarrow{E} \; &= \; q \; \left(\; \frac{\partial}{\partial x} \; \frac{x}{r^3} \; + \; \frac{\partial}{\partial y} \; \frac{y}{r^3} \; + \; \frac{\partial}{\partial z} \; \frac{z}{r^3} \; \right) \\ &= \; q \; \left(\; \frac{3}{r^3} \; - \; 3 \; \frac{x^2 \; + \; y^2 \; + \; z^2}{r^5} \; \right) \; = \; 0 \end{aligned} \tag{28}$$

and is not defined at $r \; = \; 0$. By consideration of Gauss's theorem, one can see that the divergence must diverge at $r \; = \; 0$. Thus, the electric field accumulates at the point charge.

There is no source for magnetic induction field, and this shows up in the Maxwell equation

$$\overrightarrow{\nabla} \; . \; \overrightarrow{B} \; = \; 0 \tag{29}$$

The finite magnetic induction field is purely a relativistic effect in that it represents the electric field produced by compensating charge densities which are in relative motion.

2.5 The Curl

Given a differentiable vector field, representing a flow, one can define a vector (pseudo-vector) quantity which represents the rotation of the flow. The curl is defined as the vector product

$$\overrightarrow{\nabla} \; \wedge \; \overrightarrow{A} \tag{30}$$

which is evaluated as

$$\left(\; \hat{e}_x \; \frac{\partial}{\partial x} \; + \; \hat{e}_x \; \frac{\partial}{\partial x} \; + \; \hat{e}_x \; \frac{\partial}{\partial x} \; \right) \; \wedge \; \left(\; \hat{e}_x \; A_x \; + \; \hat{e}_y \; A_y \; + \; \hat{e}_z \; A_z \; \right) \tag{31}$$

or

$$= \begin{vmatrix} \hat{e}_x & \hat{e}_y & \hat{e}_z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} = \hat{e}_x \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) - \hat{e}_y \left(\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} \right) + \hat{e}_z \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \tag{32}$$

The curl of a radial vector $\overrightarrow{A} \; = \; \overrightarrow{r} \; f(r)$ is evaluated as

$$\overrightarrow{\nabla} \; \wedge \; \overrightarrow{A} \; = \; \begin{vmatrix} \hat{e}_x & \hat{e}_y & \hat{e}_z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ x \; f(r) & y \; f(r) & z \; f(r) \end{vmatrix} \; = \; 0 \tag{33}$$

The curl of a tangential vector $\vec{t}$ given by

$$\vec{t} = (\hat{e}_x \, y - \hat{e}_y \, x) \tag{34}$$

is evaluated as

$$\vec{\nabla} \wedge \vec{t} = - 2 \, \hat{e}_z \tag{35}$$

The tangential vector represents a rotation about the z axis in a clockwise (negative) direction.

A physical example of the curl is given by the relationship between a magnetic induction $\vec{B}$ and the vector potential $\vec{A}$

$$\vec{B} = \vec{\nabla} \wedge \vec{A} \tag{36}$$

The vector potential

$$\vec{A} = \frac{B_z}{2} \left(x \, \hat{e}_y - y \, \hat{e}_x \right) \tag{37}$$

produces a magnetic field

$$\begin{aligned} \vec{B} &= \vec{\nabla} \wedge \frac{B_z}{2} \left(x \, \hat{e}_y - y \, \hat{e}_x \right) \\ &= \hat{e}_z \, B_z \end{aligned} \tag{38}$$

which is uniform and oriented along the z axis.

Another example is that of a magnetic induction field produced by a straight long current carrying wire. If the wire is oriented along the z axis, Ampere's law yields

$$\vec{B} = \frac{I}{2 \, \pi \, \rho^2} \left(x \, \hat{e}_y - y \, \hat{e}_x \right) \tag{39}$$

where

$$\rho^2 = x^2 + y^2 \tag{40}$$

The vector potentials $\vec{A}$ that produces this $\vec{B}$ can be fund a solution of

$$\vec{\nabla} \wedge \vec{A} = \vec{B} \tag{41}$$

The solutions are not unique, one solution is given by

$$\vec{A} = - \, \hat{e}_z \, \frac{I}{2 \, \pi} \, \ln \rho \tag{42}$$

2.6 Successive Applications of ∇

The gradient operator can be used successively to create higher order differentials. Frequently found higher derivatives include, the divergence of a gradient of a scalar ϕ

$$\vec{\nabla} \, . \, \vec{\nabla} \, \phi \; = \; \nabla^2 \, \phi \tag{43}$$

which defines the Laplacian of ϕ. In Cartesian coordinates one has

$$\vec{\nabla} \, . \, \vec{\nabla} \, \phi \; = \; \left(\frac{\partial^2}{\partial x^2} \; + \; \frac{\partial^2}{\partial y^2} \; + \; \frac{\partial^2}{\partial z^2} \right) \phi \tag{44}$$

The Laplacian appears in electrostatic problems. On putting combining the definition of a scalar potential ϕ in electro-statics

$$\vec{E} \; = \; - \, \vec{\nabla} \phi \tag{45}$$

and Gauss's law

$$\vec{\nabla} \, . \, \vec{E} \; = \; 4 \, \pi \, \rho \tag{46}$$

one obtains Laplace's equation

$$\nabla^2 \, \phi \; = \; - \, 4 \, \pi \, \rho \tag{47}$$

which relates the electrostatic potential to the charge density.

Another useful identity is obtained by taking the curl of a curl. It can be shown, using Cartesian coordinates, that the curl of the curl can be expressed as

$$\vec{\nabla} \, \wedge \, (\, \vec{\nabla} \, \wedge \, \vec{A} \,) \; = \; - \, \nabla^2 \, \vec{A} \; + \; \vec{\nabla} \, (\, \vec{\nabla} \, . \, \vec{A} \,) \tag{48}$$

This identity is independent of the choice of coordinate systems.

This identity is often used in electromagnetic theory by combining

$$\vec{B} \; = \; \vec{\nabla} \, \wedge \, \vec{A} \tag{49}$$

and the static form of Ampere's law

$$\vec{\nabla} \, \wedge \, \vec{B} \; = \; \frac{4 \, \pi}{c} \, \vec{j} \tag{50}$$

which yields the relation between the vector potential and the current density

$$- \, \nabla^2 \, \vec{A} \; + \; \vec{\nabla} \, (\, \vec{\nabla} \, . \, \vec{A} \,) \; = \; \frac{4 \, \pi}{c} \, \vec{j} \tag{51}$$

The above equation holds only when the fields are time independent.

Other useful identities include

$$\overrightarrow{\nabla} \wedge (\overrightarrow{\nabla} \phi) = 0 \tag{52}$$

and

$$\overrightarrow{\nabla} . (\overrightarrow{\nabla} \wedge \overrightarrow{A}) = 0 \tag{53}$$

2.7 Gauss's Theorem

Gauss's theorem relates the volume integral of a divergence of a vector to the surface integral of the vector. Since the volume integral of the divergence is a scalar, the surface integral of the vector must also be a scalar. The integration over the surface must be of the form of a scalar product of the vector and the normal to the surface area.

Consider the volume integral of $\overrightarrow{\nabla} . \overrightarrow{A}$

$$\int d^3\overrightarrow{r} (\overrightarrow{\nabla} . \overrightarrow{A}) \tag{54}$$

For simplicity, consider the integration volume as a cube with faces oriented parallel to the x, y and z axis. In this special case, Gauss's theorem can be easily proved by expressing the divergence in terms of the Cartesian components, and integrating the three separate terms. Since each term is of the form of a derivative with respect to a Cartesian coordinate, the corresponding integral can be evaluated in terms of the boundary term

$$\int_{x_-}^{x_+} dx \int_{y_-}^{y_+} dy \int_{z_-}^{z_+} dz \left(\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \right)$$
$$= \int_{y_-}^{y_+} dy \int_{z_-}^{z_+} dz \, A_x \Big|_{x_-}^{x_+} + \int_{x_-}^{x_+} dx \int_{z_-}^{z_+} dz \, A_y \Big|_{y_-}^{y_+} + \int_{x_-}^{x_+} dx \int_{y_-}^{y_+} dy \, A_z \Big|_{z_-}^{z_+} \tag{55}$$

The last six terms can be identified with the integrations over the six surfaces of the cube. It should be noted that the for a fixed direction of $\overrightarrow{A}$ the integration over the upper and lower surfaces have different signs. If the normal to the surface is always chosen to be directed outwards, this expression can be written as an integral over the surface of the cube

$$\int d^2\overrightarrow{S} . \overrightarrow{A} \tag{56}$$

Hence, we have proved Gauss's theorem for our special geometry

$$\int_V d^3\overrightarrow{r} (\overrightarrow{\nabla} . \overrightarrow{A}) = \int_S d^2\overrightarrow{S} . \overrightarrow{A} \tag{57}$$

where the surface $\vec{S}$ bounds the volume V.

The above argument can be extended to volumes of arbitrary shape, by considering the volume to be composed of an infinite number of infinitesimal cubes, and applying Gauss's theorem to each cube. The surfaces of the cubes internal to the volume occur in pairs. Since the surface integrals are oppositely directed, they cancel in pairs. This leaves only the integrals over the external surfaces of the cubes, which defines the integral over the surface of the arbitrary volume.

Example:

Gauss's theorem can be used to show that the divergence of the electric field caused by a point charge q is proportional to a Dirac delta function. Since, the electric field is given by

$$\vec{E} \; = \; \frac{q \; \vec{r}}{r^3} \tag{58}$$

and

$$\vec{\nabla} \; . \; \vec{E} \; = \; 0 \tag{59}$$

for $r \; \neq \; 0$. Then as Gauss's theorem yields

$$\begin{aligned} \int d^3\vec{r} \; \vec{\nabla} \; . \; \vec{E} \; &= \; \int d^2\vec{S} \; . \; \vec{E} \\ &= \; \int d^2\vec{S} \; . \; \frac{q \; \vec{r}}{r^3} \\ &= \; 4 \; \pi \; q \end{aligned} \tag{60}$$

it suggests that one must have

$$\vec{\nabla} \; . \; \vec{E} \; = \; 4 \; \pi \; q \; \delta^3(\vec{r}) \tag{61}$$

Thus, the divergence of the electric field is a point source represented by a Dirac delta function.

2.8 Stokes's Theorem

Stoke's theorem relates the surface integral of the curl of a vector to an integral of the vector around the perimeter of the surface.

Stokes's theorem can easily be proved by integration of the curl of the vector over a square, with normal along the z axis and sides parallel to the Cartesian axes

$$\int d^2\vec{S} \; . \; \left(\; \vec{\nabla} \; \wedge \; \vec{A} \; \right)$$

$$= \int_{x_-}^{x_+} dx \int_{y_-}^{y_+} dy \ \hat{e}_z \ . \ \hat{e}_z \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \tag{62}$$

The scalar product with the directed surface selects out the z component of the curl. One integral in each term can be evaluated, yielding

$$= \int_{y_-}^{y_+} dy \ A_y \Big|_{x_-}^{x_+} - \int_{x_-}^{x_+} dx \ A_x \Big|_{y_-}^{y_+} = \oint d\overrightarrow{r} \ . \ \overrightarrow{A} \tag{63}$$

which is of the form of an integration over the four sides of the square, in which the loop is traversed in a counterclockwise direction.

Stokes's theorem can be proved for a general surface, by subdividing it into a grid of infinitesimal squares. The integration over the interior perimeters cancel, the net result is an integration over the loop bounding the exterior perimeters.

A physical example of Stokes's theorem is found in quantum mechanics, for a charged particle in magnetic field. The wave function can be composed of a super-position of two components stemming from two paths. The two components have a phase difference which is proportional of the integral of the vector potential along the two paths :-

$$\int_{path_1} d\overrightarrow{r} \ . \ \overrightarrow{A} \tag{64}$$

and

$$\int_{path_2} d\overrightarrow{r} \ . \ \overrightarrow{A} \tag{65}$$

If these two paths are traversed consecutively, but the second path is traced in the reverse direction, then one has a loop. If the phase of the wave function at the origin is unique, up to multiples of 2 π, then the loop integral

$$\oint d\overrightarrow{r} \ . \ \overrightarrow{A} \tag{66}$$

must take on multiples of a fundamental value ϕ_0. Stokes's theorem leads to the discovery that magnetic flux must be quantized as

$$\begin{aligned} \oint d\overrightarrow{r} \ . \ \overrightarrow{A} &= n \ \phi_0 \\ \int d^2\overrightarrow{S} \ . \ \overrightarrow{B} &= n \ \phi_0 \end{aligned} \tag{67}$$

where n is an arbitrary integer and ϕ_0 is the fundamental flux quantum . This phenomenon, discovered by Dirac, is known as flux quantization.

2.9 Non-Orthogonal Coordinate Systems

One can introduce non-Cartesian coordinate systems. The most general coordinate systems do not use orthogonal unit vectors. As an example, consider a coordinate system for a plane based on two unit vectors (of fixed direction) $\hat{e}_1$ and $\hat{e}_2$. The position of a point on the plane can be labeled by the components x_1 and x_2 where

$$\vec{r} \; = \; \hat{e}_1 \, x_1 \; + \; \hat{e}_2 \, x_2 \tag{68}$$

The length l of the vector is given by

$$l^2 \; = \; x_1^2 \; + \; x_2^2 \; + \; 2 \, \hat{e}_1 \, . \, \hat{e}_2 \;\; x_1 \, x_2 \tag{69}$$

The expression for the length can be written as

$$l^2 \; = \; \sum_{i,j} \, g^{i,j} \; x_i \; x_j \tag{70}$$

where $g^{i,j}$ is known as the metric tensor and is given by

$$g^{i,j} \; = \; \hat{e}_i \, . \, \hat{e}_j \tag{71}$$

In this prescription we have given the components as the successive displacements needed to be traversed parallel to the unit vectors to arrive at the point. This is one way of specifying a vector. The components x_1 and x_2 are known as the co-variant components.

Another way of specifying the same vector is given by specifying the components x^1, x^2 as the displacements along the unit vectors, if the point is given by the intersection of the perpendiculars subtended from the axes. The components x^1 and x^2 are the contra-variant components.

What is the relationship between the co-variant and contra-variant components of the vector? Express the relationship and inverse relationship in terms of the components of the metric.

Solution:

Let θ be the angle between $\hat{e}_1$ and $\hat{e}_2$, such that

$$\hat{e}_1 \, . \, \hat{e}_2 \; = \; \cos\theta \tag{72}$$

Consider a vector of length l which is oriented at an angle ϕ relative to the unit vector $\hat{e}_1$.

The relationship between the Cartesian components of the vector and the covariant components is given by

$$\begin{aligned} l\ \cos\phi &= x_1 + x_2\ \cos\theta \\ l\ \sin\phi &= x_2\ \sin\theta \end{aligned} \tag{73}$$

The contra-variant components are given by

$$\begin{aligned} l\ \cos\phi &= x^1 \\ l\ \cos(\theta-\phi) &= x^2 \end{aligned} \tag{74}$$

Hence we find the relationship

$$\begin{aligned} x^1 &= x_1 + x_2\ \cos\theta \\ x^2 &= x_2 + x_1\ \cos\theta \end{aligned} \tag{75}$$

which can be summarized as

$$x^i = \sum_j g^{i,j}\ x_j \tag{76}$$

The inverse relation is given by

$$\begin{aligned} x_1 &= \frac{1}{\sin^2\theta}\ (\ x^1 - x^2\ \cos\theta\ ) \\ x_2 &= \frac{1}{\sin^2\theta}\ (\ x^2 - x^1\ \cos\theta\ ) \end{aligned} \tag{77}$$

which can be summarized as

$$x_i = \sum_j (g^{i,j})^{-1}\ x^j \tag{78}$$

How does the length get expressed in terms of the contra-variant components?

The length is given in terms of the contra-variant components by

$$l^2 = \sum_{i,j} (g^{i,j})^{-1}\ x^i\ x^j \tag{79}$$

It is customary to write the inverse of the metric as

$$(g^{i,j})^{-1} = g_{i,j} \tag{80}$$

so that the sub-scripts balance the superscripts when summed over.

2.9.1 Curvilinear Coordinate Systems

It is usual to identify generalized coordinates, such as (r, θ, φ), and then define the unit vectors corresponding to the direction of increasing generalized coordinates. That is $\hat{e}_r$ is the unit vector in the direction of increasing r, $\hat{e}_\theta$ as the unit vector in the direction of increasing θ and $\hat{e}_\varphi$ as the unit vector in the direction of increasing φ.

If we denote the generalized coordinates as q_i then an infinitesimal change in a Cartesian coordinate can be expressed as

$$dx_i = \sum_j \frac{\partial x_i}{\partial q_j} \, dq_j \tag{81}$$

The change in length dl can be expressed as

$$dl^2 = \sum_i dx_i^2 \tag{82}$$

which becomes

$$dl^2 = \sum_{j,j'} \left(\sum_i \frac{\partial x_i}{\partial q_j} \frac{\partial x_i}{\partial q_{j'}} \right) dq_j \, dq_{j'} \tag{83}$$

Thus the metric is found to be

$$g^{j,j'} = \left(\sum_i \frac{\partial x_i}{\partial q_j} \frac{\partial x_i}{\partial q_{j'}} \right) \tag{84}$$

The three unit vectors of the generalized coordinate system are proportional to

$$\hat{e}_{q_j} \propto \sum_i \hat{e}_i \frac{\partial x_i}{\partial q_j} \tag{85}$$

In general, the direction of the unit vectors depends on the values of the set of three generalized coordinates q_j's.

In orthogonal coordinate systems the coordinates are based on the existence of three orthogonal unit vectors. The unit vectors are orthogonal when the scalar products of the unit vectors vanish, which gives the conditions

$$\sum_i \frac{\partial x_i}{\partial q_j} \frac{\partial x_i}{\partial q_{j'}} = 0 \tag{86}$$

for $j \neq j'$. Thus, for orthogonal coordinate systems the metric is diagonal.

$$g^{j,j'} \propto \delta_{j,j'} \tag{87}$$

The metric is positive definite as the non-zero elements are given by

$$g^{j,j} \; = \; \sum_i \left(\frac{\partial x_i}{\partial q_j} \right)^2 \; > \; 0 \tag{88}$$

The inverse of the metric is also diagonal and has non-zero elements $\frac{1}{g^{i,i}}$. Thus, in this case, the co-variant and contra-variant components of a vector are simply related by

$$x^i \; = \; \frac{1}{g^{i,i}} \; x_i \tag{89}$$

An example of orthogonal curvilinear coordinates are given by spherical polar coordinates.

2.9.2 Spherical Polar Coordinates

In the spherical polar coordinates representation of an arbitrary vector is given by the generalized coordinates (r, θ, φ), such that

$$\overrightarrow{r} \; = \; \hat{e}_x \; r \; \sin\theta \; \cos\varphi \; + \; \hat{e}_y \; r \; \sin\theta \; \sin\varphi \; + \; \hat{e}_z \; r \; \cos\theta \tag{90}$$

The unit vectors are $(\hat{e}_r, \hat{e}_\theta, \hat{e}_\varphi)$ and are in the direction of increasing coordinate. Thus,

$$\begin{aligned} \hat{e}_r \; &= \; \frac{\partial \overrightarrow{r}}{\partial r} \\ &= \; \hat{e}_x \; \sin\theta \; \cos\varphi \; + \; \hat{e}_y \; \sin\theta \; \sin\varphi \; + \; \hat{e}_z \; \cos\theta \end{aligned} \tag{91}$$

and

$$\begin{aligned} \hat{e}_\theta \; &\propto \; \frac{\partial \overrightarrow{r}}{\partial \theta} \\ &= \; \hat{e}_x \; r \; \cos\theta \; \cos\varphi \; + \; \hat{e}_y \; r \; \cos\theta \; \sin\varphi \; - \; \hat{e}_z \; r \; \sin\theta \end{aligned} \tag{92}$$

The unit vector $\hat{e}_\theta$ is given by

$$\hat{e}_\theta \; = \; \hat{e}_x \; \cos\theta \; \cos\varphi \; + \; \hat{e}_y \; \cos\theta \; \sin\varphi \; - \; \hat{e}_z \; \sin\theta \tag{93}$$

Finally, we find the remaining unit vector from

$$\begin{aligned} \hat{e}_\varphi \; &\propto \; \frac{\partial \overrightarrow{r}}{\partial \varphi} \\ &= \; - \; \hat{e}_x \; r \; \sin\theta \; \sin\varphi \; + \; \hat{e}_y \; r \; \sin\theta \; \cos\varphi \end{aligned} \tag{94}$$

which is in the $x - y$ plane. The unit vector $\hat{e}_\varphi$ is given by normalizing the above vector, and is

$$\hat{e}_\varphi \; = \; - \; \hat{e}_x \; \sin\varphi \; + \; \hat{e}_y \; \cos\varphi \tag{95}$$

As can be seen by evaluation of the scalar product, these three unit vectors are mutually perpendicular. Furthermore, they form a coordinate systems in which

$$\hat{e}_r \wedge \hat{e}_\theta = \hat{e}_\varphi \tag{96}$$

Due to the orthogonality of the unit vectors, the metric is a diagonal matrix and has the non-zero matrix elements

$$\begin{aligned} g^{r,r} &= 1 \\ g^{\theta,\theta} &= r^2 \\ g^{\varphi,\varphi} &= r^2 \sin^2\theta \end{aligned} \tag{97}$$

In terms of the metric, the unit vectors are given by

$$\hat{e}_{q_j} = \frac{1}{\sqrt{g^{j,j}}} \frac{\partial \overrightarrow{r}}{\partial q_j} \tag{98}$$

2.9.3 The Gradient

In curvilinear coordinates the gradient of a scalar function ϕ is given by consideration of the infinitesimal increment caused by the change in the independent variables q_j

$$d\phi = \sum_j \left(\frac{\partial \phi}{\partial q_j} \right) dq_j \tag{99}$$

which for orthogonal coordinate systems can be written as

$$\begin{aligned} d\phi &= \sum_j \hat{e}_{q_j} \frac{1}{\sqrt{g^{j,j}}} \left(\frac{\partial \phi}{\partial q_j} \right) . \sum_{j'} \hat{e}_{q_{j'}} \sqrt{g^{j',j'}} \, dq_{j'} \\ &= \sum_j \hat{e}_{q_j} \frac{1}{\sqrt{g^{j,j'}}} \left(\frac{\partial \phi}{\partial q_j} \right) . \, d\overrightarrow{r} \end{aligned} \tag{100}$$

Thus, in the orthogonal coordinate systems the gradient is identified as

$$\overrightarrow{\nabla} \phi = \sum_j \hat{e}_{q_j} \frac{1}{\sqrt{g^{j,j}}} \left(\frac{\partial \phi}{\partial q_j} \right) \tag{101}$$

In spherical polar coordinates the gradient is given by

$$\overrightarrow{\nabla} \phi = \hat{e}_r \left(\frac{\partial \phi}{\partial r} \right) + \hat{e}_\theta \frac{1}{r} \left(\frac{\partial \phi}{\partial \theta} \right) + \hat{e}_\varphi \frac{1}{r \sin\theta} \left(\frac{\partial \phi}{\partial \varphi} \right) \tag{102}$$

2.9.4 The Divergence

Gauss's theorem can be used to define the divergence in a general orthogonal coordinate system. In particular, applying Gauss's theorem to an infinitesimal volume, one has

$$d^3\vec{r}\ \vec{\nabla}\ .\ \vec{A}\ =\ d^2\vec{S}\ .\ \vec{A} \tag{103}$$

where the elemental volume is given by

$$\begin{aligned} d^3\vec{r} &= \Pi_j\ dq_j\ \sqrt{g^{j,j}} \\ &= \sqrt{\text{Det}\ g^{j,j}}\ \Pi_j\ dq_j \end{aligned} \tag{104}$$

and the elemental surface areas are given by

$$\begin{aligned} d^2\vec{S}_i &= \Pi_{j\neq i}\ dq_j\ \sqrt{g^{j,j}} \\ &= \frac{1}{dq_i\ \sqrt{g^{i,i}}}\ \sqrt{\text{Det}\ g^{j,j}}\ \Pi_j\ dq_j \end{aligned} \tag{105}$$

Hence, from Gauss's theorem, one has the divergence given by the ratio of the sums over the scalar product of the vector with the directed surface areas divided by the volume element. Since the surfaces with normals $\hat{e}_{q_i}$ occur in pair and are oppositely directed, one finds the divergence as the derivative

$$\vec{\nabla}\ .\ \vec{A}\ =\ \frac{1}{\sqrt{\text{Det}g^{j,j}}}\ \sum_i\ \frac{\partial}{\partial q_i}\left(\frac{A_i}{\sqrt{g^{i,i}}}\ \sqrt{\text{Det}\ g^{j,j}}\right) \tag{106}$$

For spherical polar coordinates, the divergence is evaluated as

$$\begin{aligned} \vec{\nabla}\ .\ \vec{A} &= \frac{1}{r^2\ \sin\theta}\ \frac{\partial}{\partial r}\left(\ r^2\ \sin\theta\ A_r\ \right)\ +\ \frac{1}{r^2\ \sin\theta}\ \frac{\partial}{\partial\theta}\left(\ r\ \sin\theta\ A_\theta\ \right) \\ &+ \frac{1}{r^2\ \sin\theta}\ \frac{\partial}{\partial\varphi}\left(\ r\ A_\varphi\ \right) \end{aligned} \tag{107}$$

2.9.5 The Curl

In a generalized orthogonal coordinate system, Stokes's theorem can be used to define the curl. We shall apply Stokes's theorem to an infinitesimal loop integral

$$\int\ d^2\vec{S}\ .\ \left(\ \vec{\nabla}\ \wedge\ \vec{A}\ \right)\ =\ \oint\ d\vec{r}\ .\ \vec{A} \tag{108}$$

The components of the curl along the unit directions $\hat{e}_{q_j}$ can be evaluated over the surface areas $d^2\vec{S}$ with normals $\hat{e}_{q_j}$. Then we have

$$\int\ d^2\vec{S}_j\ .\ \left(\ \vec{\nabla}\ \wedge\ \vec{A}\ \right)\ =\ \left(\ \vec{\nabla}\ \wedge\ \vec{A}\ \right)_j\ \frac{\sqrt{\text{Det}g^{i,i}}}{\sqrt{g^{j,j}}}\ \Pi_{i\neq j}\ dq_i \tag{109}$$

For the surface with normal in direction 1, this is given by

$$\int d^2 \overrightarrow{S}_1 \, . \, \left(\overrightarrow{\nabla} \, \wedge \, \overrightarrow{A} \right) \; = \; \left(\overrightarrow{\nabla} \, \wedge \, \overrightarrow{A} \right)_1 \sqrt{g^{2,2}} \, \sqrt{g^{3,3}} \, dq_2 \, dq_3 \tag{110}$$

The loop integral over the perimeter of this surface becomes

$$\begin{aligned} \oint d\overrightarrow{r} \, . \, \overrightarrow{A} \; &= \; A_2 \, \sqrt{g^{2,2}} \, dq_2 \; + \; \left(A_3 \, \sqrt{g^{3,3}} \; + \; dq_2 \, \frac{\partial}{\partial q_2} \, A_3 \, \sqrt{g^{3,3}} \right) dq_3 \\ &- \; \left(A_2 \, \sqrt{g^{2,2}} \; + \; dq_3 \, \frac{\partial}{\partial q_3} \, A_2 \, \sqrt{g^{2,2}} \right) dq_2 \; - \; A_3 \, \sqrt{g^{3,3}} \, dq_3 \end{aligned} \tag{111}$$

where we have Taylor expanded the vector field about the center of the infinitesimal surface. The lowest order terms in the expansion stemming from the opposite sides of the perimeter cancel. Hence, the component of the curl along the normal to the infinitesimal surface is given by the expression

$$\left(\overrightarrow{\nabla} \, \wedge \, \overrightarrow{A} \right)_1 \; = \; \frac{1}{\sqrt{g^{2,2} g^{3,3}}} \left[\frac{\partial}{\partial q_2} \, \sqrt{g^{3,3}} \, A_3 \; - \; \frac{\partial}{\partial q_3} \, \sqrt{g^{2,2}} \, A_2 \right] \tag{112}$$

The expression for the entire curl vector can be expressed as a determinant

$$\left(\overrightarrow{\nabla} \, \wedge \, \overrightarrow{A} \right) \; = \; \frac{1}{\sqrt{\mathrm{Det} g^{j,j}}} \begin{vmatrix} \hat{e}_1 \, \sqrt{g^{1,1}} & \hat{e}_2 \, \sqrt{g^{2,2}} & \hat{e}_3 \, \sqrt{g^{3,3}} \\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\ \sqrt{g^{1,1}} \, A_1 & \sqrt{g^{2,2}} \, A_2 & \sqrt{g^{3,3}} \, A_3 \end{vmatrix} \tag{113}$$

In spherical polar coordinates, the curl is given by

$$\left(\overrightarrow{\nabla} \, \wedge \, \overrightarrow{A} \right) \; = \; \frac{1}{r^2 \, \sin\theta} \begin{vmatrix} \hat{e}_r & r \, \hat{e}_\theta & r \, \sin\theta \, \hat{e}_\varphi \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \theta} & \frac{\partial}{\partial \varphi} \\ A_r & r \, A_\theta & r \, \sin\theta \, A_\varphi \end{vmatrix} \tag{114}$$

Find an explicit expression for the angular momentum operator

$$\hat{\overrightarrow{L}} \; = \; - \, i \, \overrightarrow{r} \, \wedge \, \overrightarrow{\nabla} \tag{115}$$

in spherical polar coordinates.

2.9.6 Compounding Vector Differential Operators in Curvilinear Coordinates

When compounding differential operators, it is essential to note that operators should be considered to act on an arbitrary differentiable function. Thus, since

$$\frac{\partial}{\partial x} \, x \, f(x) \; = \; x \, \frac{\partial}{\partial x} \, f(x) \; + \; f(x) \tag{116}$$

one can compound $\frac{\partial}{\partial x}$ and x via

$$\frac{\partial}{\partial x} \, x \; = \; x \, \frac{\partial}{\partial x} \; + \; 1 \tag{117}$$

The order of the operators is important. The differential operator acts on everything in front of it, which includes the unit vectors. In Cartesian coordinates, the directions of the unit vectors are fixed thus,

$$\frac{\partial}{\partial x} \, \hat{e}_x \; = \; \frac{\partial}{\partial y} \, \hat{e}_x \; = \; \frac{\partial}{\partial z} \, \hat{e}_x \; = \; 0 \tag{118}$$

etc. For curvilinear coordinates this is no longer true. For example, in spherical polar coordinates although the directions of the unit vectors are not determined by the radial distance

$$\frac{\partial}{\partial r} \, \hat{e}_r \; = \; \frac{\partial}{\partial r} \, \hat{e}_\theta \; = \; \frac{\partial}{\partial r} \, \hat{e}_\varphi \; = \; 0 \tag{119}$$

the other derivatives of the unit vectors are not zero, as

$$\begin{aligned} \frac{\partial}{\partial \theta} \, \hat{e}_r \; &= \; \hat{e}_\theta \\ \frac{\partial}{\partial \theta} \, \hat{e}_\theta \; &= \; - \, \hat{e}_r \\ \frac{\partial}{\partial \theta} \, \hat{e}_\varphi \; &= \; 0 \end{aligned} \tag{120}$$

and

$$\begin{aligned} \frac{\partial}{\partial \varphi} \, \hat{e}_r \; &= \; \sin\theta \, \hat{e}_\varphi \\ \frac{\partial}{\partial \varphi} \, \hat{e}_\theta \; &= \; \cos\theta \, \hat{e}_\varphi \\ \frac{\partial}{\partial \varphi} \, \hat{e}_\varphi \; &= \; - \left(\, \sin\theta \, \hat{e}_r \; + \; \cos\theta \, \hat{e}_\theta \, \right) \end{aligned} \tag{121}$$

Find an explicit expression for the square of the angular momentum operator $\hat{\overrightarrow{L}}^2$ where

$$\hat{\overrightarrow{L}} \; = \; - \, i \, \overrightarrow{r} \; \wedge \; \overrightarrow{\nabla} \tag{122}$$

in spherical polar coordinates.

The Laplacian of a scalar ϕ can be evaluated by computing the divergence of the gradient of ϕ, i.e.,

$$\vec{\nabla} \,.\, \left(\vec{\nabla} \, \phi \right) \tag{123}$$

Here it is important to note that the differential operator acts on the unit vectors, before the scalar product is evaluated.

How is the Laplacian of a scalar $\nabla^2\phi$ related to $\vec{\hat{L}}^2 \phi$?

3 Partial Differential Equations

The dynamics of systems are usually described by one or more partial differential equations. A partial differential equation is characterized by being an equation for an unknown function of more than one independent variable, which expresses a relationship between the partial derivatives of the function with respect to the various independent variables. Conceptually, a solution may be envisaged as being obtained by direct integration. Since integration occurs between two limits, the solution of a partial differential equation is not unique unless its value is given at one of the limits. That is, the solution is not unique unless the constants of integration are specified. These are usually specified as boundary conditions or initial conditions.

Important examples are provided by the non-relativistic Schrödinger equation

$$- \frac{\hbar^2}{2\, m} \nabla^2 \psi + V(\underline{r}) \psi = i \hbar \frac{\partial \psi}{\partial t} \tag{124}$$

in which the wave function $\psi(\underline{r}, t)$ is usually a complex function of position and time. The one particle wave function has the interpretation that $| \psi(\underline{r}, t) |^2$ is the probability density for finding a particle at position $\underline{r}$ at time t. In order that $\psi(\underline{r}, t)$ be uniquely specified, it is necessary to specify boundary conditions. These may take the form of specifying $\psi(\underline{r}, t)$ or its derivative with respect to $\underline{r}$ on the boundary of the three dimensional region of interest. Furthermore, since this partial differential equation contains the first derivative with respect to time, it is necessary to specify one boundary condition at a temporal boundary, such as the initial time t_0. That is the entire wave function must be specified as an initial condition, $\psi(\underline{r}, t_0)$.

Another important example is given by the wave equation

$$\nabla^2 \phi - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = f(\underline{r}, t) \tag{125}$$

where $\phi(\underline{r}, t)$ describes the wave motion, c is the phase velocity of the wave and the force density $f(\underline{r}, t)$ acts as a source for the waves, inside the region of interest. Again appropriate boundary conditions for four dimensional space time $(\underline{r}, t)$ need to be specified, for the solution to be unique. Since this equation is a second order equation with respect to time, it is necessary to specify ϕ at two times. Alternatively, one may specify $\phi(\underline{r}, t_0)$ at the initial time and its derivative $\frac{\partial \phi(\underline{r}, t)}{\partial t}|_{t_0}$ at the initial time.

Poisson's equation is the partial differential equation

$$\nabla^2 \phi = - 4 \pi \rho \tag{126}$$

which specifies the scalar or electrostatic potential $\phi(\underline{r})$ produced by a charge density $\rho(\underline{r})$. The boundaries of the spatial region in which ϕ is to be determined, may also involve charge densities on the boundary surfaces or they may be surfaces over which ϕ is specified. The charge density is to be regarded as a source for the electric potential ϕ.

Maxwell's theory of electromagnetism is based on a set of equation of the form

$$
\begin{aligned}
\underline{\nabla} \, . \, \underline{E} &= 4 \, \pi \, \rho \\
\underline{\nabla} \, . \, \underline{B} &= 0 \\
\underline{\nabla} \, \wedge \, \underline{B} &= \frac{4 \, \pi}{c} \, \underline{j} \, + \, \frac{1}{c} \, \frac{\partial \underline{E}}{\partial t} \\
\underline{\nabla} \, \wedge \, \underline{E} &= - \, \frac{1}{c} \, \frac{\partial \underline{B}}{\partial t}
\end{aligned}
\tag{127}
$$

for the two vector quantities $\underline{E}$ and $\underline{B}$, where ρ and $\underline{j}$ are source terms, respectively representing the charge and current densities. These can be considered as forming a set of eight equations for the six components of $\underline{E}$ and $\underline{B}$. In general specifying more equations than components may lead to inconsistencies, however, in this case two equations can be thought of specifying consistency conditions on the initial data, such as the continuity of charge or the absence of magnetic monopoles. Since these equations are first order in time, it is only necessary to specify one initial condition on each of the $\underline{E}$ and $\underline{B}$ fields. This is in contrast to the wave equation, which is obtained by combining the equations for $\underline{E}$ and $\underline{B}$, which is a second order partial differential equation. The two initial conditions required to solve the wave equation correspond to specifying $\underline{E}$ and the derivative of $\underline{E}$ with respect to t, the last condition is equivalent to specifying $\underline{B}$ in Maxwell's equations.

All of the above equations posses the special property that they are linear partial differential equations. Furthermore, they are all second order linear partial differential equations since, the highest order derivative that enters is the second order derivative.

Consider the homogeneous equation which is obtained by setting the source terms to zero. In the absence of the source terms, each term in these equations only involve the first power of the unknown function or the first power of a (first or higher order) partial derivative of the function. The solution of the partial differential equation is not unique, unless the boundary conditions are specified. That is, one may find more than one (linearly independent) solution for the unknown function, such as ϕ_i for $i \; = \; 1 \; , \; 2 \; , \; \ldots \; , \; N$. Due to the linearity, the general solution of the homogeneous equation ϕ can be expressed as a linear combination

$$\phi \;=\; \sum_{i=1}^{N} \, C_i \, \phi_i \tag{128}$$

where the C_i are arbitrary (complex) numbers. The constant C_i may be determined if appropriate boundary conditions and initial conditions are specified. This is often referred to as the principle of linear superposition.

Now consider the inhomogeneous equation, that is the equation in which the source terms are present. If a particular solution of the inhomogeneous equation is found as ϕ_p, then it can be seen that due to the linearity it is possible to find a general solution as the sum of the particular solution and the solutions of the homogeneous equation

$$\phi \;=\; \phi_p \;+\; \sum_{i=1}^{N} \, C_i \, \phi_i \tag{129}$$

The solution may be uniquely determined if appropriate boundary and initial conditions are specified.

Non-Linear Partial Differential Equations.

By contrast, a non-linear partial differential equation involves powers of different orders in the unknown function and its derivatives. Examples are given by the sine-Gordon equation

$$\nabla^2 \, \phi \;-\; \frac{1}{c^2} \, \frac{\partial^2 \phi}{\partial t^2} \;-\; m^2 \, \sin \phi \;=\; 0 \tag{130}$$

which is a second order non-linear partial differential equation or the Korteweg-de Vries equation

$$\frac{\partial \phi}{\partial t} \;+\; \phi \, \frac{\partial \phi}{\partial x} \;+\; \frac{\partial^3 \phi}{\partial x^3} \;=\; 0 \tag{131}$$

which describes shallow water waves in a one dimensional channel. The Kortweg-de Vries equation is a third order non-linear partial differential equation as the highest order derivative that it contains is third order. In these non-linear equations, the principle of linear superposition does not hold. One can not express the general solution of the equation as a linear sum of individual solutions ϕ_i. Both these non-linear equations are special as they have travelling wave like solutions which propagate without dispersion. These special solutions are known as soliton solutions.

For the Korteweg-de Vries equation one can look for soliton solutions which propagate with velocity c,

$$\phi(x,t) \;=\; \phi(x \;-\; c \; t) \tag{132}$$

so that one has

$$(\phi - c) \frac{\partial \phi}{\partial x} + \frac{\partial^3 \phi}{\partial x^3} = 0 \tag{133}$$

which can be integrated to yield

$$\frac{\phi^2}{2} - c \, \phi + \frac{\partial^2 \phi}{\partial x^2} = \kappa \tag{134}$$

The constant of integration κ is chosen to be zero, by specifying that the $\phi \to 0$ when $| x - c t | \to \infty$. On identifying an integrating factor of

$$\frac{\partial \phi}{\partial x} \tag{135}$$

and multiplying the differential equation, by the integrating factor one obtains

$$\frac{\partial \phi}{\partial x} \frac{\phi^2}{2} - c \frac{\partial \phi}{\partial x} \phi + \frac{\partial \phi}{\partial x} \frac{\partial^2 \phi}{\partial x^2} = 0 \tag{136}$$

This can be integrated again to yield

$$\frac{\phi^3}{6} - c \frac{\phi^2}{2} + \frac{1}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 = \gamma \tag{137}$$

The boundary conditions can be used again to find $\gamma = 0$. The square root of the equation can be taken, giving the solution as an integral with $z = \frac{\phi}{3 \, c}$

$$\int^{\frac{\phi(x,t)}{3 \, c}} \frac{dz}{z \sqrt{1 - z}} = \sqrt{c} \int^{x-ct} dx' \tag{138}$$

The integral can be evaluated, using the substitution

$$z = \text{sech}^2 \, x \tag{139}$$

and

$$dz = - 2 \, \text{sech}^2 \, x \, \tanh \, x \, dx \tag{140}$$

giving

$$\phi(x,t) = \frac{3 \, c}{\cosh^2 \left(\sqrt{c} \, \frac{x - c \, t}{2} \right)} \tag{141}$$

This non-linear solution has a finite spatial extent and propagates with velocity c, and does not disperse or spread out.

The stability of shape of the soliton solution is to be contrasted with the behavior found from either linear equations with non-trivial dispersion relations or with the non-linear first order differential equation

$$\frac{\partial \phi}{\partial t} = - \phi \frac{\partial \phi}{\partial x} \tag{142}$$

which has the solution

$$\phi \;=\; f(\, x \;-\; \phi \, t \,) \tag{143}$$

where $f(x)$ is the (arbitrary) initial condition. This can be solved graphically. As the point with largest ϕ moves most rapidly, the wave must change its shape. It leads to a breaker wave and may give rise to singularities in the solution after a finite time has elapsed. That is, the solution may cease to be single valued after the elapse of a specific time.

3.1 Linear First Order Partial Differential Equations

Consider the homogeneous linear first order partial differential equation

$$\frac{\partial \phi}{\partial x} \;+\; a(x,t)\,\frac{\partial \phi}{\partial t} \;=\; 0 \tag{144}$$

with initial conditions $\phi(x,0) \;=\; f(x)$. This is known as a Cauchy problem.

We shall solve the Cauchy problem with the method of characteristics. The characteristics are defined to be curves in the (x,t) plane, $x(t)$, which satisfy the equation

$$\frac{dx(t)}{dt} \;=\; a(x(t),t) \tag{145}$$

The solution of this equation defines a family or a set of curves $x(t)$. The different curves correspond to the different constants of integration, or initial conditions $x(0) \;=\; x_0$.

The solution $\phi(x,t)$ when evaluated on a characteristic yield $\phi(x(t),t)$, and has the special property that it has a constant value along the curve $x(t)$. This can be shown by taking the derivative along the characteristic curve

$$\frac{d}{dt}\,\phi(x(t),t) \;=\; \frac{dx(t)}{dt}\,\frac{\partial \phi(x,t)}{\partial x} \;+\; \frac{\partial \phi(x,t)}{\partial t} \tag{146}$$

and as the characteristic satisfies

$$\frac{dx(t)}{dt} \;=\; a(x(t),t) \tag{147}$$

one has

$$\frac{d}{dt}\,\phi(x(t),t) \;=\; a(x,t)\,\frac{\partial \phi(x,t)}{\partial x} \;+\; \frac{\partial \phi(x,t)}{\partial t} \;=\; 0 \tag{148}$$

as $\phi(x,t)$ satisfies the homogeneous linear partial differential equation. Thus, $\phi(x,t)$ is constant along a characteristic. Hence,

$$\begin{aligned} \phi(x(t),t) \;&=\; \phi(x_0,0) \\ &=\; f(x_0) \end{aligned} \tag{149}$$

This means that if we can determine the characteristic one can compute the solution of the Cauchy problem.

Example:

Consider the Cauchy problem

$$\frac{\partial \phi}{\partial t} \; + \; c \, \frac{\partial \phi}{\partial x} \; = \; 0 \tag{150}$$

with initial conditions

$$\phi(x,0) \; = \; f(x) \tag{151}$$

The characteristic is determined from the ordinary differential equation (it has only one variable)

$$\frac{dx}{dt} \; = \; c \tag{152}$$

which has solutions

$$x(t) \; = \; c \, t \; + \; x_0 \tag{153}$$

Thus, the characteristic consist of curves of uniform motion with constant velocity c.

The solution $\phi(x,t)$ is constant on the curve passing through $(x_0, 0)$, and is determined from

$$\phi(x,t) \; = \; \phi(x(t),t) \; = \; f(x_0) \tag{154}$$

However, on inverting the equation for the characteristic one finds

$$x_0 \; = \; x \; - \; c \, t \tag{155}$$

so one has

$$\phi(x,t) \; = \; f(\; x \; - \; c \, t \;) \tag{156}$$

which clearly satisfies both the initial condition and the differential equation. The above solution corresponds to a wave travelling in the positive direction with speed c.

Example:

Consider the Cauchy problem

$$\frac{\partial \phi}{\partial t} \; + \; x \, \frac{\partial \phi}{\partial x} \; = \; 0 \tag{157}$$

with initial conditions

$$\phi(x,0) \; = \; f(x) \tag{158}$$

The characteristic is determined by the ordinary differential equation

$$\frac{dx}{dt} = x \tag{159}$$

which has a solution

$$x(t) = x_0 \exp[\, t \,] \tag{160}$$

On inverting the equation for the characteristic and the initial condition, one has

$$x_0 = x(t) \exp[\, - t \,] \tag{161}$$

Then, as the solution is constant along the characteristic curve

$$\phi(x(t), t) = f(x_0) \tag{162}$$

one has

$$\phi(x, t) = f(\, x \exp[\, - t \,] \,) \tag{163}$$

This is the solution that satisfies both the partial differential equation and the initial condition.

Inhomogeneous First Order Partial Differential Equations.

The inhomogeneous linear first order partial differential equation can be solved by a simple extension of the method of characteristics. Consider, the partial differential equation

$$\frac{\partial \phi}{\partial t} + a(x,t) \frac{\partial \phi}{\partial x} = b(x,t) \tag{164}$$

where the inhomogeneous term $b(x,t)$ acts as a source term. The initial condition is given by

$$\phi(x, 0) = f(x) \tag{165}$$

The characteristics are given by the solution of

$$\frac{dx}{dt} = a(x,t) \tag{166}$$

and $x(0) = x_0$. The solution along the characteristic is not constant due to the presence of the inhomogeneous term, but instead satisfies

$$\begin{aligned} \frac{d\phi(x(t),t)}{dt} &= \frac{\partial \phi}{\partial t} + \frac{dx(t)}{dt} \frac{\partial \phi}{\partial x} \\ &= \frac{\partial \phi}{\partial t} + a(x,t) \frac{\partial \phi}{\partial x} \\ &= b(x,t) \end{aligned} \tag{167}$$

However, the solution can be found by integration along the characteristic curve. This yields,

$$\phi(x(t),t) \;=\; f(x_0) \;+ \int_0^t \; dt' \; b(x(t'),t') \tag{168}$$

On inverting the relation between $x(t)$ and x_0, and substituting the resulting relation for $f(x_0)$ in the above equation one has the solution.

Example:

Consider the inhomogeneous Cauchy problem

$$\frac{\partial \phi}{\partial t} \;+\; c \, \frac{\partial \phi}{\partial x} \;=\; \lambda \, x \tag{169}$$

where the solution has to satisfy the initial condition $\phi(x,0) \;=\; f(x)$. The characteristics are found as

$$x(t) \;=\; x_0 \;+\; c \, t \tag{170}$$

and the solution of the partial differential equation along the characteristic is given by

$$\begin{aligned}\phi(x(t),t) \;&=\; f(x_0) \;+\; \lambda \int_0^t \; dt' \; x(t') \\ &=\; f(x_0) \;+\; \lambda \; (\; x_0 \; t \;+\; \frac{c}{2} \, t^2 \;)\end{aligned} \tag{171}$$

Since the characteristic can be inverted to yield the initial condition as $x_0 \;=\; x \;-\; c \, t$, one has the solution

$$\phi(x,t) \;=\; f(\; x \;-\; c \, t \;) \;+\; \lambda \, t \left(\; x \;-\; \frac{c \, t}{2} \; \right) \tag{172}$$

which completely solves the problem.

Homework:

Find the solution of the inhomogeneous Cauchy problem

$$\frac{\partial \phi}{\partial t} \;+\; c \, \frac{\partial \phi}{\partial x} \;=\; - \; \frac{1}{\tau} \; \phi(x,t) \tag{173}$$

subject to the initial condition

$$\phi(x,0) \;=\; f(x) \tag{174}$$

Solution:

The characteristic is given by

$$x(t) \ = \ x_0 \ + \ c \ t \tag{175}$$

The ordinary differential equation for $\phi(x(t), t)$ evaluated on a characteristic is

$$\frac{d\phi(x(t),t)}{dt} \ = \ - \ \frac{1}{\tau} \ \phi(x(t),t) \tag{176}$$

which has the solution

$$\begin{aligned} \phi(x(t),t) \ &= \ \phi(x(0),0) \ \exp[\ - \ \frac{t}{\tau}\ ] \\ &= \ f(\ x \ - \ c\ t\ ) \ \exp[\ - \ \frac{t}{\tau}\ ] \end{aligned} \tag{177}$$

which is a damped forward travelling wave.

3.2 Classification of Partial Differential Equations

Second order partial differential equations can be classified into three types, Elliptic, Parabolic and Hyperbolic. The classification is based upon the shape of surfaces on which the solution ϕ is constant, or on which ϕ has the maximal variation. These surfaces correspond to the wave fronts in space time $(\underline{r}, t)$, and the normals to the surfaces which correspond to the direction of propagation of waves and are called the characteristics. That is, one finds the combination corresponding to the light ray of geometrical optics.

To motivate the discussion, consider a general second order partial differential equation

$$A \ \frac{\partial^2 \phi}{\partial x^2} \ + \ 2 \ B \ \frac{\partial^2 \phi}{\partial x \ \partial t} \ + \ C \ \frac{\partial^2 \phi}{\partial t^2} \ + \ D \ \frac{\partial \phi}{\partial x} \ + \ E \ \frac{\partial \phi}{\partial t} \ + \ F \ = \ 0 \tag{178}$$

where a, B, C, D, E and F are smooth differentiable functions of x and t. Suppose we are trying to obtain a Frobenius series of ϕ in the independent variables x and t. If $\phi(x, 0)$ is given, then all the derivatives $\frac{\partial^n \phi(x,0)}{\partial x^n}$ can be obtained by direct differentiation. If the first order derivative $\frac{\partial \phi(x,t)}{\partial t}\Big|_{t=0}$, then the derivatives $\frac{\partial^{n+1} \phi(x,t)}{\partial t \ \partial x^n}\Big|_{t=0}$ can also be obtained by direct differentiation.

These two pieces of initial data allow the second derivative $\left.\frac{\partial^2\phi(x,t)}{\partial t^2}\right|_{t=0}$ to be evaluated, by using the differential equation,

$$\frac{\partial^2\phi}{\partial x^2} \;=\; -\,2\,\frac{B}{A}\,\frac{\partial^2\phi}{\partial x\,\partial t} \;-\; \frac{C}{A}\,\frac{\partial^2\phi}{\partial t^2} \;-\; \frac{D}{A}\,\frac{\partial\phi}{\partial x} \;-\; \frac{E}{A}\,\frac{\partial\phi}{\partial t} \;-\; \frac{F}{A} \tag{179}$$

Also by repeated differentiation of the differential equation with respect to t, all the higher order derivative can be obtained. Hence, one can find the solution as an expansion

$$\phi(x,t') \;=\; \phi(x,0) \;+\; t'\,\left.\frac{\partial\phi(x,t)}{\partial t}\right|_{t=0} \;+\; \frac{t'^2}{2}\,\left.\frac{\partial^2\phi(x,t)}{\partial t^2}\right|_{t=0} \;+\;\ldots \tag{180}$$

Thus, on specifying $\phi(x,0)$ and the derivative $\left.\frac{\partial\phi(x,t)}{\partial t}\right|_{t=0}$ allows $\phi(x,t)$ to be determined. However, it is essential that the appropriate derivatives exist.

Characteristics.

Consider a family of curves $\xi(x,t) \;=\; const.$ and another family of curves $\eta(x,t) \;=\; const.$ which act as a local coordinate system. These set of curves must not be parallel, therefore we require that the Jacobian be non-zero or

$$J\left(\frac{\xi,\eta}{x,y}\right) \;=\; \frac{\partial\xi}{\partial x}\,\frac{\partial\eta}{\partial y} \;-\; \frac{\partial\xi}{\partial y}\,\frac{\partial\eta}{\partial x} \;\neq\; 0 \tag{181}$$

The family of curves do not need to be mutually orthogonal.

The differential equation can be solved in the (ξ,η) local coordinate system. We shall define the solution in the new coordinates to be

$$\phi(x,t) \;=\; \tilde{\phi}(\xi,\eta) \tag{182}$$

Let us assume that the differential equation has the function $\tilde{\phi}(\xi = 0,\eta)$ and the derivative $\left.\frac{\partial\phi(\tilde{\xi},\eta)}{\partial\xi}\right|_{xi=0}$ are given. By differentiation with respect to η one can determine

$$\begin{gathered}\frac{\partial\tilde{\phi}(0,\eta)}{\partial\eta}\\ \frac{\partial^2\tilde{\phi}(0,\eta)}{\partial\eta^2}\end{gathered} \tag{183}$$

and

$$\left.\frac{\partial \tilde{\phi}(\xi,\eta)}{\partial \xi}\right|_{\xi=0}$$
$$\left.\frac{\partial^2 \tilde{\phi}(\xi,\eta)}{\partial \xi \, \partial \eta}\right|_{\xi=0} \tag{184}$$

To obtain all the higher order derivatives, one must express the partial differential equation in terms of the new variables. Thus, one has

$$\left(\frac{\partial \phi}{\partial t}\right)_x = \left(\frac{\partial \tilde{\phi}}{\partial \xi}\right)_\eta \left(\frac{\partial \xi}{\partial t}\right)_x + \left(\frac{\partial \tilde{\phi}}{\partial \eta}\right)_\xi \left(\frac{\partial \xi}{\partial t}\right)_x \tag{185}$$

and

$$\begin{aligned}\left(\frac{\partial^2 \phi}{\partial t^2}\right)_x &= \left(\frac{\partial \tilde{\phi}}{\partial \xi}\right)_\eta \left(\frac{\partial^2 \xi}{\partial t^2}\right)_x + \left(\frac{\partial \tilde{\phi}}{\partial \eta}\right)_\xi \left(\frac{\partial^2 \xi}{\partial t^2}\right)_x \\ &+ \left(\frac{\partial^2 \tilde{\phi}}{\partial \xi^2}\right) \left(\frac{\partial \xi}{\partial t}\right)_x^2 + 2 \left(\frac{\partial^2 \tilde{\phi}}{\partial \xi \, \partial \eta}\right) \left(\frac{\partial \xi}{\partial t}\right)_x \left(\frac{\partial \eta}{\partial t}\right)_x + \left(\frac{\partial^2 \tilde{\phi}}{\partial \eta^2}\right) \left(\frac{\partial \xi}{\partial t}\right)_x^2\end{aligned} \tag{186}$$

etc. Thus, the differential equation can be written as

$$\begin{aligned}&\left(\frac{\partial^2 \tilde{\phi}}{\partial \xi^2}\right) \left(A \left(\frac{\partial \xi}{\partial x}\right)^2 + 2 \, B \left(\frac{\partial \xi}{\partial x}\right) \left(\frac{\partial \xi}{\partial t}\right) + C \left(\frac{\partial \xi}{\partial t}\right)^2 \right) \\ +\ & 2 \left(\frac{\partial^2 \tilde{\phi}}{\partial \xi \, \partial \eta}\right) \left(A \left(\frac{\partial \xi}{\partial x}\right) \left(\frac{\partial \eta}{\partial x}\right) + B \left[\left(\frac{\partial \xi}{\partial x}\right) \left(\frac{\partial \eta}{\partial t}\right) + \left(\frac{\partial \eta}{\partial x}\right) \left(\frac{\partial \xi}{\partial t}\right) \right] + C \left(\frac{\partial \xi}{\partial t}\right) \left(\frac{\partial \eta}{\partial t}\right) \right) \\ +\ & \left(\frac{\partial^2 \tilde{\phi}}{\partial \eta^2}\right) \left(A \left(\frac{\partial \eta}{\partial x}\right)^2 + 2 \, B \left(\frac{\partial \eta}{\partial x}\right) \left(\frac{\partial \eta}{\partial t}\right) + C \left(\frac{\partial \eta}{\partial t}\right)^2 \right) \\ +\ & \left(\frac{\partial \tilde{\phi}}{\partial \xi}\right) \left(A \left(\frac{\partial^2 \xi}{\partial x^2}\right) + 2 \, B \left(\frac{\partial^2 \xi}{\partial x \, \partial t}\right) + C \left(\frac{\partial^2 \xi}{\partial t^2}\right) + D \left(\frac{\partial \xi}{\partial x}\right) + E \left(\frac{\partial \xi}{\partial t}\right) \right) \\ +\ & \left(\frac{\partial \tilde{\phi}}{\partial \eta}\right) \left(A \left(\frac{\partial^2 \eta}{\partial x^2}\right) + 2 \, B \left(\frac{\partial^2 \eta}{\partial x \, \partial t}\right) + C \left(\frac{\partial^2 \eta}{\partial t^2}\right) + D \left(\frac{\partial \eta}{\partial x}\right) + E \left(\frac{\partial \eta}{\partial t}\right) \right) \\ +\ & F \tilde{\phi} + G = 0\end{aligned} \tag{187}$$

The ability to solve this equation, with the initial data on $\xi = 0$ rests on whether or not

$$A \left(\frac{\partial \xi}{\partial x}\right)^2 + 2 \, B \left(\frac{\partial \xi}{\partial x}\right) \left(\frac{\partial \xi}{\partial t}\right) + C \left(\frac{\partial \xi}{\partial t}\right)^2 \neq 0 \tag{188}$$

If the above expression never vanishes for any real function $\xi(x,t)$, then the solution can be found. All higher order derivatives of $\tilde{\phi}$ can be found by repeated differentiation.

If a real function $\xi(x,t)$ exists for which

$$A \left(\frac{\partial \xi}{\partial x} \right)^2 \; + \; 2 \; B \left(\frac{\partial \xi}{\partial x} \right) \left(\frac{\partial \xi}{\partial t} \right) \; + \; C \left(\frac{\partial \xi}{\partial t} \right)^2 \; = \; 0 \tag{189}$$

then the problem is not solvable if the initial conditions are specified on this curve.

The condition of the solvability of the partial differential equation is that the quadratic expression

$$A \left(\frac{\partial \xi}{\partial x} \right)^2 \; + \; 2 \; B \left(\frac{\partial \xi}{\partial x} \right) \left(\frac{\partial \xi}{\partial t} \right) \; + \; C \left(\frac{\partial \xi}{\partial t} \right)^2 \tag{190}$$

is non-vanishing. This condition is governed by the discriminant

$$B^2 \; - \; A \; C \tag{191}$$

and can result results in three regimes.

Hyperbolic Equations.

The case where $B^2 \; - \; A \; C \; > \; 0$ corresponds to the case of hyperbolic equations. In this case, one finds that the condition vanishes on the curve

$$\left(\frac{\partial \xi}{\partial x} \right) / \left(\frac{\partial \xi}{\partial t} \right) \; = \; \frac{\left[\; - \; B \; \pm \; \sqrt{B^2 \; - \; A \; C} \; \right]}{A} \tag{192}$$

However, the slope of the curve $\xi(x,t) \; = \; conts.$ is given

$$dx \left(\frac{\partial \xi}{\partial x} \right) \; + \; dt \left(\frac{\partial \xi}{\partial t} \right) \; = \; 0 \tag{193}$$

Hence, on the curve

$$\left(\frac{dx}{dt} \right) \; = \; - \; \frac{\left(\frac{\partial \xi}{\partial t} \right)}{\left(\frac{\partial \xi}{\partial x} \right)} \tag{194}$$

or

$$\left(\frac{dt}{dx} \right) \; = \; \frac{\left[\; B \; \mp \; \sqrt{B^2 \; - \; A \; C} \; \right]}{A} \tag{195}$$

the solution can not be determined from Cauchy initial boundary conditions. These are the characteristics of the equation. In the local coordinate system corresponding to the positive sign we see that

$$A \left(\frac{\partial \xi}{\partial x} \right)^2 + 2 \, B \left(\frac{\partial \xi}{\partial x} \right) \left(\frac{\partial \xi}{\partial t} \right) + C \left(\frac{\partial \xi}{\partial t} \right)^2 = 0 \tag{196}$$

and also the other coordinates $\eta(x,t)$ can be found by choosing the negative sign. On this family of curves one also finds

$$A \left(\frac{\partial \eta}{\partial x} \right)^2 + 2 \, B \left(\frac{\partial \eta}{\partial x} \right) \left(\frac{\partial \eta}{\partial t} \right) + C \left(\frac{\partial \eta}{\partial t} \right)^2 = 0 \tag{197}$$

In this special coordinate system, one finds the partial differential equation simplifies and has the canonical form

$$\frac{\partial^2 \tilde{\phi}}{\partial \xi \, \partial \eta} + \alpha \, \frac{\partial \tilde{\phi}}{\partial \xi} + \beta \, \frac{\partial \tilde{\phi}}{\partial \eta} + \gamma \, \tilde{\phi} + \delta = 0 \tag{198}$$

where α, β, γ and δ are functions of ξ and η.

An example of a hyperbolic equation is given by the wave equation

$$\left(\frac{\partial^2 \phi}{\partial x^2} \right) - \frac{1}{c^2} \left(\frac{\partial^2 \phi}{\partial t^2} \right) = 0 \tag{199}$$

where $A = 1$ and $B = 0$ and $C = - \frac{1}{c^2}$. The equation for the characteristics is given by

$$\left(\frac{\partial \xi}{\partial x} \right)^2 - \frac{1}{c^2} \left(\frac{\partial \xi}{\partial t} \right)^2 = 0 \tag{200}$$

which factorizes as

$$\left(\frac{\partial \xi}{\partial x} \right) + \frac{1}{c} \left(\frac{\partial \xi}{\partial t} \right) = 0 \tag{201}$$

and

$$\left(\frac{\partial \eta}{\partial x} \right) - \frac{1}{c} \left(\frac{\partial \eta}{\partial t} \right) = 0 \tag{202}$$

which has solutions

$$\xi = x - c \, t \tag{203}$$

and

$$\eta = x + c \, t \tag{204}$$

The wave equation reduces to

$$\left(\frac{\partial^2 \tilde{\phi}}{\partial \xi \, \partial \eta} \right) = 0 \tag{205}$$

and has the solution

$$\begin{aligned}\tilde{\phi}(\xi,\eta) &= f(\xi) + g(\eta) \\ &= f(\,x - c\,t\,) + g(\,x + c\,t\,)\end{aligned} \tag{206}$$

which corresponds to a forward and backward travelling wave.

Parabolic Equations.

If the discriminant vanishes in a finite region, $B^2 - A\,C = 0$, then it is clear that neither A nor C can vanish as in this case B must also vanish, and one would only have an ordinary differential equation. If $A \neq 0$, one has the single solution

$$\left(\frac{\partial\xi}{\partial x}\right)/\left(\frac{\partial\xi}{\partial t}\right) = -\,B/A \tag{207}$$

corresponding to the double root. Hence, there is only a single family of characteristics ξ defined by

$$\frac{dx}{dt} = \frac{A}{B} \tag{208}$$

On transforming to the coordinate system determined by the characteristics ξ, one has the coefficient of $\frac{\partial^2\tilde{\phi}}{\partial\xi^2}$ vanishes, but $\frac{\partial^2\tilde{\phi}}{\partial\xi\,\partial\eta}$ must also vanish since the discriminant vanishes. The equation can be put in canonical form

$$\frac{\partial^2\tilde{\phi}}{\partial\eta^2} + \alpha\,\frac{\partial\tilde{\phi}}{\partial\xi} + \beta\,\frac{\partial\tilde{\phi}}{\partial\eta} + \gamma\,\tilde{\phi} + \delta = 0 \tag{209}$$

An example of a parabolic partial differential equation is given by the diffusion equation,

$$\frac{\partial^2\phi}{\partial x^2} - \frac{\partial\phi}{\partial t} = 0 \tag{210}$$

in which $A = 1$ and $B = C = 0$.

Elliptic Equations.

In the case when $B^2 - A\,C < 0$ the partial differential equation is elliptic.

In the case, when the discriminant is negative, there are no real roots and thus there are no real solutions of the equation and there is always a solution of the partial differential equation if the initial conditions are given.

The elliptic equation can be put in canonical form. First, the coefficient of

$$\frac{\partial^2 \tilde{\phi}}{\partial \xi \, \partial \eta} \tag{211}$$

is chosen to be put equal to zero. This requires that

$$\left(\frac{\partial \xi}{\partial x} \right) \left[A \left(\frac{\partial \eta}{\partial x} \right) + B \left(\frac{\partial \eta}{\partial t} \right) \right] + \left(\frac{\partial \xi}{\partial t} \right) \left[B \left(\frac{\partial \eta}{\partial x} \right) + C \left(\frac{\partial \eta}{\partial t} \right) \right] = 0 \tag{212}$$

The curve ξ that does this satisfies

$$\left(\frac{dt}{dx} \right) = - \frac{\left(\frac{\partial \xi}{\partial x} \right)}{\left(\frac{\partial \xi}{\partial t} \right)} = \frac{B \left(\frac{\partial \eta}{\partial x} \right) + C \left(\frac{\partial \eta}{\partial t} \right)}{A \left(\frac{\partial \eta}{\partial x} \right) + B \left(\frac{\partial \eta}{\partial t} \right)} \tag{213}$$

Secondly, equation is transformed such that the coefficients of $\frac{\partial^2 \tilde{\phi}}{\partial \xi^2}$ and $\frac{\partial^2 \tilde{\phi}}{\partial \eta^2}$ are made equal, while the coefficient of $\frac{\partial^2 \tilde{\phi}}{\partial \xi \partial \eta}$ is maintained to be zero. For convenience, we shall relabel the coordinates found from the first transformation as (x, t), and the coefficients as A and C etc. The required transformation is determined by the condition that the coefficients are equal

$$A \left(\frac{\partial \xi}{\partial x} \right)^2 + C \left(\frac{\partial \xi}{\partial t} \right)^2 = A \left(\frac{\partial \eta}{\partial x} \right)^2 + C \left(\frac{\partial \eta}{\partial t} \right)^2 \tag{214}$$

and zero

$$A \left(\frac{\partial \xi}{\partial x} \right) \left(\frac{\partial \eta}{\partial x} \right) + C \left(\frac{\partial \xi}{\partial t} \right) \left(\frac{\partial \eta}{\partial t} \right) = 0 \tag{215}$$

where one has used $B = 0$. Furthermore as $A \, C > B^2$ then A and C have the same sign. These equations can be combined to yield

$$A \left[\left(\frac{\partial \xi}{\partial x} \right) + i \left(\frac{\partial \eta}{\partial x} \right) \right]^2 = - C \left[\left(\frac{\partial \xi}{\partial t} \right) + i \left(\frac{\partial \eta}{\partial t} \right) \right]^2 \tag{216}$$

This condition is equivalent to

$$\begin{aligned} \sqrt{A} \left(\frac{\partial \xi}{\partial x} \right) &= \sqrt{C} \left(\frac{\partial \eta}{\partial t} \right) \\ \sqrt{C} \left(\frac{\partial \xi}{\partial t} \right) &= - \sqrt{A} \left(\frac{\partial \eta}{\partial x} \right) \end{aligned} \tag{217}$$

The existence of a solution of the two equation for both ξ and η is addressed by assuming that η is determined. Once η is determined, then ξ can be determined from

$$\xi(x,t) \;=\; \text{const.} \;+\; \int_{x_0,t_0}^{x,t} \left[\sqrt{\frac{C}{A}} \left(\frac{\partial \eta}{\partial t} \right) dx \;-\; \sqrt{\frac{A}{C}} \left(\frac{\partial \eta}{\partial x} \right) dt \right] \tag{218}$$

The solution exists if the integral is independent of the path of integration. This requires

$$\frac{\partial}{\partial t} \left[\sqrt{\frac{C}{A}} \left(\frac{\partial \eta}{\partial t} \right) \right] \;=\; - \, \frac{\partial}{\partial x} \left[\sqrt{\frac{A}{C}} \left(\frac{\partial \eta}{\partial x} \right) \right] \tag{219}$$

which is just the condition that ξ is an analytic function, so a solution can always be found.

An example of an elliptic equation is given by Laplace's equation

$$\frac{\partial^2 \phi}{\partial x^2} \;+\; \frac{\partial^2 \phi}{\partial y^2} \;=\; 0 \tag{220}$$

in which $A \;=\; C \;=\; 1$ and $B \;=\; 0$.

The characteristic equation is

$$\begin{aligned} 0 \;&=\; \left(\frac{\partial \xi}{\partial x} \right)^2 \;+\; \left(\frac{\partial \xi}{\partial y} \right)^2 \\ &=\; \left[\left(\frac{\partial \xi}{\partial x} \right) \;+\; i \left(\frac{\partial \xi}{\partial y} \right) \right] \left[\left(\frac{\partial \xi}{\partial x} \right) \;-\; i \left(\frac{\partial \xi}{\partial y} \right) \right] \end{aligned} \tag{221}$$

which has solutions

$$\begin{aligned} \xi \;&=\; x \;+\; i\, y \\ \eta \;&=\; x \;-\; i\, y \end{aligned} \tag{222}$$

In terms of these complex characteristics, the equation reduces to

$$\left(\frac{\partial^2 \tilde{\phi}}{\partial \xi \, \partial \eta} \right) \;=\; 0 \tag{223}$$

and thus the solution is given by

$$\begin{aligned} \tilde{\phi}(\xi,\eta) \;&=\; F(\xi) \;+\; G(\eta) \\ &=\; F(\, x \;+\; i\, y \,) \;+\; G(\, x \;-\; i\, y \,) \end{aligned} \tag{224}$$

These are harmonic functions. The real and imaginary part of these solutions separately satisfy Laplace's equation.

3.3 Boundary Conditions

Boundary conditions usually take three forms:-

Cauchy Conditions.

Cauchy conditions consist of specifying the value of the unknown function and the normal derivative (gradient) on the boundary.

Dirichlet Conditions.

Dirichlet conditions correspond to specifying the value of the unknown function on the boundary.

Neumann Conditions.

Neumann conditions consist of specifying the value of the normal derivative (gradient) on the boundary.

Hyperbolic equations possess unique solutions if Cauchy conditions are specified on an open surface.

Elliptic equations possess unique solutions if either Dirichlet or Neumann conditions are specified over a closed surface.

Parabolic equations posses unique solutions if either Dirichlet or Neumann conditions are specified over an open surface.

3.4 Separation of Variables

A partial differential equation may some time be solvable by the method of separation of variables. In this case, the partial differential equation can be broken down into a set of differential equations, one equation for each independent variable.

For example. the wave equation in Cartesian coordinates takes the form

$$\left(\frac{\partial^2 \phi}{\partial x^2} \right) + \left(\frac{\partial^2 \phi}{\partial y^2} \right) + \left(\frac{\partial^2 \phi}{\partial z^2} \right) - \frac{1}{c^2} \left(\frac{\partial^2 \phi}{\partial t^2} \right) = 0 \tag{225}$$

This can be reduced to three one dimensional differential equations by assuming that

$$\phi(x,y,z,t) \;=\; X(x)\,Y(y)\,Z(z)\,T(t) \tag{226}$$

which, on substituting into the differential equation leads to

$$X(x)\,Y(y)\,Z(z)\,T(t)\left[\frac{1}{X(x)}\left(\frac{\partial^2 X}{\partial x^2}\right)+\frac{1}{Y(y)}\left(\frac{\partial^2 Y}{\partial y^2}\right)+\frac{1}{Z(z)}\left(\frac{\partial^2 Z}{\partial z^2}\right)-\frac{1}{c^2}\,\frac{1}{T}\left(\frac{\partial^2 T}{\partial t^2}\right)\right] \;=\; 0 \tag{227}$$

or on diving by ϕ one has

$$\left[\frac{1}{X(x)}\left(\frac{\partial^2 X}{\partial x^2}\right)+\frac{1}{Y(y)}\left(\frac{\partial^2 Y}{\partial y^2}\right)+\frac{1}{Z(z)}\left(\frac{\partial^2 Z}{\partial z^2}\right)\right] \;=\; \frac{1}{c^2}\,\frac{1}{T}\left(\frac{\partial^2 T}{\partial t^2}\right) \tag{228}$$

The left hand side is independent of t and is a constant as t is varied while the right hand side is only a function of t. Hence, we have

$$\frac{1}{c^2}\,\frac{1}{T}\left(\frac{\partial^2 T}{\partial t^2}\right) \;=\; K \tag{229}$$

where K is the constant of separation. One then finds that the t dependence is governed by

$$\frac{1}{c^2}\left(\frac{\partial^2 T}{\partial t^2}\right) \;=\; K\;T(t) \tag{230}$$

and is given by the solution of a one dimensional problem. The equation for the spatial terms is given by

$$\left[\frac{1}{X(x)}\left(\frac{\partial^2 X}{\partial x^2}\right)\;+\;\frac{1}{Y(y)}\left(\frac{\partial^2 Y}{\partial y^2}\right)\;+\;\frac{1}{Z(z)}\left(\frac{\partial^2 Z}{\partial z^2}\right)\right] \;=\; K \tag{231}$$

The function $X(x)$ can be determined by noting that

$$\left[\frac{1}{Y(y)}\left(\frac{\partial^2 Y}{\partial y^2}\right)\;+\;\frac{1}{Z(z)}\left(\frac{\partial^2 Z}{\partial z^2}\right)\right]\;-\;K \;=\; -\;\frac{1}{X(x)}\left(\frac{\partial^2 X}{\partial x^2}\right) \tag{232}$$

Hence, the left hand side is constant while the independent variable x is varied. Thus, it is a constant L

$$\frac{1}{X(x)}\left(\frac{\partial^2 X}{\partial x^2}\right) \;=\; L \tag{233}$$

which is the one dimensional problem

$$\left(\frac{\partial^2 X}{\partial x^2}\right) \;=\; L\;X(x) \tag{234}$$

which can easily be solved. The remaining terms are governed by

$$\left[\frac{1}{Y(y)} \left(\frac{\partial^2 Y}{\partial y^2} \right) + \frac{1}{Z(z)} \left(\frac{\partial^2 Z}{\partial z^2} \right) \right] = K - L \tag{235}$$

which involves the two constants of separation K and L. This equation can be solved by noting that

$$\frac{1}{Z(z)} \left(\frac{\partial^2 Z}{\partial z^2} \right) - K + L = - \frac{1}{Y(y)} \left(\frac{\partial^2 Y}{\partial y^2} \right) \tag{236}$$

which can be reduced from a two dimensional to a one dimensional problem by noting that the left hand side is independent of y and is thus a constant, say, $- M$. Then

$$\left(\frac{\partial^2 Y}{\partial y^2} \right) = M \, Y(y) \tag{237}$$

which can be solved. Finally, one has

$$\frac{1}{Z(z)} \left(\frac{\partial^2 Z}{\partial z^2} \right) = K - L - M \tag{238}$$

which can also be solved.

Thus, on solving the one dimensional problems we have found a specific solution of the form

$$\phi_{K,L,M}(x, y, z.t) = T_K(t) \, X_L(x) \, Y_M(y) \, Z_{K-L-M}(z) \tag{239}$$

Since we have a linear partial differential equation one has a general solution of the form of a linear superposition

$$\begin{aligned} \phi(x,y,z,t) &= \sum_{K,L,M} C_{K,L,M} \, \phi_{K,L,M}(x,y,z,t) \\ &= \sum_{K,L,M} C_{K,L,M} \, T_K(t) \, X_L(x) \, Y_M(y) \, Z_{K-L-M}(z) \end{aligned} \tag{240}$$

The constant coefficients $C_{K,L,M}$ are chosen such as to satisfy the boundary conditions.

Example:

The quantum mechanical three dimensional harmonic oscillator has energy eigenstates described by the equation

$$- \frac{\hbar^2}{2 \, m} \nabla^2 \Psi + \frac{m \, \omega^2}{2} r^2 \, \Psi = E \, \Psi \tag{241}$$

This can be solved in Cartesian coordinates by using

$$r^2 \; = \; x^2 \; + \; y^2 \; + \; z^2 \tag{242}$$

and the ansatz for the eigenfunction

$$\Psi(x,y,z) \; = \; X(x) \; Y(y) \; Z(z) \tag{243}$$

which leads to three equations

$$\begin{aligned} - \frac{\hbar^2}{2\ m} \frac{\partial^2 X(x)}{\partial x^2} \; + \; \frac{m\ \omega^2}{2} \ x^2 \ X(x) \; &= \; E_x \ X(x) \\ - \frac{\hbar^2}{2\ m} \frac{\partial^2 Y(y)}{\partial y^2} \; + \; \frac{m\ \omega^2}{2} \ y^2 \ Y(y) \; &= \; E_y \ Y(y) \\ - \frac{\hbar^2}{2\ m} \frac{\partial^2 Z(z)}{\partial z^2} \; + \; \frac{m\ \omega^2}{2} \ z^2 \ Z(z) \; &= \; E_z \ Z(z) \end{aligned} \tag{244}$$

where the constants of separation satisfy $E \; = \; E_x \; + \; E_y \; + \; E_z$.

Example:

The energy eigenfunction for a particle of mass m with a radial potential $V(r)$ can be written as

$$- \frac{\hbar^2}{2\ m} \ \nabla^2 \Psi \; + \; V(r) \ \Psi \; = \; E \ \Psi \tag{245}$$

and in spherical polar coordinates reduces to

$$- \frac{\hbar^2}{2\ m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2 \ \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{r^2 \ \sin^2\theta} \frac{\partial^2 \Psi}{\partial \varphi^2} \right] + V(r) \Psi \; = \; E \ \Psi \tag{246}$$

This can be reduced to three one dimensional problems by separation of variables. The eigenfunction is assumed to be of the form

$$\Psi(r,\theta,\varphi) \; = \; R(r) \ \Theta(\theta) \ \Phi(\varphi) \tag{247}$$

On substituting this form into the equation and multiplying by $r^2 \ \sin^2\theta$ and dividing be Ψ it can be found that the azimuthal function satisfies

$$\frac{\partial^2 \Phi}{\partial \varphi^2} \; = \; - \ m^2 \ \Phi(\varphi) \tag{248}$$

where the constant of separation is identified as m^2. The solution is denoted by $\Phi_m(\varphi)$. On substituting for the φ dependence in terms of the constant of separation and multiplying by $\sin\theta\ \Theta(\theta)$, one finds that θ dependence is also separable and governed by

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)-\frac{m^2}{\sin^2\theta}\Theta(\theta) = -\,l\,(\,l\,+\,1\,)\,\Theta(\theta) \tag{249}$$

where the constant of separation is written as $l\,(\,l\,+\,1\,)$. The solution depends on the values of (l,m) and is denoted by $\Theta_{l,m}(\theta)$. The radial dependence $R(r)$ satisfies the one dimensional problem

$$-\frac{\hbar^2}{2\,m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{\hbar^2\,l\,(\,l\,+\,1\,)}{2\,m\,r^2}R(r)+V(r)\,R(r) = E\,R(r) \tag{250}$$

It is seen that $R(r)$ depends on l and not m, and is denoted by $R_l(r)$. Thus, in this case the solution of the partial differential equation can be reduced to the solution of three one dimensional problems or ordinary differential equations, involving two constants of separation (l,m). The general solution can be written as the linear superposition

$$\Psi(r,\theta,\varphi) = \sum_{l,m} C_{l,m}\,R_l(r)\,\Theta_{l,m}(\theta)\,\Phi_m(\varphi) \tag{251}$$

of solutions with the different possible (l,m) values, and with expansion coefficients $C_{l,m}$.

4 Ordinary Differential Equations

An ordinary differential equation is an equation involving one unknown function ϕ of a single variable and it's derivatives. In physical applications, the variable is either a position coordinate x or time t. Since the equation involves a derivative of first or higher order, finding solution requires the equivalent of at least one integration of the unknown function $\phi(x)$. Hence, in order that the constants of integration be uniquely specified the equation must be supplemented by at least one boundary condition. Generally, as many derivatives occur in the ODE, many different boundary conditions are also needed. The number of boundary conditions needed usually correspond to the degree of the highest order derivative. The boundary conditions usually consist of specifying a combination of the unknown function and its derivatives at a particular value of the variable, x_0.

Ordinary differential equations may be either linear or non-linear differential equations. A linear ODE is an equation in which each term in the equation only contains terms of first order in the unknown function or its derivative. For example,

$$\frac{\partial^2 \phi}{\partial t^2} \; + \; \sin \omega \; t \; \phi(t) \; = \; \cos \omega \; t \tag{252}$$

is a linear differential equation. An equation is non-linear if it contains powers of the unknown function or its derivatives other than linear. For example,

$$\frac{\partial^2 \phi}{\partial x^2} \; - \; m^2 \; \sin \phi(x) \; = \; 0 \tag{253}$$

is a non-linear differential equation. It occurs in connection with the sine-Gordon field theory, which involves the temporal and spatial variation of the physical field ϕ. Non-linear differential equations do not have systematic methods of finding solutions. Sometimes a specific solution can be found by introducing an integrating factor. In the above case, an integrating factor of $\frac{\partial \phi}{\partial x}$ can be used to convert the equation into the form of an exact integral

$$\frac{\partial \phi}{\partial x} \, \frac{\partial^2 \phi}{\partial x^2} \; - \; m^2 \, \frac{\partial \phi}{\partial x} \; \sin \phi(x) \; = \; 0 \tag{254}$$

which can be integrated to yield

$$\frac{1}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 \; + \; m^2 \; \cos \phi \; = \; C \tag{255}$$

where C is a constant of integration. The constant of integration must be determined from the boundary conditions. A suitable boundary condition may be given by

$$\lim_{x \to \infty} \; \phi(x) \; \to \; 0 \tag{256}$$

In this case one may identify $C = m^2$. Hence, the non-linear differential equation of second order in the derivative has been reduced to a non-linear differential equation only involving the first order derivative of ϕ.

On using the trigonometric identity

$$(1 - \cos\phi) = 2 \sin^2 \frac{\phi}{2} \tag{257}$$

one can take the square root of the equation to yield

$$\left(\frac{\partial \phi}{\partial x} \right) = \pm 2 m \sin \frac{\phi}{2} \tag{258}$$

This is a first order non-linear differential equation. This can be solved by writing

$$\frac{(\frac{\partial \phi}{\partial x})}{\sin \frac{\phi}{2}} = 2 m \tag{259}$$

which can be integrated by changing variable to $t = \tan(\frac{\phi}{4})$. A limit of the integration can be chosen to coincide with the point at which the boundary condition is specified

$$2 \ln\tan \left(\frac{\phi}{4} \right) \Big|_0^x = \pm 2 m x \tag{260}$$

which involves the term $\ln\tan(\frac{\phi(0)}{4})$ which is another constant of integration. If this is specified to have a value $\ln A$, the above equation can be inverted to yield

$$\phi(x) = 4 \tan^{-1} \left(A \exp \left[\pm m x \right] \right) \tag{261}$$

This solution represents a static soliton excitation. Solitons of this kind exist in a system of infinitely many gravitational pendula. In this case, the pendula are joined rigidly to one wire. The rotation of a pendulum provides a twist in the supporting wire which transmits a torsional force on the neighboring wire. The angle that the pendula make with the direction of the gravitation is denoted by ϕ. The gravitational force is periodic in the angle ϕ and is responsible for the non-linear term. The above solution represents a rotation of successive pendula over the top. In addition to this one expects small amplitude oscillations of the weights around the bottom. Since ϕ is expected to be small one can linearize the equation, that is we may be able to write b

$$\sin\phi \approx \phi \tag{262}$$

to obtain

$$\frac{\partial^2 \phi}{\partial x^2} - m^2 \phi(x) = 0 \tag{263}$$

This is a second order linear differential equation. It can be solved to yield the solution

$$\phi(x) = A \sin m (x - x_0) \tag{264}$$

involving two constants of integration which are provided by two boundary conditions. This solution represents a snapshot of the ripples of the coupled pendula. We have assumed that the amplitude of the ripples are such that $A \ll 1$.

4.1 Linear Ordinary Differential Equations

Linear differential equations have the form

$$\sum_{n=1}^{n=N} a_n(x) \frac{\partial^n \phi}{\partial x^n} = f(x) \tag{265}$$

where the set of functions $a_n(x)$ and $f(x)$ are known. The largest value of n for which the function $a_n(x)$ is non-zero is denoted by N, then the linear differential equation is of N-th order. If the term $f(x)$ is zero the equation is homogeneous, whereas if the term $fx)$ is non-zero the equation is inhomogeneous.

Homogeneous linear differential equations satisfy the principle of superposition. Namely if $\phi_1(x)$ satisfies the equation and $\phi_2(x)$ also satisfies the same equation, then the linear combination

$$\phi(x) = C_1 \phi_1(x) + C_2 \phi_2(x) \tag{266}$$

also satisfies the same linear differential equation. In general, the non-uniqueness of solutions to an equation is due to the failure to specify appropriate boundary conditions on $\phi(x)$. This non-uniqueness can be utilized to construct solutions that satisfy the appropriate boundary conditions.

A particular solution of an inhomogeneous linear differential equation, $\phi_p(x)$, is not unique as, if any solution of the homogeneous equation is added to the particular solution is added it

$$\phi(x) = \phi_p(x) + \sum_n C_n \phi_n(x) \tag{267}$$

then this ϕ also satisfies the same inhomogeneous equation. The non-uniqueness does not hold when appropriate boundary conditions are specified.

For an ordinary differential equation of N-th order it is usually necessary to specify N boundary conditions in order to obtain a unique solution. These boundary conditions eliminate the N constants of integration that are found when integrating the equation N times. Exceptions to this rule may occur if the coefficient of the highest differential may vanish at a point. This, essentially, reduces the order of the differential equation locally. If the boundary conditions are not used, one can develop N independent solutions of the N-th order linear differential equation.

4.1.1 Singular Points

A homogeneous linear differential equation can be re-written such that the coefficient of the highest order derivative is unity. That is it can be written in the form

$$\sum_n \frac{a_n(x)}{a_N(x)} \frac{\partial^n \phi}{\partial x^n} = 0 \tag{268}$$

For a second order differential equation we shall use the notation

$$\frac{d^2 \phi}{dx^2} + P(x) \frac{d\phi}{dx} + Q(x) \phi = 0 \tag{269}$$

If both $P(x)$ and $Q(x)$ are finite at the point $x = x_0$ the point x_0 is an ordinary point. If either $P(x)$, $Q(x)$ or both diverge at the point $x = x_0$ the point x_0 is a singular point. Example of a singular point occurs in quantum mechanics, for example the behavior of the radial part of the Hydrogen atom wave function is governed by the ordinary differential equation

$$- \frac{\hbar^2}{2 m} \frac{1}{r^2} \left(\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right) R(r) + \left[V(r) + \frac{\hbar^2 l (l + 1)}{2 m r^2} \right] R(r) = E R(r) \tag{270}$$

where the centrifugal potential diverges as $r \rightarrow 0$. This is an example of a singular point. Physically, what is expected to occur is that the terms $V(r)$ and E are negligible, near this singular point, and that the radial kinetic energy will balance the centrifugal potential.

$$- \frac{\hbar^2}{2 m} \frac{1}{r^2} \left(\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right) R(r) + \frac{\hbar^2 l (l + 1)}{2 m r^2} R(r) \approx 0 \tag{271}$$

Then, one expects that for $r \sim 0$ the radial wave function will be such that

$$\lim_{r \rightarrow 0} R(r) \propto r^\alpha \tag{272}$$

where $\alpha = l$ or $\alpha = - (l + 1)$. Another example occurs in the one dimensional harmonic oscillator which is governed by

$$- \frac{\hbar^2}{2} \frac{\partial^2 \psi}{\partial x^2} + \frac{m \omega^2 x^2}{2} \psi = E \psi \tag{273}$$

when $x \to \pm\infty$. In this case, one expects that the kinetic energy term should balance the potential energy term. This is usually handled by introducing the variable $z = \frac{1}{x}$.

The type of singularity can be classified as being regular or irregular.

A regular singular point x_0 is a singular point in which both $(x - x_0) P(x)$ and $(x - x_0)^2 Q(x)$ remain finite in the limit $x \to x_0$.

An irregular point x_0 is a singular point in which either $(x - x_0) P(x)$ or $(x - x_0)^2 Q(x)$ diverge in the limit $x \to x_0$.

4.2 The Frobenius Method

Given a linear differential equation one can generate an approximate solution around a point x_0 in the form of a power series in $(x - x_0)$. This is the Frobenius method. The idea is to develop $P(x)$ and $Q(x)$ in a power series around x_0 and then express the solution as a power series, with arbitrary coefficients C_n. The arbitrary coefficients are determined by demanding that each power of $(x - x_0)^n$ vanish identically when the series solution is substituted into the equation. Essentially, we are demanding that the power series satisfy the differential equation by yielding zero, and that the zero only can be expanded as a polynomial if all the coefficients are zero. This produces a set of linear algebraic equations, one for each value of n, which determine the set of unknown coefficients C_n. For simple equations, these coefficients can be determined from a recursion relation.

We shall consider the series expansion of the solution ϕ about the point x_0, in the form

$$\phi(x) = (x - x_0)^\alpha \sum_{n=0} C_n (x - x_0)^n \tag{274}$$

Then one has

$$\begin{aligned} \frac{\partial \phi(x)}{\partial x} &= \alpha (x - x_0)^{\alpha-1} \sum_{n=0} C_n (x - x_0)^n + (x - x_0)^\alpha \sum_{n=1} n \, C_n (x - x_0)^{n-1} \\ &= \sum_{n=1} C_n (x - x_0)^{\alpha+n-1} \left(n + \alpha \right) \end{aligned} \tag{275}$$

and

$$\frac{\partial^2 \phi(x)}{\partial x^2} = \alpha (\alpha - 1)(x - x_0)^{\alpha-2} \sum_{n=0} C_n (x - x_0)^n$$

$$
\begin{aligned}
&+ \quad 2\,\alpha\,(\,x\,-\,x_0\,)^{\alpha-1}\sum_{n=1} n\,C_n\,(\,x\,-\,x_0\,)^{n-1} \\
&+ \quad (\,x\,-\,x_0\,)^{\alpha}\sum_{n=2} n\,(\,n\,-\,1\,)\,C_n\,(\,x\,-\,x_0\,)^{n-2} \\
&= \sum_{n=0} C_n\,(\,x\,-\,x_0\,)^{\alpha+n-2}\Big(\,n\,(\,n\,-\,1\,)\,+\,2\,n\,\alpha\,+\,\alpha\,(\,\alpha\,-\,1\,)\,\Big) \\
&= \sum_{n=0} C_n\,(\,x\,-\,x_0\,)^{\alpha+n-2}\,(\,n\,+\,\alpha\,)\,(\,n\,+\,\alpha\,-\,1\,)
\end{aligned}
\tag{276}
$$

etc.

4.2.1 Ordinary Points

If x_0 is an ordinary point then $P(x)$ and $Q(x)$ can be expanded around x_0

$$
\begin{aligned}
P(x) &= \sum_{m=0} P_m\,(\,x\,-\,x_0\,)^m \\
Q(x) &= \sum_{m=0} Q_m\,(\,x\,-\,x_0\,)^m
\end{aligned}
\tag{277}
$$

On substituting all these into the differential equation, one obtains the equation

$$
\begin{aligned}
0 \quad &= \quad \sum_{n=0}(\,x\,-\,x_0\,)^{\alpha+n-2}\,C_n\Big(\,n\,+\,\alpha\,\Big)\Big(\,n\,+\,\alpha\,-\,1\,\Big) \\
&+ \quad \sum_{n=0}(\,x\,-\,x_0\,)^{\alpha+n-1}\sum_{m=0}^{m=n} P_m\,C_{n-m}\Big(\,n\,-\,m\,+\,\alpha\,\Big) \\
&+ \quad \sum_{n=0}(\,x\,-\,x_0\,)^{\alpha+n}\sum_{m=0}^{m=n} Q_m\,C_{n-m}
\end{aligned}
\tag{278}
$$

On relabelling n by $n+2$ in the first equation and n by $n+1$ in the second equation, so that the summations have formally similar exponents, one obtains

$$
\begin{aligned}
0 \quad &= \quad \sum_{n=0}(\,x\,-\,x_0\,)^{\alpha+n}\,C_{n+2}\Big(\,n\,+\,2\,+\,\alpha\,\Big)\Big(\,n\,+\,\alpha\,+\,1\,\Big) \\
&+ \quad \sum_{n=0}(\,x\,-\,x_0\,)^{\alpha+n}\sum_{m=0}^{m=n+1} P_m\,C_{n-m+1}\Big(\,n\,-\,m\,+\,\alpha\,+\,1\Big) \\
&+ \quad \sum_{n=0}(\,x\,-\,x_0\,)^{\alpha+n}\sum_{m=0}^{m=n} Q_m\,C_{n-m}
\end{aligned}
$$

$$
\begin{aligned}
&+ \ (\ x \ - \ x_0 \ )^{\alpha-2} \ C_0 \ \alpha \ (\ \alpha \ - \ 1 \ ) \\
&+ \ (\ x \ - \ x_0 \ )^{\alpha-1} \ \alpha \left(\ C_1 \ (\ \alpha \ + \ 1) \ + \ P_0 \ C_0 \ \right)
\end{aligned}
\tag{279}
$$

On equating two polynomials, the coefficients of the various powers are to be equated. Hence we have the set of algebraic equations consisting of two equations

$$
\begin{aligned}
0 \ &= \ \alpha \ (\ \alpha \ - \ 1 \ ) \ C_0 \\
0 \ &= \ \alpha \left(\ C_1 \ (\ \alpha \ + \ 1) \ + \ P_0 \ C_0 \ \right)
\end{aligned}
\tag{280}
$$

and the set of equations valid for integer $n \ > \ 0$

$$
\begin{aligned}
0 \ = \ & C_{n+2} \left(\ n \ + \ 2 \ + \ \alpha \ \right) \left(\ n \ + \ \alpha \ + \ 1 \ \right) \\
+ \ & \sum_{m=0}^{m=n+1} P_m \ C_{n-m+1} \left(\ n \ - \ m \ + \ \alpha \ + \ 1 \right) \\
+ \ & \sum_{m=0}^{m=n} Q_m \ C_{n-m}
\end{aligned}
\tag{281}
$$

The first equation is known as the indicial equation, and has solutions $\alpha \ = \ 0$ or $\alpha \ = \ 1$. The indicial equation can be obtained directly be examining only the lowest order mono-nomial. Due to the principle of superposition the coefficient C_0 can be chosen arbitrarily.

In the case $\alpha \ = \ 0$, the coefficient C_1 is arbitrary.

For $\alpha \ = 1$ the coefficient C_1 is determined uniquely in terms of C_0 by

$$
C_1 \ = \ - \frac{P_0 \ C_0}{\alpha \ + \ 1} \ = \ - \frac{P_0 \ C_0}{2}
\tag{282}
$$

The set of equations, for each positive index n determines C_{n+2} in terms of all the lower order expansion coefficients. For example, for $n = 0$ one has

$$
C_2 \ = \ - \ \frac{1}{(\alpha+2)(\alpha+1)} \left(\ (\alpha+1) \ P_0 \ C_1 \ + \ (P_1 \ \alpha + Q_0) \ C_0 \ \right)
\tag{283}
$$

For $\alpha = 0$ the first few terms of the solution can be written as

$$\begin{aligned}
\phi_a(x) \;&=\; C_0 \; (\; 1 \; - \; \frac{Q_0}{2!} \; (\; x \; - \; x_0 \;)^2 \; + \; \ldots \;) \\
&+ \; C_1 \; (\; x \; - \; x_0 \;) \; (\; 1 \; - \; \frac{P_0}{2!} \; (\; x \; - \; x_0 \;) \; + \; \ldots \;)
\end{aligned} \tag{284}$$

while for $\alpha \; = \; 0$ one has

$$\phi_b(x) \;=\; C_0 \; (\; x \; - \; x_0 \;) \; (\; 1 \; - \; \frac{P_0}{2!} \; (\; x \; - \; x_0 \;) \; + \; \ldots \;) \tag{285}$$

Thus, we have found only two independent solutions of the second order differential equation. A general solution can be expressed as a linear combination of $\phi_a(x)$ with $C_1 \; = \; 0$ and $\phi_b(x)$.

Example:

An example of an equation that can be solved by the Frobenius method is Airy's equation. It arises in the context of a quantum mechanical particle in a uniform electric field. The equation for the motion of the particle along the field direction is given by

$$- \; \frac{\hbar^2}{2 \; m} \; \frac{\partial^2}{\partial z^2} \; \Psi(z) \; - \; e \; E_z \; z \; \Psi(z) \; = \; E \; \Psi(z) \tag{286}$$

where E_z is the field strength and E is the energy. Before solving this equation, it is useful to change coordinates. Let us note that the classical turning point is determined by the point at which the potential $- \; e \; E_z \; z$ is equal to the energy E. That is, if the turning point is denoted by z_0, then the turning point is determined from

$$- \; e \; E_z \; z_0 \; = \; E \tag{287}$$

We shall change variables so that the position s is measured relative to the turning point

$$s \; = \; z \; - \; z_0 \tag{288}$$

in which case the equation takes the form

$$- \; \frac{\hbar^2}{2 \; m} \frac{\partial^2}{\partial s^2} \Psi \; - \; e \; E_z \; s \; \Psi \; = \; 0 \tag{289}$$

The form of the equation can be further simplified by identifying a length scale ξ defined by

$$\xi^3 \; = \; \frac{\hbar^2}{2 \; m \; | \; e \; | \; E_z} \tag{290}$$

and then introducing a dimensionless length $x = \frac{z}{\xi}$ one obtains

$$\frac{\partial^2}{\partial x^2} \phi(x) - x \phi(x) = 0 \tag{291}$$

where $\phi(x) = \phi(\frac{z - z_0}{\xi}) = \Psi(z)$.

Airy's equation has no singularities at finite values of x, except at infinity. We shall find a solution by series expansion around $x = 0$. Let, us assume that the solution has the form

$$\begin{aligned} \phi(x) &= x^\alpha \sum_{n=0}^{\infty} C_n x^n \\ &= \sum_{n=0}^{\infty} C_n x^{n+\alpha} \end{aligned} \tag{292}$$

which is substituted into the differential equation. One finds

$$\sum_{n=0}^{\infty} (n + \alpha) (n + \alpha - 1) C_n x^{n+\alpha-2} - \sum_{n=0}^{\infty} C_n x^{n+\alpha+1} = 0 \tag{293}$$

The value of α is determined from the indicial equation. It is found by examining the terms of lowest power in the above equation. This, by definition, has to be a term in which $n = 0$. The term of lowest power is identified as the term $x^{\alpha-2}$ and the coefficients are given by

$$\alpha (\alpha - 1) = 0 \tag{294}$$

Thus, we either have $\alpha = 0$ or $\alpha = 1$.

For $\alpha = 0$ the equation becomes

$$\sum_{n=0}^{\infty} n (n - 1) C_n x^{n-2} - \sum_{n=0}^{\infty} C_n x^{n+1} = 0 \tag{295}$$

Or since the first two terms on the left hand side are zero one has

$$\sum_{n=2}^{\infty} n (n - 1) C_n x^{n-2} - \sum_{n=0}^{\infty} C_n x^{n+1} = 0 \tag{296}$$

Changing the summation variable from $m = n - 3$ one has

$$\sum_{m=-1}^{\infty} (m + 3) (m + 2) C_{m+3} x^{m+1} - \sum_{n=0}^{\infty} C_n x^{n+1} = 0 \tag{297}$$

or

$$2\,C_{-1} \;+\; \sum_{m=0}^{\infty} \left((\,m\;+\;3\,)\,(\,m\;+\;2\,)\,C_{m+3} \;-\; C_m \right) x^{m+1} \;=\; 0 \qquad (298)$$

On equating the coefficients of the various powers to zero, one obtains

$$C_{-1} \;=\; 0 \qquad (299)$$

which is consistent with our assumption that the series expansion starts with C_0. The higher order coefficients are related via

$$C_{m+3} \;=\; \frac{C_m}{(\,m\;+\;3\,)\,(\,m\;+2\,)} \qquad (300)$$

Hence, we have a relation between the terms in which the powers of x are of the form x^{3r}. One has

$$\begin{aligned} C_{3r} &= \frac{C_{3r-3}}{(\,3\,r\,)\,(\,3\,r\;-\;1\,)} \\ &= \frac{C_{3r-6}}{(\,3\,r\,)\,(\,3\,r\;-\;1\,)\,(\,3\,r\;-\;3\,)\,(\,3\,r\;-\;4\,)} \end{aligned} \qquad (301)$$

This leads to the unique determination of all the coefficients whose orders are divisible by three.

The other solution of the indicial equation is $\alpha\;=1$. This solution corresponds to the terms in the series of which start with C_1. The coefficients satisfy

$$C_{m+3} \;=\; \frac{C_m}{(\,m\;+\;3\,)\,(\,m\;+2\,)} \qquad (302)$$

or on writing $m\;=\;3\,r\;+\;1$ one has one has

$$\begin{aligned} C_{3r+1} &= \frac{C_{3r-2}}{(\,3\,r\;+\;1\,)\,(\,3\,r\,)} \\ &= \frac{C_{3r-5}}{(\,3\,r\;+\;1\,)\,(\,3\,r\,)\,(\,3\,r\;-\;2\,)\,(\,3\,r\;-\;3\,)} \end{aligned} \qquad (303)$$

The general solution is given by

$$\phi(x) \;=\; C_0 \left[\,1\;+\;\frac{x^3}{2.3}\;+\;\frac{x^6}{2.3.5.6}\;+\ldots\;+\;\frac{x^{3r}}{2.3.\ldots.(\,3\,r\;-\;1\,)\,(\,3\,r\,)}\;+\;\ldots\,\right]$$

$$
\begin{aligned}
& + \ C_1 \left[x + \frac{x^4}{3.4} + \frac{x^7}{3.4.6.7} + \ldots + \frac{x^{3r+1}}{3.4.\ldots.(3r)(3r+1)} \right] \\
& = \ C_0 \left[1 + \sum_{r=1}^{\infty} \frac{x^{3r}}{2.3.\ldots(3r-1)(3r)} \right] \\
& + \ C_1 \left[x + \sum_{r=1}^{\infty} \frac{x^{3r+1}}{3.4.\ldots.(3r)(3r-1)} \right]
\end{aligned}
\tag{304}
$$

Because of the denominator of the general term in the series, the series converge for all values of x. The solutions show oscillations with increasing frequency and decreasing amplitude for increasingly negative values of x. The solutions are montonic for positive values of x.

4.2.2 Regular Singularities

The Frobenius method, when applied at a regular singular point, x_0, yields an indicial equation that has a non-trivial solution. The series expansion shows a non-analytic behavior at x_0. Fuchs's theorem states that it is always possible to find one series solution for ordinary or regular singular points. For a regular singular point, where

$$
P(x) = \frac{p_{-1}}{(x - x_0)} + p_0 + \ldots \tag{305}
$$

and

$$
Q(x) = \frac{q_{-2}}{(x - x_0)^2} + \frac{q_{-1}}{(x - x_0)} + q_0 + \ldots \tag{306}
$$

the indicial equation can be found by examining the lowest term in the expansion $C_0(x - x_0)^\alpha$. The indicial equation is found as

$$
\alpha(\alpha - 1) + p_{-1}\alpha + q_{-2} = 0 \tag{307}
$$

which is a quadratic equation and gives a solution

$$
\alpha = \frac{1}{2} \left(1 - p_{-1} \pm \sqrt{(1 - p_{-1})^2 - 4 q_{-2}} \right) \tag{308}
$$

Example:

Consider the differential equation

$$
- \frac{d^2R}{dr^2} - \frac{2}{r}\frac{dR}{dr} + \frac{l(l+1)}{r^2} R = 0 \tag{309}
$$

which has a regular singular point at $r = 0$. On applying the Frobenius method with

$$R(r) = r^\alpha \left(\sum_{n=0} C_n \, r^n \right) \tag{310}$$

The indicial equation can be found directly by examining the coefficient of the lowest order mononomial $C_0 r^\alpha$. Thus, we have

$$- \alpha (\alpha - 1) C_0 \, r^{\alpha-2} - 2 \frac{\alpha}{r} C_0 \, r^{\alpha-1} + \frac{l (l + 1)}{r^2} C_0 \, r^\alpha = 0 \tag{311}$$

Thus, the indicial equation leads to

$$\alpha (\alpha + 1) = l (l + 1) \tag{312}$$

or $\alpha = l$ or $\alpha = - (l + 1)$. The singularity governs the behavior of the independent solutions at $r = 0$. In this case, only C_0 is non-zero. All higher order expansion coefficients satisfy equations which only have the solutions $C_n = 0$. This is because the equation is homogeneous in r. That is, if we count the powers of r in each term where each derivative $\frac{\partial}{\partial r}$ is counted as r^{-1}, then each term has the same power. If the equation is homogeneous it does not mix up the different powers, so the solutions must be simple powers.

Example:

For a slightly different equation, such as

$$- \frac{d^2 R}{dr^2} - \frac{2}{r} \frac{dR}{dr} + \frac{l (l + 1)}{r^2} R = k^2 \, R \tag{313}$$

it is convenient to change variables to $x = k \, r$. The equation for $R(x/k)$ becomes

$$- \frac{d^2 R}{dx^2} - \frac{2}{x} \frac{dR}{dx} + \frac{l (l + 1)}{x^2} R = R \tag{314}$$

The solution is assumed to have the form

$$R(x \; k) = x^\alpha \sum_{n=0}^{\infty} C_n \, x^n \tag{315}$$

and this is substituted into the differential equation, leading to a polynomial equation

$$- \sum_{n=0}^{\infty} (n + \alpha) (n + \alpha - 1) C_n \, x^{(\alpha+n-2)} - \frac{2}{x} \sum_{n=0}^{\infty} (n + \alpha) C_n \, x^{n+\alpha-1)} + \left(\frac{l (l + 1)}{x^2} - 1 \right) \sum_{n=0}^{\infty} C_n \, x^{(n+\alpha)} = 0 \tag{316}$$

Combining the terms of the same power we have

$$\sum_{n=0}^{\infty} \bigg((n + \alpha) (n + \alpha + 1) - l (l + 1) \bigg) C_n \, x^{(\alpha+n-2)} = \sum_{n=0}^{\infty} C_n \, x^n$$
$$\sum_{n=0}^{\infty} (n + \alpha - l) (n + \alpha + l + 1) C_n \, x^{(\alpha+n-2)} = \sum_{n=2}^{\infty} C_{n-2} \, x^{n-2} \tag{317}$$

If one were to move all the non-zero terms to one side of the equation, it is seen that this equation is equivalent to equating a polynomial with zero. A polynomial is only equal to zero, for all values of a continuous variable x, if the coefficients are of the polynomial are all identical to zero. That is the coefficients of the terms with like powers must be identical. On equating coefficients of the same power one has

$$(n + \alpha - l) (n + \alpha + l + 1) C_n = - C_{n-2} \tag{318}$$

Then, if one assumes that $C_0 \neq 0$, on equating the terms with $n = 0$ one finds the indicial equation,

$$\alpha (\alpha + 1) - l (l + 1) = 0 \tag{319}$$

with solutions $\alpha = l$ or $\alpha = - (l + 1)$. On equating the coefficients with $n = 1$, i.e. the coefficients of the terms proportional to $x^{\alpha+1}$, then one finds

$$\bigg[(\alpha + 2) (\alpha + 1) - l (l + 1) \bigg] C_1 = 0 \tag{320}$$

Since, for $\alpha = l$ or $\alpha = - (l + 1)$ the term in the parenthesis is non-zero one must have $C_1 = 0$, except if $l = 0$.

However, the general set of linear equations reduces to the recursion relation

$$(n + \alpha - l) (n + \alpha + l + 1) C_n = (- 1) C_{n-2} \tag{321}$$

This series does not terminate, and so one has

$$C_n = (- 1) \frac{1}{(n + \alpha - l) (n + \alpha + l + 1)} C_{n-2} \tag{322}$$

which can be iterated to yield

$$C_n = (- 1)^{\frac{n}{2}} \frac{(\alpha - l)!! (\alpha + l + 1)!!}{(n + \alpha - l)!! (n + \alpha + l + 1)!!} C_0 \tag{323}$$

where the double factorial is defined as

$$n!! \; = \; n \; (\; n \; - \; 2 \;)!! \tag{324}$$

and for even n, $n \; = \; 2 \; m$, can be written as

$$(\; 2 \; m \;)!! \; = \; 2^m \; m! \tag{325}$$

and for odd n, $n \; = \; 2 \; m \; + \; 1$, one has

$$(\; 2 \; m \; + \; 1 \;)!! \; = \; \frac{(\; 2 \; m \; + \; 1 \;)!}{2^m \; m!} \tag{326}$$

Instead of using the explicit expression for odd n we shall use the relation for even n to define the factorial expression for half integer n. That is, we shall define the half integer factorial via

$$\left(\; 2 \; m \; + \; 1 \; \right)!! \; = \; 2^{m + \frac{1}{2}} \; \left(\; m + \frac{1}{2} \; \right)! \tag{327}$$

Thus the solution regular at the origin can be represented by an infinite power series

$$\begin{aligned} R_l(r) \; &= \; x^l \; C_0 \; \sum_{m=0}^{\infty} \; \frac{(\; 2 \; l \; + \; 1 \;)!!}{(\; 2 \; m \;)!! \; (\; 2 \; m \; + \; 2 \; l \; + \; 1 \;)!!} \; (\; - \; 1 \;)^m \; x^{2m} \\ &= \; x^l \; C_0 \; \sum_{m=0}^{\infty} \; \frac{(\; 2 \; l \; + \; 1 \;)!!}{2^m \; m! \; (\; 2 \; m \; + \; 2 \; l \; + \; 1 \;)!!} \; (\; - \; 1 \;)^m \; x^{2m} \\ &= \; x^l \; C_0 \; \sum_{m=0}^{\infty} \; \frac{l!}{2^{2m} \; m! \; (\; m \; + \; l \; + \; \frac{1}{2} \;)!} \; (\; - \; 1 \;)^m \; x^{2m} \\ &= \; x^l \; C_0 \; \sum_{m=0}^{\infty} \; \frac{l!}{m! \; (\; m \; + \; l \; + \; \frac{1}{2} \;)!} \; (\; - \; 1 \;)^m \; \left(\frac{x}{2} \right)^{2m} \end{aligned} \tag{328}$$

where we have defined the factorial for half integer n. It can be seen, from the ratio test, that this series converges as the ratio of successive terms is $- \; \frac{1}{m^2}$, for large m. The first few terms of the solution is given by

$$R_l(r) \; = C_0 \; (\; k \; r \;)^l \; \left[\; 1 \; - \; \frac{(\; k \; r \;)^2}{2 \; (2 \; l \; + \; 3 \;)} \; + \ldots \; \right] \tag{329}$$

This series solution is related to the Bessel function of half integer order, also known as the spherical Bessel function.

Homework:

Show that the series solution for $R_l(x)$ satisfies the recursion relations

$$R_{l+1}(x) \ + \ R_{l-1}(x) \ = \ \frac{2\ l \ + \ 1}{x} \ R_l(x) \tag{330}$$

and

$$l \ R_{l-1}(x) \ - \ (\ l \ + \ 1 \ ) \ R_{l+1}(x) \ = \ (\ 2 \ l \ + \ 1 \ ) \ \frac{\partial R_l(x)}{\partial x} \tag{331}$$

Homework:

Verify that

$$j_0(x) \ = \ \frac{\sin x}{x} \tag{332}$$

and

$$j_1(x) \ = \ \frac{\sin x \ - \ x \ \cos x}{x^2} \tag{333}$$

are solutions of the differential equation for $l \ = \ 0$ and $l \ = \ 1$. Show that on expanding these solutions in powers of x, one recovers (up to an arbitrary multiplicative constant) the Frobenius series solutions which are nonsingular at $x \ = \ 0$.

Homework:

Using the above recursion relations, find explicit expressions for the solutions for $l \ = 2$ and $l \ = \ 3$.

Homework: 8.5.5

Homework: 8.5.6

Homework: 8.5.12

Example:

Consider the differential equation

$$(\ 1 \ - \ x^2 \ ) \ \frac{\partial^2 \phi}{\partial x^2} \ - \ 2 \ x \ \frac{\partial \phi}{\partial x} \ + \ l \ (\ l \ + \ 1 \ ) \ \phi \ = \ 0 \tag{334}$$

This equation has regular singular points at $x = \pm 1$. We require that the solution is finite for all values of x in the interval $(-1, 1)$. The Frobenius series is assumed to be of the form

$$\phi(x) = x^\alpha \sum_{n=0}^{\infty} C_n \, x^n \tag{335}$$

Substitution of this form in the equation leads to

$$\begin{aligned} & (1 - x^2) \sum_{n=0}^{\infty} C_n \, (n + \alpha) (n + \alpha - 1) \, x^{(n+\alpha-2)} \\ - 2 \, x & \sum_{n=0}^{\infty} C_n \, (n + \alpha) \, x^{(n+\alpha-1)} + l (l + 1) \sum_{n=0}^{\infty} C_n \, x^{(n+\alpha)} = 0 \end{aligned} \tag{336}$$

or

$$\begin{aligned} & \sum_{n=0}^{\infty} C_n \, (n + \alpha) (n + \alpha - 1) \, x^{(n+\alpha-2)} = \\ = & \sum_{n=2}^{\infty} C_{n-2} \left((n + \alpha - 2) (n + \alpha - 1) - l (l + 1) \right) x^{(n+\alpha-2)} \end{aligned} \tag{337}$$

Hence we have

$$C_n \, (n + \alpha) (n + \alpha - 1) = C_{n-2} \, (n + \alpha - l - 2) (n + \alpha + l - 1) \tag{338}$$

where we have defined $C_{-2} = C_{-1} = 0$.

The indicial equation is found by setting $n = 0$, and yields

$$\alpha (\alpha - 1) = 0 \tag{339}$$

Choosing $\alpha = 0$ one obtains solutions of even symmetry, and the coefficients are related via

$$C_n = \frac{(n - l - 2) (n + l - 1)}{n (n - 1)} \, C_{n-2} \tag{340}$$

For large n the coefficients are of the same order of magnitude, and by the ratio test,

$$\lim_{n \to \infty} \frac{C_{n+2} \, x^{n+2}}{C_n \, x^n} = x^2 \tag{341}$$

In fact, it can be shown that the series diverges when $x = \pm 1$, unless the coefficients are zero for large n. However, when l is an integer, say N, the series truncates,

$$0 = C_{N+2} = \frac{(N - l) (N + l + 1)}{(N + 2) (N + 1)} C_N \tag{342}$$

and the solution for $\alpha = 0$ is an even polynomial

$$\phi_l(x) = C_0 \left[1 + \frac{C_2}{C_0} x^2 + \frac{C_4}{C_0} x^4 + \ldots \right] \tag{343}$$

in which the highest term is of power $N = l$.

For $\alpha = 1$ the solution is odd in x and we have and the coefficients are related via

$$C_n = \frac{(n - l + 1) (n + l)}{n (n + 1)} C_{n-2} \tag{344}$$

For large n the coefficients are of the same order of magnitude, and by the ratio test, so the series may diverge when $x = \pm 1$, unless the coefficients are zero for large n. In fact, this is the case for arbitrary l. However, when l is an integer, say N, the series truncates,

$$0 = C_{N+2} = \frac{(N - l + 1) (N + l)}{(N + 2) (N + 1)} C_N \tag{345}$$

and the solution is x multiplied by an even polynomial in which the highest term is of power $N = l - 1$.

$$\phi_l(x) = x\, C_0 \left[1 + \frac{C_2}{C_0} x^2 + \frac{C_4}{C_0} x^4 + \ldots \right] \tag{346}$$

Hence, in the case $\alpha = 1$, the solution is an odd polynomial of order l.

Homework:

Show that the solution for finite l can be written as

$$\phi_l(x) = \sum_{s=0}^{s=s_{max}} A_s\, x^{(l-2s)} \tag{347}$$

where

$$s_{max} = \left\{ \begin{array}{cc} \frac{l}{2} & l \text{ even} \\ \frac{l-1}{2} & l \text{ odd} \end{array} \right\} \tag{348}$$

and the coefficients are given by

$$A_s = - \frac{(l - 2 s + 1) (l - 2 s + 2)}{2 s (2 l - 2 s + 1)} A_{s-1}$$

$$A_s = (- 1)^s \frac{l!}{(l - 2 s)! \, 2^s \, s! \, (2 l - 2 s + 1) \ldots (2 l - 1)} A_0$$

$$A_s = (- 1)^s \frac{l! \, (2 l - 2 s)! \, 2^l \, l!}{(l - 2 s)! \, 2^s \, s! \, (2 l)! \, 2^{(l-s)} \, (l - s)!} A_0 \tag{349}$$

Thus, the coefficients are given by

$$A_s = \frac{(- 1)^s}{s!} \frac{(l!)^2}{(2 l)!} \frac{(2 l - 2 s)!}{(l - 2 s)! \, (l - s)!} A_0 \tag{350}$$

and the series solution is given by

$$\phi_l(x) = \frac{(l)!^2}{(2 l)!} A_0 \sum_{s=0}^{s_{max}} \frac{(- 1)^s}{s!} \frac{(2 l - 2 s)!}{(l - 2 s)! \, (l - s)!} x^{(l-2s)} \tag{351}$$

Homework:

Show that the series solution, for integer l, satisfies the recursion relation

$$(2 l + 1) \, x \, \phi_l(x) = (l + 1) \, \phi_{l+1}(x) + l \, \phi_{l-1}(x) \tag{352}$$

Example:

An example of the Frobenius method providing a solution of an eigenvalue equation, is given by the following equation

$$\frac{\partial^2 \phi}{\partial x^2} + \left(\frac{1}{x} - 1 \right) \frac{\partial \phi}{\partial x} + \frac{m}{x} \phi = 0 \tag{353}$$

which is Laguerre's differential equation. This represents an eigenfunction when the series truncates to yield a polynomial, as certain boundary conditions have to be satisfied as $x \rightarrow \infty$. In the case that the boundary conditions are satisfied because the series truncates, the parameter m is the eigenvalue. The point $x = 0$ is a regular point.

The Frobenius solution is found by assuming a solution in the form of an expansion

$$\phi(x) = x^\alpha \sum_{n=0}^{\infty} C_n \, x^n \tag{354}$$

On substituting this into the differential equation one a polynomial equation which is equal to zero

$$0 = \sum_{n=0}^{\infty} C_n \left(n + \alpha \right) \left(n + \alpha - 1 \right) x^{\alpha+n-2}$$

$$+ \sum_{n=0}^{\infty} C_n \left(n + \alpha \right) (x^{\alpha+n-2} - x^{\alpha+n-1}) + \sum_{n=0}^{\infty} m \, C_n \, x^{\alpha+n-1} \tag{355}$$

On collecting terms one finds that

$$0 = \sum_{n=0}^{\infty} C_n \, (n + \alpha)^2 \, x^{\alpha+n-2} + \sum_{n=0}^{\infty} (m - n - \alpha) \, C_n \, x^{\alpha+n-1} \tag{356}$$

On writing $n = n' - 1$ in the second term and noting that the sum starts at $n' = 1$ one has

$$0 = \sum_{n=0}^{\infty} C_n \, (n + \alpha)^2 \, x^{\alpha+n-2} + \sum_{n'=1}^{\infty} (m - n' - \alpha + 1) \, C_{n'-1} \, x^{\alpha+n'-2} \tag{357}$$

or

$$0 = \sum_{n=0}^{\infty} \left(C_n \, (n + \alpha)^2 + (m - n - \alpha + 1) \, C_{n-1} \right) x^{\alpha+n-2} \tag{358}$$

if one defines $C_{-1} = 0$. This polynomial is only zero if the coefficients of the various powers are all equal to zero.

Examining the coefficient of the lowest power, $x^{\alpha-2}$, and equating the coefficient of the mononomial to zero, one finds the indicial equation

$$\alpha^2 \, C_0 = 0 \tag{359}$$

which only involves the lowest order expansion coefficient C_0. Since, by definition C_0 is the coefficient of the lowest order term in the expansion, it is non-zero, otherwise all the coefficients are zero. Hence, we must have

$$\alpha^2 = 0 \tag{360}$$

which only yields one solution for α.

On examining the higher order coefficient of the polynomial, i.e. the coefficient of the power in x^{n-2}, and equating the coefficient to zero, one has

$$0 = n^2 \, C_n + (m - n + 1) \, C_{n-1} \tag{361}$$

Hence, we have the recursion relation

$$C_n \; = \; \frac{(\; n \; - \; m \; - \; 1 \;)}{n^2} \; C_{n-1} \tag{362}$$

This yields the higher order coefficients in terms of the lower order coefficients. In fact, on iterating one can obtain the formal relation

$$C_n \; = \; (\; - \; 1 \;)^n \; \frac{m!}{(\; m \; - \; n \;)! \; (n!)^2} \; C_0 \tag{363}$$

for $m \; > \; n$. The Frobenius method only allows us to find this one solution, since there is only one solution for α and C_1 is uniquely determined by C_0.

For large n the recursion relation can be approximated by

$$C_n \; \sim \; \frac{1}{n} \; C_{n-1} \tag{364}$$

or

$$C_n \; \sim \; \frac{C_0}{n!} \tag{365}$$

Hence, for large x the series can be approximated by an exponential as

$$\begin{aligned} \phi(x) \quad & \sim \quad \sum_{n=0}^{\infty} \; C_0 \; \frac{x^n}{n!} \\ & \sim \quad C_0 \; \exp[\; x \;] \end{aligned} \tag{366}$$

If the series truncates at the N-th order term one must have $C_M \; = \; 0$ for all $M \; > \; N$. This can only be the case if $C_{N+1} \; = \; 0$ and $C_N \; \neq \; 0$. In this case, the recursion relation becomes

$$0 \; = \; C_{N+1} \; = \; \frac{(\; N \; - \; m \;)}{(\; N \; + \; 1 \;)^2} \; C_N \tag{367}$$

which requires $N \; = \; m$. In the case of integer m, the Frobenius series truncates to an m-th order polynomial, and m is the eigenvalue. The polynomial converges and therefore represents a good solution.

Example:

The Hermite polynomials $\phi_m(x)$ satisfy the equation

$$\frac{\partial^2 \phi_m(x)}{\partial x^2} \; - \; 2 \; x \; \frac{\partial \phi_m(x)}{\partial x} \; + \; 2 \; m \; \phi_m(x) \; = \; 0 \tag{368}$$

on the interval $(-\infty, +\infty)$. On using the Frobenius method one employs the ansatz

$$\phi_m(x) \; = \; x^\alpha \; \sum_{n=0}^{\infty} \; C_n \; x^n \tag{369}$$

and substitutes this into the differential equation

$$\sum_{n=0}^{\infty} C_n \, (\, n + \alpha \,) \, (\, n + \alpha - 1 \,) \, x^{n+\alpha-2} + 2 \sum_{n=0}^{\infty} C_n \, (\, m - n - \alpha \,) \, x^{n+\alpha} \; = \; 0 \tag{370}$$

Setting $n \; = \; n' \; - \; 2$ in the last term

$$\sum_{n=0}^{\infty} C_n \, (\, n + \alpha \,) \, (\, n + \alpha - 1 \,) \, x^{n+\alpha-2} + 2 \sum_{n'=2}^{\infty} C_{n'-2} \, (\, m + 2 - n' - \alpha \,) \, x^{n'+\alpha-2} \; = \; 0 \tag{371}$$

We shall define $C_{-1} \; = \; C_{-2} \; = 0$, and then find that

$$\sum_{n=0}^{\infty} \left(C_n \, (\, n + \alpha \,) \, (\, n + \alpha - 1 \,) + 2 \; C_{n-2} \, (\, m + 2 - n - \alpha \,) \right) x^{n+\alpha-2} \; = \; 0 \tag{372}$$

The indicial equation is found from examining the coefficient of lowest non-zero mononomial $x^{\alpha-2}$, where $n \; = \; 0$,

$$\alpha \; (\; \alpha \; - \; 1 \;) \; C_0 \; = \; 0 \tag{373}$$

hence, either $\alpha \; = \; 0$ or $\alpha \; = \; 1$.

For $\alpha \; = \; 0$ one has the recursion relation

$$C_n \; = \; 2 \, \frac{n \; - \; 2 \; - \; m}{n \; (\; n \; - \; 1 \;)} \, C_{n-2} \tag{374}$$

Thus, the solution is even in x. On writing $n \; = \; 2 \; s$ one has

$$\begin{aligned} C_{2s} \; &= \; 2 \, \frac{2 \; s \; - \; 2 \; - \; m}{2 \; s \; (\; 2 \; s \; - \; 1 \;)} \, C_{2s-2} \\ &= \; (\; - \; 1 \;)^s \, \frac{(\; m \; - \; 2 \; s \; + \; 2 \;) \; (\; m \; - \; 2 \; s \; + \; 4 \;) \; \ldots \; (\; m \; - \; 2 \;) \; m}{(2s)!} \, 2^s \; C_0 \\ &= \; (\; - \; 1 \;)^s \, \frac{(m)!!}{(\; m \; - \; 2 \; s \;)!! \; (2s)!} \, 2^s \; C_0 \\ &= \; (\; - \; 1 \;)^s \, \frac{(\frac{m}{2})!}{(\frac{m}{2} - s)! \; (2s)!} \, 2^{2s} \; C_0 \end{aligned} \tag{375}$$

It can be seen that the series truncates when

$$0 \; = \; C_{N+2} \; = \; 2 \, \frac{N \; - \; m}{(\; N \; + \; 2 \;) \; (\; N \; + \; 1 \;)} \, C_N \tag{376}$$

that is, the series terminates if $m = N$ and the series is a polynomial of order N.

We note that if the series does not truncate the large n behavior of the coefficients is governed by

$$C_n \sim \frac{2}{n} C_{n-2} \tag{377}$$

so one has

$$C_{2s} \sim \frac{1}{s!} C_0 \tag{378}$$

and the series would exponentiate at large x.

4.3 Linear Dependence

In the Frobenius method we look for a power series solution, by substituting the power series into the equation. Let us examine only the first N terms in the series solution. After some re-organization one finds a polynomial equation, in which the polynomial is equated to zero. This equation is solved by insisting that if the polynomial in x is equal to zero then all the coefficients of the polynomial are zero. This then leads to the recursion relation etc., and if the series converges in the limit $N \to \infty$ one has a solution.

A crucial point of the procedure is the insistence that if the polynomial is equal to zero then the only solution is that all the coefficients of the various mononomials are zero. This is a statement that the various mononomials x^n are linearly independent.

The linear independence can be proved by examining a general N-th order polynomial which is equal to zero

$$\sum_{n=0}^{n+N} C_n x^n = 0 \tag{379}$$

which is supposed to hold over a continuous range of x values. Then as this holds for $x = 0$ one finds that the coefficient C_0 must be zero. On taking the differential of the polynomial one obtains

$$\sum_{n=1}^{n=N} n C_n x^{n-1} = 0 \tag{380}$$

which must also hold at $x = 0$. Hence one obtains $C_1 = 0$. By taking all N higher order differentials this can be extended to show that all the $C_n = 0$.

Thus, we have shown that if the polynomial is equal to zero the coefficients of the various mononomials are equal to zero. Thus, it is impossible to write

$$k_N \; x^N \; = \; \sum_{n=0}^{n=N-1} \; k_n \; x^n \tag{381}$$

for any set of k_n which contains non-zero values. This is formalized by the statement that a set of functions $\phi_n \; = \; x^n$ are linearly independent if the only solution of

$$\sum_n \; k_n \; \phi_n \; = \; 0 \tag{382}$$

is that $k_n \; = \; 0$ for all n. On the other hand if one has a set of functions ϕ_α such as the set containing all the N-th lowest order mononomials, such as x^n, and the function $\phi_{N+1} \; = \; a \; x^2 \; + \; b \; x \; + \; c$ then there are non zero or non trivial solutions of the equation

$$\sum_{\alpha=0}^{N+1} \; k_\alpha \; \phi_\alpha \; = \; 0 \tag{383}$$

such as

$$\begin{aligned} k_0 &= c \\ k_1 &= b \\ k_2 &= a \\ k_{N+1} &= 1 \end{aligned} \tag{384}$$

In this case, the set of functions ϕ_α are linearly dependent as at least one of them can be expressed as a linear combination of the others.

The concept of linear dependence and linear independence can be extended to other sets of functions. A set of N functions ϕ_α are linearly independent if the only solution of the equation

$$\sum_{\alpha=1}^{N} \; k_\alpha \; \phi_\alpha \; = \; 0 \tag{385}$$

is that

$$k_\alpha \; = \; 0 \qquad \qquad \forall \; \alpha \tag{386}$$

Otherwise, if a non-trivial solution exists the set of functions are linearly dependent.

A simple test of linear dependence is provided by the Wronskian. Consider the generalization of the proof that the mono-nomials are linearly independent. Namely consider

$$\sum_{\alpha=1}^{N} k_\alpha \, \phi_\alpha \; = \; 0 \tag{387}$$

and the successive derivatives with respect to x starting with

$$\sum_{\alpha=1}^{N} k_\alpha \, \frac{\partial \phi_\alpha}{\partial x} \; = \; 0 \tag{388}$$

and

$$\sum_{\alpha=1}^{N} k_\alpha \, \frac{\partial^2 \phi_\alpha}{\partial x^2} \; = \; 0 \tag{389}$$

etc. The set of all these equations must be satisfied if the original equation is satisfied for a continuous range of x, since the derivatives of the equation can be found by subtracting the equation at infinitesimally different values of x ie, $x + dx$ and x, and then dividing by dx. The set of N coefficients k_α are completely determined from N independent equations, so we shall truncate the set of equations with

$$\sum_{\alpha=1}^{N} k_\alpha \, \frac{\partial^{N-1} \phi_\alpha}{\partial x^{N-1}} \; = \; 0 \tag{390}$$

Since the functions ϕ_α and the derivatives are known, this is a set of N linear equations for N unknowns and can be written as a matrix equation

$$\begin{pmatrix} \phi_1 & \phi_2 & \dots & \dots & \phi_N \\ \frac{\partial \phi_1}{\partial x} & \frac{\partial \phi_2}{\partial x} & \dots & \dots & \frac{\partial \phi_N}{\partial x} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \frac{\partial^{N-1} \phi_1}{\partial x^{N-1}} & \frac{\partial^{N-1} \phi_2}{\partial x^{N-1}} & \dots & \dots & \frac{\partial^{N-1} \phi_N}{\partial x^{N-1}} \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \\ . \\ . \\ k_N \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ . \\ . \\ 0 \end{pmatrix} \tag{391}$$

This matrix equation has a solution given by

$$\begin{pmatrix} k_1 \\ k_2 \\ . \\ . \\ k_N \end{pmatrix} = \begin{pmatrix} \phi_1 & \phi_2 & \dots & \dots & \phi_N \\ \frac{\partial \phi_1}{\partial x} & \frac{\partial \phi_2}{\partial x} & \dots & \dots & \frac{\partial \phi_N}{\partial x} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \frac{\partial^{N-1} \phi_1}{\partial x^{N-1}} & \frac{\partial^{N-1} \phi_2}{\partial x^{N-1}} & \dots & \dots & \frac{\partial^{N-1} \phi_N}{\partial x^{N-1}} \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ 0 \\ . \\ . \\ 0 \end{pmatrix} \tag{392}$$

The matrix has an inverse if it's determinant is non-zero. In this case, the only solution consists of the trivial solution $k_n \; = \; 0$ for all n. If the determinant is non-zero the set of functions ϕ_n are linearly independent.

If the determinant is zero, then non-zero solutions exist for k_n for some n and the set of functions ϕ_n are linearly dependent.

The determinant of the N by N matrix composed of the N functions and their first $N-1$ derivatives is known as the Wronskian, W

$$W \;=\; \begin{vmatrix} \phi_1 & \phi_2 & \ldots & \ldots & \phi_N \\ \frac{\partial \phi_1}{\partial x} & \frac{\partial \phi_2}{\partial x} & \ldots & \ldots & \frac{\partial \phi_N}{\partial x} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \frac{\partial^{N-1} \phi_1}{\partial x^{N-1}} & \frac{\partial^{N-1} \phi_2}{\partial x^{N-1}} & \ldots & \ldots & \frac{\partial^{N-1} \phi_N}{\partial x^{N-1}} \end{vmatrix} \tag{393}$$

As examples one can find that the functions $\sin x$ and $\cos x$ are linearly independent as

$$\begin{vmatrix} \sin x & \cos x \\ \cos x & -\sin x \end{vmatrix} \;=\; -1 \tag{394}$$

which is non zero. Although, $\sin x$ is related to $\cos x$ via

$$\sin x \;=\; \pm \sqrt{(\,1 \;-\; \cos^2 x\,)} \tag{395}$$

this relation is non-linear.

It is easy to show that the functions $\exp x$, $\exp -x$ and $\cosh x$ are linearly dependent as

$$\begin{vmatrix} \exp x & \exp -x & \cosh x \\ \exp x & -\exp -x & \sinh x \\ \exp x & \exp -x & \cosh x \end{vmatrix} \;=\; 0 \tag{396}$$

which shows that it is possible to find a linear relationship between the functions such as

$$\exp x \;+\; \exp -x \;=\; 2\;\cosh x \tag{397}$$

The concept of linear dependence and linear independence is common to the theory of vectors in d-dimensional spaces. A set of vectors $\hat{\phi}_n$ are linearly independent if non-zero constants k_n can not be found such that

$$\sum_{n=1}^{n=d} k_n\;\hat{\phi}_n \;=\; 0 \tag{398}$$

In such cases, the set of $\hat{\phi}_n$ can be used as a basis for the d-dimensional space, in that an arbitrary vector $\overrightarrow{\Phi}$ can be expanded as

$$\overrightarrow{\Phi} \;=\; \sum_{n=1}^{n=d} C_n\;\hat{\phi}_n \tag{399}$$

That is, the vector $\overrightarrow{\Phi}$ and the set of basis vectors are form a linearly dependent set. To see the relation we should identify $k_{d+1} \ = \ 1$ as the multiplier of $\hat{\phi}_{d+1} \ = \ \overrightarrow{\Phi}$ and $k_n \ = \ C_n$ as the multipliers for the rest of the $\hat{\phi}_n$. Thus, the k_n or C_n can be considered as the components of the vector and the set of linearly independent $\hat{\phi}_n$ as providing the basis vectors.

This is to be considered as analogous to he expansion of an arbitrary polynomial $\Phi(x)$ of degree d in terms of the mononomials $\phi_n \ = \ x^n$ so that

$$\begin{aligned} \Phi(x) &= \sum_{n=1}^{n=d} C_n \ x^n \\ &= \sum_{n=1}^{n=d} C_n \ \phi_n \end{aligned} \tag{400}$$

where the set of linearly independent mononomials can be considered as forming the basis functions ϕ_n.

4.3.1 Linearly Independent Solutions

For an N-th order linear differential equation one expects that there exist N linearly independent solutions ϕ_n. The general solution is expected to be able to be written as a linear superposition of the N linearly independent solutions as

$$\phi \ = \ \sum_{n=1}^{n=N} C_n \ \phi_n \tag{401}$$

where the N arbitrary coefficients C_n roughly correspond to the information contained in the N constants of integration. If a set of appropriate boundary conditions are applied, the coefficients C_n can be determined such that the solution ϕ satisfies the boundary conditions.

Given an N-th order differential equation for ϕ

$$\sum_{n=0}^{n=N} a_n(x) \ \frac{\partial^n \phi}{\partial x^n} \ = \ 0 \tag{402}$$

then it is easy to show that N is the maximum number of linearly independent solutions. This can be proved by contradiction. Assume that there are $N+1$ or more linearly independent solutions represented by the set of $N+1$ functions

ϕ_n. Then form the Wronskian as the determinant of an $N+1$ by $N+1$ matrix

$$W = \begin{vmatrix} \phi_1 & \phi_2 & \dots & \dots & \phi_{N+1} \\ \frac{\partial\phi_1}{\partial x} & \frac{\partial\phi_2}{\partial x} & \dots & \dots & \frac{\partial\phi_{N+1}}{\partial x} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \frac{\partial^N\phi_1}{\partial x^N} & \frac{\partial^N\phi_2}{\partial x^N} & \dots & \dots & \frac{\partial\phi_{N+1}}{\partial x} \end{vmatrix} \tag{403}$$

On substituting from the differential equation for the N-th order derivative one finds the Wronskian is zero as the last row can be expressed as a linear combination of the $(N-1)$ higher rows. Hence, the set of $N+1$ solutions are linearly dependent contrary to our initial assumption. Thus, at most there are only N linearly independent solutions of the general N-th order differential equation.

4.3.2 Abel's Theorem

If there are two linearly independent solutions ϕ_1 and ϕ_2 of the second order differential equation

$$\frac{\partial^2\phi}{\partial x^2} + p(x)\,\frac{\partial\phi}{\partial x} + q(x)\,\phi = 0 \tag{404}$$

then the Wronskian W may be a function of x

$$W = \begin{vmatrix} \phi_1 & \phi_2 \\ \frac{\partial\phi_1}{\partial x} & \frac{\partial\phi_2}{\partial x} \end{vmatrix} = \phi_1\,\frac{\partial\phi_2}{\partial x} - \phi_2\,\frac{\partial\phi_1}{\partial x}$$

Abel's theorem states that the x dependence of the Wronskian $W(x)$ is determined from the differential equation through $p(x)$. Taking the derivative of the Wronskian one finds

$$\begin{aligned} \frac{\partial W}{\partial x} &= \frac{\partial}{\partial x}\left(\phi_1\,\frac{\partial\phi_2}{\partial x}\right) - \frac{\partial}{\partial x}\left(\phi_2\,\frac{\partial\phi_1}{\partial x}\right) \\ &= \phi_1\,\frac{\partial^2\phi_2}{\partial x^2} - \phi_2\,\frac{\partial^2\phi_1}{\partial x^2} \end{aligned} \tag{405}$$

On substituting the differential equation

$$\frac{\partial^2\phi}{\partial x^2} = -\,p(x)\,\frac{\partial\phi}{\partial x} - q(x)\,\phi \tag{406}$$

for the second derivatives one obtains

$$\begin{aligned} \frac{\partial W}{\partial x} &= -\,\phi_1\,p(x)\,\frac{\partial\phi_2}{\partial x} + \phi_2\,p(x)\,\frac{\partial\phi_1}{\partial x} \\ &= -\,p(x)\,W(x) \end{aligned} \tag{407}$$

This can be integrated to yield

$$W(x) \;=\; W(a)\;\exp\left[\;-\;\int_a^x\;dt\;p(t)\;\right] \tag{408}$$

Thus, if $W(a)$ is non-zero because the solutions are linearly independent then as long as $p(t)$ is not complex then $W(x)$ is always non-zero and the solutions are always linearly independent. For linearly independent solutions the Wronskian is determined up to an arbitrary multiplicative constant as the solutions are only determined up to a multiplicative constant. Furthermore, if $p(x) \;=\; 0$ then the Wronskian is simply a constant.

4.3.3 Other Solutions

Given of $N-1$ linearly independent solutions ϕ_n and the Wronskian W of an N-th order differential one can reduce the order of the equation to an $N-1$-th ordinary differential equation. This is most useful for the case where $N \;=\; 2$. In this case given a solution ϕ_1 and a Wronskian W one can find a second solution ϕ_2. Starting with $W(x)$

$$\begin{aligned}
W \;&=\; \phi_1\,\frac{\partial\phi_2}{\partial x}\;-\;\phi_2\,\frac{\partial\phi_1}{\partial x} \\
&=\; (\;\phi_1(x)\;)^2\left(\frac{\frac{\partial\phi_2}{\partial x}}{\phi_1}\;-\;\frac{\phi_2}{\phi_1^2}\,\frac{\partial\phi_1}{\partial x}\right) \\
&=\; (\;\phi_1(x)\;)^2\,\frac{\partial}{\partial x}\left(\frac{\phi_2}{\phi_1}\right)
\end{aligned} \tag{409}$$

Thus,

$$\frac{\partial}{\partial x}\left(\frac{\phi_2}{\phi_1}\right) \;=\; \frac{W(x)}{\phi_1(x)^2} \tag{410}$$

and so one obtains the second solution of the second order differential equation through one integration

$$\phi_2(x) \;=\; \phi_1(x)\int^x dt\;\frac{W(t)}{\phi_1(t)^2} \tag{411}$$

Since the Wronskian is known up to an arbitrary multiplicative constant the second solution is also determined up to a multiplicative constant.

A simple example is given by the solution of

$$\frac{\partial^2\phi}{\partial x^2}\;+\;\phi\;=\;0 \tag{412}$$

which on knowing one solution $\phi_1 = \sin x$ one can find a second solution. Since $p(x) = 0$ the Wronskian is just a constant W, hence

$$\begin{aligned}\phi_2(x) &= \sin x \int^x \frac{dt\ W}{\sin^2 t} \\ &= W\ \sin x \left(- \cot x \right) \\ &= - W\ \cos x \end{aligned} \tag{413}$$

Thus, $\cos x$ is a second linearly independent solution of the equation.

5 Stürm Liouville Theory

Consider the Stürm-Liouville eigenvalue equation for the unknown function ϕ in the form

$$a_2(x)\,\frac{\partial^2\phi}{\partial x^2} \;+\; a_1(x)\,\frac{\partial\phi}{\partial x} \;+\; a_0(x)\,\phi \;=\; \lambda\,u(x)\,\phi \tag{414}$$

where λ is an unknown number, and all the functions are defined on an interval between $x = a$ and $x = b$. The solutions are expected to satisfy boundary conditions. The functions $a_0(x)$ and $u(x)$ are non zero in the interval (a,b). For convenience we shall consider the case where $u(x) > 0$. The case of negative $u(x)$ can be treated by changing the definition of λ to accommodate the sign change. The number λ is regarded as unknown and is called the eigenvalue. The possible values of the eigenvalue are found from the condition that a solution $\phi(x)$ exists which satisfies the boundary conditions. When the solutions $\phi_\lambda(x)$ are found to exist the eigenvalues have particular values. The set of eigenvalues may take on either discrete or continuous values. The function $\phi_\lambda(x)$ is called an eigenfunction, and each eigenfunction corresponds to a particular eigenvalue λ. Sometimes a particular eigenvalue λ may correspond to two or more different eigenfunctions. In this case, the eigenvalue is said to be degenerate. Any linear combination of the degenerate eigenfunctions is also an eigenfunction with the same eigenvalue. The number of linearly independent eigenfunctions corresponding to this eigenvalue is the degeneracy of the eigenvalue.

It is usual to re-write the Stürm-Liouville equation in the form

$$\frac{\partial\phi}{\partial x}\left(\,p(x)\,\frac{\partial\phi}{\partial x}\,\right) \;+\; q(x)\,\phi \;=\; \lambda\,w(x)\,\phi \tag{415}$$

which is equivalent to

$$p(x)\,\frac{\partial^2\phi}{\partial x^2} \;+\; \frac{\partial p(x)}{\partial x}\,\frac{\partial\phi}{\partial x} \;+\; q(x)\,\phi \;=\; \lambda\,w(x)\,\phi \tag{416}$$

Hence, we can identify

$$\begin{aligned}\frac{a_1(x)}{a_2(x)} &= \frac{\frac{\partial p}{\partial x}}{p(x)}\\ \frac{a_0(x)}{a_1(x)} &= \frac{q(x)}{p(x)}\\ \frac{u(x)}{a_2(x)} &= \frac{w(x)}{p(x)}\end{aligned} \tag{417}$$

Thus, we can find $p(x)$ by integration between two limits of integration in the interval

$$\ln p(t) \Big|_a^x = \int_a^x dt \, \frac{a_1(t)}{a_2(t)} \tag{418}$$

or

$$p(x) = p(a) \, \exp \left[\int_a^x dt \, \frac{a_1(t)}{a_2(t)} \right] \tag{419}$$

It is because of this that we required that $a_2(t)$ be non-vanishing in (a, b).

A well known example of a Stürm-Liouville eigenvalue equation is provided by

$$\frac{\partial^2 \phi}{\partial x^2} = \lambda \, \phi \tag{420}$$

on the interval $(0, L)$ where the boundary conditions are that the functions ϕ must vanish at the boundaries

$$\phi(0) = \phi(L) = 0 \tag{421}$$

In this case, we see that $p(x) = w(x) = 1$ and $q(x) = 0$. For each arbitrary real value of λ one can find two solutions of the differential equation which do not satisfy the two boundary conditions

$$f_{\pm\lambda}(x) = \exp \left[\pm \sqrt{\lambda} \, x \right] \tag{422}$$

The functions $f_{\pm\lambda}(x)$ can be combined to yield functions $\phi_\lambda(x)$ that satisfies the boundary condition at $x = 0$ as

$$\phi_\lambda(x) = \exp \left[+ \sqrt{\lambda} \, x \right] - \exp \left[- \sqrt{\lambda} \, x \right] \tag{423}$$

so $\phi(0) = 0$. The second boundary condition is not satisfied for arbitrary values of λ as

$$\phi_\lambda(L) = 2 \, \sinh \sqrt{\lambda} \, L \tag{424}$$

which is non-zero for real values of $\sqrt{\lambda}$ or positive λ. However, for negative values of λ one finds that this equation can have solutions

$$\phi_\lambda(L) = 2 \, i \, \sin \sqrt{|\lambda|} \, L \tag{425}$$

for values of λ such that

$$\sqrt{|\lambda|} \, L = n \, \pi \tag{426}$$

for integer n. The eigenfunctions can be written as

$$\phi_n(x) = \sin \frac{n \, \pi \, x}{L} \tag{427}$$

and the eigenvalues form a discrete set of negative numbers

$$\lambda_n \; = \; - \left(\frac{n \; \pi}{L} \right)^2 \tag{428}$$

Thus, the values of the eigenvalues λ_n are determined by the condition that $\phi_n(x)$ exists and satisfy the boundary conditions.

Homework:

Find the general solutions of the above equation, using the Frobenius method, without imposing boundary conditions.

If boundary conditions are applied, can the series be used directly to find the possible set of eigenvalues?

Example:

A second example is given by the Stürm-Liouville eigenvalue equation

$$\frac{\partial^2 \phi}{\partial x^2} \; - \; x^2 \; \phi \; = \; \lambda \; \phi \tag{429}$$

subject to the boundary conditions that $\phi(x)$ vanishes in the limits $x \; \rightarrow \; \pm \; \infty$. Here $p(x) \; = \; w(x) \; = 1$ and $q(x) \; = \; - \; x^2$. The eigenvalue equation can be solved near the origin by the Frobenius method. The indicial equation is simply

$$\alpha \; (\; \alpha \; - \; 1 \;) \; = \; 0 \tag{430}$$

and thus the solutions have the form of either

$$\phi_0 \; = \; \sum_{n=0} C_n \; x^n \tag{431}$$

or

$$\phi_1 \; = \; x \; \sum_{n=0} C_n \; x^n \tag{432}$$

Furthermore, from the recursion relation one finds that the odd coefficients vanish and that the even coefficients must satisfy

$$n \; (\; n \; - \; 1 \;) \; C_n \; - \; C_{n-4} \; = \; \lambda \; C_{n-2} \tag{433}$$

Thus, the solutions are either even $\phi_0(-x) \; = \; \phi_0(x)$ or odd $\phi_1(-x) \; = \; - \; \phi_1(x)$ in x. The Frobenius method can not be expected to converge in the limits $x \; \rightarrow \; \pm \; \infty$. Thus, we need to examine the asymptotic large x behavior. In this case, one can neglect the eigenvalue compared to the x^2 term. The approximate equation is given by

$$\frac{\partial^2 \phi}{\partial x^2} \; - \; x^2 \; \phi \; \sim \; 0 \tag{434}$$

This equation can be approximately factorized as

$$\left(\frac{\partial}{\partial x} \; - \; x \right) \left(\frac{\partial}{\partial x} \; + \; x \right) \phi \; \sim \; 0 \tag{435}$$

Then, we can expect that

$$\frac{\partial \phi}{\partial x} \; + \; x \; \phi \; \sim \; 0 \tag{436}$$

so that the asymptotic large x variation is given by

$$\phi(x) \; \sim \; \exp \left[\; - \; \frac{x^2}{2} \; \right] \tag{437}$$

which satisfies the boundary conditions.

Thus, we may look for solutions of the forms of power series in increasing powers of x^2 times a decreasing exponential function. That is we either have the even function

$$\phi_0(x) \; = \; \sum_{n=0} P_{2n} \; x^{2n} \; \exp \left[\; - \; \frac{x^2}{2} \; \right] \tag{438}$$

or the odd function

$$\phi_1(x) \; = \; x \; \sum_{n=0} P_{2n} \; x^{2n} \; \exp \left[\; - \; \frac{x^2}{2} \; \right] \tag{439}$$

Using this form we can determine the power series with coefficients P_n by using the Frobenius method.

To simplify the solution we shall substitute $\phi(x) \; = \; p(x) \; \exp \left[\; - \; \frac{x^2}{2} \; \right]$ into the equation and after cancelling out the common exponential factor one finds

$$\frac{\partial^2 p(x)}{\partial x^2} \; - \; 2 \; x \; \frac{\partial p(x)}{\partial x} \; - \; p(x) \; = \; \lambda \; p(x) \tag{440}$$

Then the indicial equation for $p(x)$ is

$$\alpha \; (\; \alpha \; - \; 1 \;) \; = \; 0 \tag{441}$$

The recursion relation becomes

$$(\; 2 \; n + 2 + \alpha \;) \; (\; 2 \; n + 1 + \alpha \;) \; P_{2n+2} - (\; 2 \; n + 2 \; \alpha + \lambda + 1 \;) \; P_{2n} \; = \; 0 \tag{442}$$

For large n, such $n \gg \lambda$ the coefficients are related by

$$P_{2n+2} \sim \frac{P_{2n}}{2\,n} \tag{443}$$

so

$$P_{2n} \sim \frac{P_0}{2^n\,(n)!} \tag{444}$$

In this case the series can be approximately summed to yield

$$p(x) \sim p_0 \exp\left[+ \frac{x^2}{2} \right] \tag{445}$$

which diverges exponentially. Thus, we note that the recursion relation for P_n must truncate at some finite value of N in order that the solution has the correct exponentially decaying behavior for asymptotically large values of x. However, the series only truncates for particular values of λ. The value of λ can be determined by examining the recursion relation of the largest term in the polynomial. Physically this is because the term proportional to x^N, and the exponential factor, dominates the function $\phi(x)$ at large x. Hence, we find that if $P_{2N+2} = 0$ then

$$\lambda_N = -\,(\,2\,N + 2\,\alpha + 1\,) \tag{446}$$

Thus, the value of λ is determined by the highest power in the finite polynomial.

In the above two examples, the set of eigenfunctions share the common property that

$$\int_a^b dx\;\phi_n(x)\;w(x)\;\phi_m(x) = 0 \tag{447}$$

where $\lambda_n \neq \lambda_m$. This is a general property of a set of eigenfunctions of the Stürm-Liouville equation. This theorem implies that the successive eigenfunctions change sign an increasing number of times. That is the eigenfunctions can be classified by their number of nodes.

Homework:

Show that the set eigenfunctions

$$\phi_m(x) = \sqrt{\frac{2}{L}}\;\sin\frac{n\,\pi\,x}{L} \tag{448}$$

obey the equation

$$\int_0^L dx\;\phi_m(x)\;\phi_n(x) = 0 \tag{449}$$

if $\lambda_m \neq \lambda_n$.

5.1 Degenerate Eigenfunctions

If more than one eigenfunction corresponds to the same eigenvalue, the eigenvalue is said to be degenerate. The number of linearly independent eigenfunctions are the degeneracy of the eigenvalue. The set of eigenfunctions are said to be degenerate.

Example:

An example of degenerate eigenfunctions is given by the solutions of

$$\frac{\partial \phi}{\partial x} \; = \; - \; k^2 \; \phi \tag{450}$$

without boundary conditions. The eigenvalue $- \; k^2$ is a real negative number and is twofold degenerate, as it corresponds to the two linearly independent eigenfunctions

$$\begin{aligned} \phi_1(x) \; &= \; \sin \; k \; x \\ \phi_2(x) \; &= \; \cos \; k \; x \end{aligned} \tag{451}$$

Since any linear combinations of these are also eigenfunctions, one finds that the complex functions

$$\begin{aligned} \phi'_1(x) \; &= \; \exp \left[\; + \; i \; k \; x \; \right] \\ \phi'_2(x) \; &= \; \exp \left[\; - \; i \; k \; x \; \right] \end{aligned} \tag{452}$$

are also eigenfunctions corresponding to the same eigenvalue.

5.2 The Inner Product

The inner product of two functions $\Psi(x)$ and $\Phi(x)$ is defined as the weighted integral

$$\int_a^b dx \; \Psi^*(x) \; w(x) \; \Phi(x) \tag{453}$$

Two functions are said to be orthogonal if their inner product is zero. The inner product of a function with itself is the normalization of the function. If $w(x)$ is a real, non-zero, function the normalization is a real number. It is customary to demand that all functions $\Psi(x)$ are normalized to unity. Thus, we insist that

$$\int dx \; \Psi^*(x) \; w(x) \; \Psi(x) \; = \; 1 \tag{454}$$

A function can always be normalized as, according to the principle of linear superposition it can always be multiplied by a constant complex number C. This appears as a factor $| C |^2$ in the inner product. The magnitude of the real number $| C |^2$ is chosen such that the functions are normalized.

This inner product is analogous to the scalar product of two vectors

$$\vec{A} \, . \, \vec{B} \tag{455}$$

which is usually evaluated in terms of its components. That is on expanding the vector in terms of the basis vectors $\hat{e}_n$ via

$$\vec{A} \; = \; \sum_{n=1}^{d} A_n \, \hat{e}_n \tag{456}$$

and noting that the basis vectors form an orthogonal set so that

$$\hat{e}_n \, . \, \hat{e}_m \; = \; \delta_{n,m} \tag{457}$$

one has

$$\vec{A} \, . \, \vec{B} \; = \; \sum_{n=1}^{d} A_n \, B_n \tag{458}$$

The inner product of two functions can be evaluated in the same way. First the functions are expanded in terms of the basis functions $\phi_n(x)$ with components A_n and B_n

$$\Phi(x) \; = \; \sum_{n=1}^{d} A_n \, \phi_n(x) \tag{459}$$

and

$$\Psi(x) \; = \; \sum_{n=1}^{d} B_n \, \phi_n(x) \tag{460}$$

Then, if the basis functions form an orthonormal set so that

$$\int_a^b dx \; \phi^*_n(x) \; w(x) \; \phi_m(x) \; = \; \delta_{n,m} \tag{461}$$

then the inner product is evaluated as

$$\begin{aligned} \int_a^b dx \; \Psi^*(x) \; w(x) \; \Phi(x) \; &= \; \sum_{n,m} B^*_n \, \delta_{n,m} \, A_m \\ &= \; \sum_n B^*_n \, A_n \end{aligned} \tag{462}$$

which is similar to the scalar product of two vectors.

5.3 Orthogonality of Eigenfunctions

The orthogonality property of eigenfunctions of a Stürm-Liouville equation can be derived by examining the properties of two solutions, ϕ_1 and ϕ_2 corresponding to the respective eigenvalues λ_1 and λ_2. Then

$$\frac{\partial}{\partial x} \left(p(x) \frac{\partial \phi_1}{\partial x} \right) + q(x) \phi_1 = \lambda_1 w(x) \phi_1 \tag{463}$$

and

$$\frac{\partial}{\partial x} \left(p(x) \frac{\partial \phi_2}{\partial x} \right) + q(x) \phi_2 = \lambda_2 w(x) \phi_2 \tag{464}$$

The complex conjugate of the second equation is just

$$\frac{\partial}{\partial x} \left(p(x) \frac{\partial \phi_2^*}{\partial x} \right) + q(x) \phi_2^* = \lambda_2^* w(x) \phi_2^* \tag{465}$$

as $p(x)$, $q(x)$ and $w(x)$ are real. Pre-multiplying the above equation by $\phi_1(x)$ and pre-multiplying the first equation by the complex conjugate $\phi_2^*(x)$ and subtracting one obtains

$$\phi_1(x) \frac{\partial}{\partial x} \left(p(x) \frac{\partial \phi_2^*(x)}{\partial x} \right) - \phi_2^*(x) \frac{\partial}{\partial x} \left(p(x) \frac{\partial \phi_1(x)}{\partial x} \right) = (\lambda_2^* - \lambda_1) \phi_1(x) w(x) \phi_2^*(x) \tag{466}$$

In this the terms proportional to $q(x)$ have cancelled identically. Taking the above equation and integrating over the interval between a and b, one has

$$\int_a^b dx \; \phi_1(x) \frac{\partial}{\partial x} \left(p(x) \frac{\partial \phi_2^*(x)}{\partial x} \right) - \phi_2^*(x) \frac{\partial}{\partial x} \left(p(x) \frac{\partial \phi_1(x)}{\partial x} \right)$$
$$= (\lambda_2^* - \lambda_1) \int_a^b dx \; \phi_2^*(x) \, w(x) \, \phi_1(x) \tag{467}$$

where the term on the right hand side is recognized as the inner product. The term on the left hand side is evaluated by splitting into two parts and integrating each term by parts. The terms of the form

$$\frac{\partial \phi_2^*}{\partial x} \, p(x) \, \frac{\partial \phi_1}{\partial x} \tag{468}$$

cancel identically, leaving only the boundary terms

$$\phi_1(x) \, p(x) \frac{\partial \phi_2^*(x)}{\partial x} \Big|_a^b - \phi_2^*(x) \, p(x) \frac{\partial \phi_1(x)}{\partial x} \Big|_a^b$$
$$= (\lambda_2^* - \lambda_1) \int_a^b dx \; \phi_2^*(x) \, w(x) \, \phi_1(x) \tag{469}$$

However, on either using boundary conditions such that the functions vanish on the boundaries

$$\phi(a) \; = \; \phi(b) \; = \; 0 \tag{470}$$

or boundary conditions where the derivative vanishes at the boundaries

$$\frac{\partial \phi}{\partial x} \bigg|_a \; = \; \frac{\partial \phi}{\partial x} \bigg|_b \; = \; 0 \tag{471}$$

then one finds that

$$(\; \lambda_2^* \; - \; \lambda_1 \;) \int_a^b dx \; \phi_2^*(x) \; w(x) \; \phi_1(x) \; = \; 0 \tag{472}$$

This is the central result. It proves the theorem. First if $\phi_2 \; = \; \phi_1$ then the normalization integral is finite and non-zero, so $\lambda_1^* \; = \lambda_1$. Thus, the eigenvalues of the Stürm-Liouville equation are real. Using this we have

$$(\; \lambda_2 \; - \; \lambda_1 \;) \int_a^b dx \; \phi_2^*(x) \; w(x) \; \phi_1(x) \; = \; 0 \tag{473}$$

Thus, if $\lambda_1 \; \neq \; \lambda_2$ one must have

$$\int_a^b dx \; \phi_2^*(x) \; w(x) \; \phi_1(x) \; = \; 0 \tag{474}$$

Thus, the eigenfunctions belonging to different eigenvalues are orthogonal. As we shall see later, if an eigenvalue is degenerate one can use the properties of the degeneracy to construct a set of mutually orthogonal eigenfunctions corresponding to the same eigenvalue. The maximum number of the mutually orthogonal functions is equal to the degeneracy. This means that the eigenfunctions of the Stürm-Liouville equation can be used to create a very convenient set of basis functions, in function space.

5.4 Orthogonality and Linear Independence

Given a set of mutually orthogonal functions $\phi_n(x)$, one can easily show that they are linearly independent. For if one has

$$\sum_n k_n \; \phi_n(x) \; = \; 0 \tag{475}$$

then one can take the inner product with any one of them, say $\phi_m(x)$, to find

$$\sum_n k_n \int_a^b dx \; \phi_m^*(x) \; w(x) \; \phi_n(x) \; = \; 0$$

$$\begin{aligned} \sum_n k_n \, \delta_{n,m} &= 0 \\ k_m &= 0 \end{aligned} \tag{476}$$

Thus, the only solution of the equation is that all the k_m are identically zero. Hence, any set of mutually orthogonal functions are linearly independent.

5.5 Gram-Schmidt Orthogonalization

If we have a set of eigenfunctions of a Stürm-Liouville equation, some of the eigenvalues might be degenerate. The eigenfunctions corresponding to the same eigenvalue generally might not be orthogonal. The Gram-Schmidt orthogonalization process can be used to construct a set of mutually orthogonal eigenfunctions. Consider the set of normalized eigenfunctions $\phi_1(x)$, $\phi_2(x)$, $\phi_3(x)$,....corresponding to an eigenvalue λ. The method produces a set of orthogonal and normalized eigenfunctions $\psi_1(x)$, $\psi_2(x)$, $\psi_3(x)$,.... The first eigenfunction is chosen to be

$$\psi_1(x) = \phi_1(x) \tag{477}$$

The second eigenfunction is to be constructed from $\phi_2(x)$. However, since the inner product with $\phi_1(x)$ is non-zero, there is a component of $\phi_2(x)$ which is parallel to $\phi_1(x)$. Thus, we can subtract the component of $\phi_2(x)$ which is parallel to $\phi_1(x)$ and then normalize the function by multiplying by a constant C_2

$$\psi_2(x) = C_2 \left(\phi_2(x) - \psi_1(x) \left(\int_a^b dt \; \psi_1^*(t) \; w(t) \; \phi_2(t) \right) \right) \tag{478}$$

This is an eigenfunction corresponding to the eigenvalue λ as the eigenvalue equation is linear. The constant C_2 or rather $| \, C_2 \, |^2$ in $\psi_2(x)$ is determined from the normalization condition

$$\int_a^b dx \; \psi_2^*(x) \; w(x) \; \psi_2(x) = 1 \tag{479}$$

It can be seen that $\psi_2(x)$ is orthogonal to $\psi_1(x)$ by direct substitution in

$$\int_a^b dx \; \psi_1^*(x) \; w(x) \; \psi_2(x) = 0 \tag{480}$$

and using the fact that $\psi_1(x)$ is normalized to unity

$$\int_a^b dx \; \psi_1^*(x) \; w(x) \; \psi_1(x) = 1 \tag{481}$$

The next eigenfunction $\psi_3(x)$ is constructed from $\phi_3(x)$ by orthogonalizing it to $\psi_2(x)$ and $\psi_1(x)$. That is, we write

$$\psi_3(x) \;=\; C_3 \left(\phi_3(x) - \psi_2(x) \int_a^b dt\, \psi_2^*(t)\, w(t)\, \phi_3(t) - \psi_1(x) \int_a^b dt\, \psi_1^*(t)\, w(t)\, \phi_3(t) \right) \tag{482}$$

The eigenfunction $\psi_3(x)$ has no components parallel to $\psi_1(x)$ or to $\psi_2(x)$, since $\psi_2(x)$ and $\psi_1(x)$ have been normalized previously. The constant C_3 is then determined from the normalization condition

$$\int_a^b dx\; \psi_3^*(x)\; w(x)\; \psi_3(x) \;=\; 1 \tag{483}$$

This procedure is iterated, by orthogonalizing $\phi_n(x)$ to all the previous orthonormal functions $\psi_m(x)$ for $n \;>\; m$

$$\psi_n(x) \;=\; C_n \left(\phi_n(x) \;-\; \sum_{m=1}^{m=n-1} \psi_m(x) \int_a^b dt\; \psi_m^*(t)\; w(t)\; \phi_n(t) \right) \tag{484}$$

and then determining the normalization $\mid C_n \mid^2$ from the condition

$$\int_a^b dx\; \psi_n^*(x)\; w(x)\; \psi_n(x) \;=\; 1 \tag{485}$$

If the set of eigenfunctions is composed of M functions corresponding to the same eigenvalue this procedure only has to be iterated M times.

The method does not have to be applied to a set of linearly independent eigenfunctions. If it is applied to a set of M linearly dependent eigenfunctions, where $M \;>\; N$ and the degeneracy of the eigenvalue is N, then the Gram-Schmidt orthogonalization procedure will lead to a maximum of N orthonormal functions. The way this happens is that if the n-th initial eigenfunction $\phi_n(x)$ is linearly dependent on the previous set of initial eigenfunctions, the orthogonalization procedure will lead to $\psi_n(x) \;=\; 0$.

Thus, it is always possible to construct a set of orthonormal basis functions from the set of Sturm-Liouville eigenfunctions. We shall always assume that the set of eigenfunctions of a Stürm-Liouville equation have been chosen as an orthonormal set.

As an example of Gram-Schmitt orthogonalization, consider the set of polynomials, $\phi_n(x)$ 1, x, x^2, x^3, ... defined on the real interval between $(-1, 1)$ and with weight factor one. Since the interval and the weighting factor is evenly distributed around $x \;=\; 0$, we shall see that the orthogonal polynomials $\psi_n(x)$ are either even or odd, because the even polynomials are automatically orthogonal with the odd polynomials.

The method starts with normalizing $\phi_0(x)$ to yield $\psi_0(x)$ as

$$\psi_0(x) \;=\; C_0\;\phi_0(x) \;=\; C_0\;1 \tag{486}$$

The normalization constant C_0 is determined from

$$\begin{aligned} 1 &= \int_{-1}^{1} dx \mid \psi_0(x) \mid^2 \\ &= \mid C_0 \mid^2 \int_{-1}^{1} dx \mid \phi_0(x) \mid^2 \\ &= \mid C_0 \mid^2 \int_{-1}^{1} dx \\ &= \mid C_0 \mid^2 \, 2 \end{aligned} \tag{487}$$

or $\mid C_0 \mid \;=\; \frac{1}{\sqrt{2}}$. Thus, since all our quantities are real we might as well choose all the phases to be real and have

$$\psi_0(x) \;=\; \frac{1}{\sqrt{2}} \tag{488}$$

The lowest order normalized polynomial $\psi_0(x)$ is an even function of x.

Proceeding to construct the next orthogonal polynomial from $\phi_1(x) \;=\; x$, one has

$$\begin{aligned} \psi_1 &= C_1 \left(\phi_1(x) \;-\; \psi_0(x) \int_{-1}^{1} dt\;\phi_1(t)\;\psi_0(t) \right) \\ &= C_1 \left(x \;-\; \frac{1}{2} \int_{-1}^{1} dt\;t \right) \\ &= C_1\;x \end{aligned} \tag{489}$$

since x is odd and 1 is an even function of x. The normalization is found to be

$$C_1 \;=\; \sqrt{\frac{3}{2}} \tag{490}$$

Thus, the orthogonal polynomial $\psi_1(x) \;=\; \sqrt{\frac{3}{2}}\;x$ and is an odd function of x.

The next polynomial is constructed from $\phi_2(x) = x^2$ this is an even function and is automatically orthogonal to all odd functions of x. Thus, we only need to orthogonalize it against $\psi_0(x)$

$$\begin{aligned}
\psi_2 &= C_2 \left(x^2 - \frac{1}{\sqrt{2}} \int_{-1}^{1} dt \; t^2 \; \frac{1}{\sqrt{2}} \right) \\
&= C_2 \left(x^2 - \frac{1}{3} \right)
\end{aligned} \tag{491}$$

and C_2 is found as

$$C_2 = \sqrt{\frac{45}{8}} \tag{492}$$

The orthogonalization of the next polynomial is non-trivial. The process starts with $\phi_3(x) = x^3$, so one finds

$$\begin{aligned}
\psi_3(x) &= C_3 \left(x^3 - x \, \frac{3}{2} \int_{-1}^{1} dt \; t^4 \right) \\
&= C_3 \left(x^3 - \frac{3}{5} \, x \right)
\end{aligned} \tag{493}$$

etc.

This set of polynomials, apart from multiplicative constants, are the same as the set of Legendre polynomials $P_n(x)$

$$\begin{aligned}
P_0(x) &= 1 \\
P_1(x) &= x \\
P_2(x) &= \frac{3 \, x^2 - 1}{2} \\
P_3(x) &= \frac{5 \, x^3 - 3 \, x}{2} \\
P_n(x) &= \frac{(2n)! \; x^n + \ldots}{2^n \; (n!)^2}
\end{aligned} \tag{494}$$

The Legendre polynomials are normalized differently. The Legendre polynomials are normalized by insisting that $P_n(0) = 1$.

Homework:

Construct the first four orthogonal polynomials on the interval $(-\infty, +\infty)$ with weight factor $w(x) = \exp[- x^2]$. Show, by direct substitution in the equation, that these are the same polynomials $p(x)$ that occur in the eigenfunctions $\phi(x) = p(x) \exp[- \frac{x^2}{2}]$ of

$$\frac{\partial^2 \phi}{\partial x^2} - x^2 \phi = \lambda \phi \tag{495}$$

subject to the boundary conditions that the functions $\phi(x)$ vanishes in the limits $x \to \pm \infty$.

Homework:

Use the Gram-Schmidt procedure to obtain an orthonormal set of functions $\psi_n(x)$ from the degenerate eigenfunctions on the interval $(0, L)$

$$\begin{aligned} \phi_0(x) &= \exp \left[i \frac{n \pi x}{L} \right] \\ \phi_1(x) &= \cos \frac{n \pi x}{L} \\ \phi_2(x) &= \sin \frac{n \pi x}{L} \end{aligned} \tag{496}$$

Are the initial set $\phi_n(x)$ and the final set $\psi_n(x)$ linearly independent?

5.6 Completeness of Eigenfunctions

A set of linearly independent basis vectors in a vector space is defined to be complete if any vector in the space can be expressed as a linear combination of the basis vectors. The set of linearly independent basis vectors are incomplete if they are not complete. In the case of an incomplete set of basis vectors, then a linear combination of the basis vectors can only describe a subset of the vectors residing in the vector space.

In general the number of linearly independent basis vectors that form a complete set is equal to the dimension of the vector space. Also, if the basis is not complete, then the set of vectors that can be expressed as a linear combination of the incomplete basis set forms a vector space which has dimensions equal to the number of linearly independent basis vectors in the incomplete set.

For example, in two dimensions, any vector can be expanded in terms of a basis composed of two non-collinear unit vectors, $\hat{e}_1$ and $\hat{e}_2$. The non-collinearity condition is an expression of the linear independence of the basis vectors. Thus, any vector in the two dimensional plane can be written as

$$\vec{C} = C_1 \hat{e}_1 + C_2 \hat{e}_2 \tag{497}$$

For the two dimensional space, the set of the two basis vectors span the entire vector space and the basis is said to be complete. However, in a three dimensional vector space, the above combination only describes a two dimensional plane in the three dimensional volume. The two dimensional basis vectors do not span the three dimensional vector space and the set of two basis vectors is therefore said to be incomplete.

To be able to express any vector in the three dimensional volume, it is necessary to expand our basis by adding one non-coplanar unit vector. In this case, one can express a general vector as

$$\overrightarrow{A} = \sum_{i=1}^{3} A_i \hat{e}_i \tag{498}$$

In this case of a three dimensional vector space, the set of the three basis vectors is complete.

One can generalize the above definitions to a linearly independent set of basis functions. Thus, for example, given a set of mononomials $\phi_m = x^m$ which serve as basis functions one can describe polynomials as residing in the space of polynomials. Thus, with a complete set of basis functions 1, x and x^2, one can describe any polynomial in a three dimensional space as a linear combination of the three linearly independent basis mononomials

$$p(x) = p_0 + p_1 x + p_2 x^2 \tag{499}$$

where the expansion coefficients (p_0, p_1, p_2) are the "components" or "coordinates" of the polynomial.

Likewise, if we use the set of functions given by the eigenfunctions $\phi_m(x)$ of a Stürm-Liouville equation one can, if needed through the Gram-Schmidt process, construct an orthogonal set of basis functions. We shall always assume that the basis functions are orthonormal. Then a well behaved general function can be expressed as a linear combination of the basis functions

$$\Psi(x) = \sum_n C_n \phi_n(x) \tag{500}$$

By a general well behaved function, we require that our function satisfy the same boundary conditions as the basis functions. Also, the inner product of $\Psi(x)$ with itself must exist. These functions lie in the space C_2, i.e., the space of square integrable complex functions.

It is easy to show that a function $\Psi(x)$ in this space has a unique expansion in terms of the basis. That is the expansion coefficients are uniquely determined since by use of the inner product of $\Psi(x)$ with any one of the basis functions, say $\phi_m(x)$, one can uniquely determine the expansion coefficient C_m.

$$\begin{aligned}
\int_a^b dx \; \phi^*_m(x) \; w(x) \; \Psi(x) &= \sum_n C_n \int_a^b dx \; \phi^*_m(x) \; w(x) \; \phi_n(x) \\
&= \sum_n C_n \; \delta_{n,m} \\
&= C_m
\end{aligned} \tag{501}$$

That is, the expansion coefficient C_m is uniquely determined by the inner product of $\Psi(x)$ and $\phi_m(x)$.

For an arbitrary well behaved function $\Psi(x)$ one can write

$$\begin{aligned}
\Psi(x) &= \sum_n C_n \; \phi_n(x) \\
&= \sum_n \int_a^b dt \; \phi^*_n(t) \; w(t) \; \Psi(t) \; \phi_n(x) \\
&= \int_a^b dt \; \Psi(t) \; \sum_n \phi^*_n(t) \; w(t) \; \phi_n(x)
\end{aligned} \tag{502}$$

Thus, the delta function $\delta(x-t)$ is identified as the sum

$$\delta(x-t) = \sum_n \phi^*_n(t) \; w(t) \; \phi_n(x) \tag{503}$$

Alternatively, if the delta function $\delta(x-x')$ is expanded as

$$\delta(x-x') = \sum_n C_n \; \phi_n(x) \tag{504}$$

then we have

$$\int_a^b dx \; \phi^*_m(x) \; w(x) \; \delta(x-x') = C_m \tag{505}$$

which is simply evaluated as

$$C_m = \phi^*_m(x') \; w(x') \tag{506}$$

Thus, the Dirac delta function has an expansion of the form

$$\delta(x-x') = \sum_n \phi^*_n(x') \; w(x') \; \phi_n(x) \tag{507}$$

Since the delta function is symmetrical in x and x' one can also write

$$\delta(x - x') \; = \; \sum_n \; \phi_n^*(x') \; w(x) \; \phi_n(x) \tag{508}$$

because the left hand side is zero unless $x \; = \; x'$.

An example of the completeness relation is given by the doubly degenerate eigenfunctions

$$\phi_k(x) \; = \; \frac{1}{\sqrt{2 \; \pi}} \; \exp \left[\; + \; i \; k \; x \; \right] \tag{509}$$

of the eigenvalue equation

$$\frac{\partial^2 \phi}{\partial x^2} \; = \; - \; k^2 \; \phi \tag{510}$$

Degenerate eigenfunctions corresponding to positive and negative values of k. The completeness relation is given by

$$\delta(x - x') \; = \; \frac{1}{2 \; \pi} \; \int_{-\infty}^{+\infty} dk \; \exp \left[\; - \; i \; k \; x' \; \right] \; \exp \left[\; + \; i \; k \; x \; \right] \tag{511}$$

The integral can be evaluated by breaking it into two segments

$$\begin{aligned} \delta(x - x') \; = \; & \frac{1}{2 \; \pi} \; \int_0^{+\infty} dk \; \exp \left[\; - \; i \; k \; x' \; \right] \; \exp \left[\; + \; i \; k \; x \; \right] \\ & + \; \frac{1}{2 \; \pi} \; \int_0^{+\infty} dk \; \exp \left[\; + \; i \; k \; x' \; \right] \; \exp \left[\; - \; i \; k \; x \; \right] \end{aligned} \tag{512}$$

and then a convergence factor $\exp[\; - \; k \; \epsilon \;]$ is added and the limit $\epsilon \; \rightarrow \; 0$ is taken. Thus,

$$\begin{aligned} \delta(x - x') \; & = \; \frac{1}{2 \; \pi} \; \int_0^{+\infty} dk \; \exp \left[\; + \; i \; k \; (\; x \; - \; x' \;) \; - \; k \; \epsilon \; \right] \\ & \quad + \; \frac{1}{2 \; \pi} \; \int_0^{+\infty} dk \; \exp \left[\; - \; i \; k \; (\; x \; - \; x' \;) \; - \; k \; \epsilon \; \right] \\ & = \; - \; \frac{1}{2 \; \pi} \; \frac{1}{i \; (\; x \; - \; x' \;) \; - \; \epsilon} \; + \; \frac{1}{2 \; \pi} \; \frac{1}{i \; (\; x \; - \; x' \;) \; + \; \epsilon} \\ & = \; \frac{1}{\pi} \; \frac{\epsilon}{(\; x \; - \; x' \;)^2 \; + \; \epsilon^2} \end{aligned}$$

This agrees with the definition of the delta function as a limit of a series functions

$$\delta(x - x') \; = \; \lim_{\epsilon \rightarrow 0} \; \frac{1}{\pi} \; \frac{\epsilon}{(\; x \; - \; x' \;)^2 \; + \; \epsilon^2} \tag{513}$$

The theory of the Fourier integral transform consists of the expansion of an arbitrary function $f(x)$

$$f(x) \; = \; \int_{-\infty}^{+\infty} dk \; \tilde{f}(k) \; \frac{1}{\sqrt{2 \; \pi}} \; \exp \left[\; + \; i \; k \; x \; \right] \tag{514}$$

and the inverse transform

$$\tilde{f}(k) \; = \; \int_{-\infty}^{+\infty} dx \; \frac{1}{\sqrt{2 \; \pi}} \; \exp \left[\; - \; i \; k \; x \; \right] \; f(x) \tag{515}$$

Completeness of the eigenfunctions of a Stürm-Liouville equation has to be proved on a case by case basis. The proof usually consists of showing that the expansion in a series of eigenfunctions

$$\sum_{n=0}^{N} C_n \; \phi_n(x) \tag{516}$$

converges to $f(x)$, when $N \; \rightarrow \; \infty$ at each point x. However it is possible, by relaxing the condition for convergence at every point x, to extend the space of functions $f(x)$ to functions which have a finite number of discontinuities and do not satisfy the boundary conditions. In this case, one requires convergence in the mean. This just requires that

$$\lim_{N \; \rightarrow \; \infty} \int_a^b dx \; \left| \; f(x) \; - \; \sum_n^N \; C_n \; \phi_n(x) \; \right|^2 \; w(x) \; \rightarrow \; 0 \tag{517}$$

Since, for finite N one has

$$\begin{aligned} & \int_a^b dx \; \left| \; f(x) \; - \; \sum_n^N \; C_n \; \phi_n(x) \; \right|^2 \; w(x) \; \geq \; 0 \\ = \; & \int_a^b dx \; | \; f(x) \; |^2 \; w(x) \; - \; \sum_n \; C_n^* \; \int_a^b \; \phi_n^*(x) \; w(x) \; f(x) \\ & - \; \sum_n \; C_n \; \int_a^b \; f^*(x) \; w(x) \; \phi_n(x) \; + \; \sum_n \; | \; C_n \; |^2 \geq \; 0 \\ = \; & \int_a^b dx \; | \; f(x) \; |^2 \; w(x) \; - \; \sum_n \; | \; C_n \; |^2 \geq \; 0 \end{aligned} \tag{518}$$

one finds that convergence requires that the equality sign in Bessel's inequality holds as $N \; \rightarrow \; \infty$.

Another useful inequality is the Schwartz inequality

$$\int_a^b dx \mid f(x) \mid^2 w(x) \int_a^b dy \mid \phi_n(y) \mid^2 w(y) \ \geq \ \left| \int_a^b dt \ f^*(t) \ w(t) \ \phi_n(t) \right|^2 \tag{519}$$

which is evaluated as

$$\int_a^b dx \mid f(x) \mid^2 w(x) \ \geq \ \mid C_n \mid^2 \tag{520}$$

which is a statement that the squared length of a vector must be greater than the square of any one component.

We shall now examine a few physically important examples of Stürm-Liouville equations.

6 Fourier Transforms

The plane waves are eigenfunctions of the Stürm-Lioville equation

$$\frac{\partial^2 \phi_k}{\partial x^2} \; = \; - \; k^2 \; \phi \tag{521}$$

on the interval $(-\infty, \infty)$ has solutions

$$\phi_k(x) \; = \; \frac{1}{\sqrt{2 \, \pi}} \; \exp \left[\; i \; k \; x \; \right] \tag{522}$$

The eigenfunctions satisfy the orthogonality relations

$$\begin{aligned} \int_{-\infty}^{\infty} dx \; \phi^*_{k'}(x) \; \phi_k(x) \; &= \; \int_{-\infty}^{\infty} \frac{dx}{2 \, \pi} \; \exp \left[\; i \; (\; k \; - \; k' \;) \; x \; \right] \\ &= \; \delta(\; k \; - \; k' \;) \end{aligned} \tag{523}$$

These eigenfunctions form a complete set, so an arbitrary function $f(x)$ can be expanded as a linear superposition of the type

$$f(x) \; = \; \int_{-\infty}^{\infty} dk \; \tilde{f}(k) \; \frac{1}{\sqrt{2 \, \pi}} \; \exp \left[\; + \; i \; k \; x \; \right] \tag{524}$$

This expansion coincides with the inverse Fourier Transform. The expansion coefficient $\tilde{f}(k)$ is given by the Fourier Transform

$$\tilde{f}(k) \; = \; \int_{-\infty}^{\infty} dx \; f(x) \; \frac{1}{\sqrt{2 \, \pi}} \; \exp \left[\; - \; i \; k \; x \; \right] \tag{525}$$

Example:

The response of a system to a delta function pulse at time $t \; = \; 0$ can be represented by a response function $\chi(t)$. For a particular system the response is given by

$$\chi(t) \; = \; \chi_0 \; \exp \left[\; i \; \omega_0 \; t \; \right] \; \exp \left[\; - \; \Gamma \; t \; \right] \Theta(t) \tag{526}$$

where $\Theta(t)$ is the Heaviside step function which expresses causality

$$\begin{aligned} \Theta(t) \; &= \; 1 \qquad \text{for } t \; > \; 0 \\ \Theta(t) \; &= \; 0 \qquad \text{for } t \; < \; 0 \end{aligned} \tag{527}$$

Find the frequency-dependent response function given by the Fourier Transform $\tilde{\chi}(\omega)$. The divergences only occur in the lower complex frequency plane.

The frequency-dependent response is obtained from

$$\begin{aligned}
\tilde{\chi}(\omega) &= \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} dt\, \chi(t)\, \exp\left[\, +\, i\,\omega\, t\,\right] \\
&= \frac{1}{\sqrt{2\,\pi}} \int_{0}^{\infty} dt\, \chi_0\, \exp\left[\, -\, i\,\omega_0\, t\,\right] \exp\left[\, -\, \Gamma\, t\,\right] \exp\left[\, +\, i\,\omega\, t\,\right] \\
&= \frac{i}{\sqrt{2\,\pi}} \frac{\chi_0}{\omega\, -\, \omega_0\, +\, i\,\Gamma}
\end{aligned} \tag{528}$$

The frequency dependent response is finite for real frequencies, but diverges at $\omega\, =\, \omega_0\, -\, i\,\Gamma$ in the lower half complex plane.

6.1 Fourier Transform of Derivatives

The Fourier transform of a derivative of a function can be simply expressed in terms of the Fourier transform of the function. Let $f(x)$ be a function which has the Fourier transform $\tilde{f}(k)$, where

$$\tilde{f}(k)\, =\, \int_{-\infty}^{\infty} dx\, f(x)\, \frac{1}{\sqrt{2\,\pi}}\, \exp\left[\, -\, i\, k\, x\,\right] \tag{529}$$

Then the Fourier transform of the derivative is defined by

$$\int_{-\infty}^{\infty} dx\, \frac{\partial f(x)}{\partial x}\, \frac{1}{\sqrt{2\,\pi}}\, \exp\left[\, -\, i\, k\, x\,\right] \tag{530}$$

Integrating by parts, one obtains

$$= f(x)\, \frac{1}{\sqrt{2\,\pi}}\, \exp\left[\, -\, i\, k\, x\,\right]\Bigg|_{-\infty}^{\infty} -\, i\, k \int_{-\infty}^{\infty} dx\, f(x)\, \frac{1}{\sqrt{2\,\pi}}\, \exp\left[\, -\, i\, k\, x\,\right] \tag{531}$$

which if $f(x)$ vanishes as $x\, \rightarrow\, \pm\,\infty$ yields the Fourier transform of the derivative as

$$\begin{aligned}
&= -\, i\, k \int_{-\infty}^{\infty} dx\, f(x)\, \frac{1}{\sqrt{2\,\pi}}\, \exp\left[\, -\, i\, k\, x\,\right] \\
&= i\, k\, \tilde{f}(k)
\end{aligned} \tag{532}$$

The Fourier transform of the n-th order derivative can be obtained by repeated differentiation by parts and is given by

$$\int_{-\infty}^{\infty} dx \left(\frac{\partial^n f(x)}{\partial x^n} \right) \frac{1}{\sqrt{2\ \pi}} \exp \left[-\ i\ k\ x \right] \\ = (\ i\ k\ )^n\ \tilde{f}(k) \tag{533}$$

Example:

The wave equation can be solved by Fourier transformation. Consider the wave equation

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} \tag{534}$$

subject to an initial conditions

$$\phi(x, 0) = f(x) \tag{535}$$

and

$$\left(\frac{\partial \phi(x,t)}{\partial t} \right) \Bigg|_{t=0} = g(x) \tag{536}$$

Fourier transforming the equation with respect to x, one has

$$\begin{aligned} \int_{-\infty}^{+\infty} dx \frac{1}{\sqrt{2\ \pi}} \exp \left[-\ i\ k\ x \right] \frac{\partial^2 \phi}{\partial x^2} &= \frac{1}{c^2} \int_{-\infty}^{+\infty} dx \frac{1}{\sqrt{2\ \pi}} \exp \left[-\ i\ k\ x \right] \frac{\partial^2 \phi}{\partial t^2} \\ -\ k^2\ \tilde{\phi}(k,t) &= \frac{1}{c^2} \frac{\partial^2 \tilde{\phi}(k,t)}{\partial t^2} \end{aligned} \tag{537}$$

At $t = 0$ the Fourier transform of the initial conditions are given by

$$\begin{aligned} \tilde{\phi}(k, 0) &= \int_{-\infty}^{+\infty} dx \frac{1}{\sqrt{2\ \pi}} \exp \left[-\ i\ k\ x \right] \phi(x, 0) \\ &= \int_{-\infty}^{+\infty} dx \frac{1}{\sqrt{2\ \pi}} \exp \left[-\ i\ k\ x \right] f(x) \\ &= \tilde{f}(k) \end{aligned} \tag{538}$$

and

$$\left(\frac{\partial \tilde{\phi}(k,t)}{\partial t} \right) \Bigg|_{t=0} = \int_{-\infty}^{+\infty} dx \, \frac{1}{\sqrt{2 \, \pi}} \, \exp \left[- \, i \, k \, x \right] \left(\frac{\partial \phi(x,t)}{\partial t} \right) \Bigg|_{t=0}$$
$$= \int_{-\infty}^{+\infty} dx \, \frac{1}{\sqrt{2 \, \pi}} \, \exp \left[- \, i \, k \, x \right] g(x)$$
$$= \tilde{g}(k) \tag{539}$$

Hence, we have to solve the second order differential equation

$$- \, k^2 \, \tilde{\phi}(k,t) = \frac{1}{c^2} \, \frac{\partial^2 \tilde{\phi}(k,t)}{\partial t^2} \tag{540}$$

subject to the two initial conditions given by

$$\tilde{\phi}(k,0) = \tilde{f}(k) \tag{541}$$

and

$$\left(\frac{\partial \tilde{\phi}(k,t)}{\partial t} \right) \Bigg|_{t=0} = \tilde{g}(k) \tag{542}$$

The second order ordinary differential equation has the general solution

$$\tilde{\phi}(k,t) = A \, \exp \left[\, i \, c \, k \, t \, \right] + B \, \exp \left[- \, i \, c \, k \, t \, \right] \tag{543}$$

where A and B are arbitrary constants. The initial conditions determine A and B from the initial conditions as

$$\tilde{f}(k) = A + B \tag{544}$$

and

$$\tilde{g}(k) = i \, c \, k \, (\, A - B \,) \tag{545}$$

Hence, we have determined the constants as

$$A = \frac{1}{2} \left(\tilde{f}(k) - i \, \frac{\tilde{g}(k)}{c \, k} \right) \tag{546}$$

and

$$B = \frac{1}{2} \left(\tilde{f}(k) + i \, \frac{\tilde{g}(k)}{c \, k} \right) \tag{547}$$

Thus, the Fourier Transform of the solution is given by

$$\tilde{\phi}(k,t) \;=\; \frac{1}{2}\Bigg[\left(\tilde{f}(k) - i\,\frac{\tilde{g}(k)}{c\,k}\right)\,\exp\Big[+\,i\,c\,k\,t\Big] + B\left(\tilde{f}(k) + i\,\frac{\tilde{g}(k)}{c\,k}\right)\exp\Big[-\,i\,c\,k\,t\Big]\Bigg] \tag{548}$$

and then the solution is given by the inverse Fourier Transform

$$\phi(x,t) \;=\; \int_{-\infty}^{+\infty} dk\;\tilde{\phi}(k,t)\;\frac{1}{\sqrt{2\,\pi}}\;\exp\Big[\;+\;i\;k\;x\;\Big] \tag{549}$$

or

$$\begin{aligned}\phi(x,t) \;&=\; \frac{1}{2}\int_{-\infty}^{+\infty} dk\left(\;\tilde{f}(k)\;-\;i\;\frac{\tilde{g}(k)}{c\,k}\;\right)\frac{1}{\sqrt{2\,\pi}}\;\exp\Big[\;i\;k\;(\;x\;+\;c\;t\;)\;\Big]\\ &+\;\frac{1}{2}\int_{-\infty}^{+\infty} dk\left(\;\tilde{f}(k)\;+\;i\;\frac{\tilde{g}(k)}{c\,k}\;\right)\frac{1}{\sqrt{2\,\pi}}\;\exp\Big[\;i\;k\;(\;x\;-\;c\;t\;)\;\Big]\end{aligned} \tag{550}$$

The integrals can be evaluated from the definition of the inverse Fourier Transform yielding

$$\begin{aligned}\phi(x,t) \;&=\; \frac{1}{2}\left[\;f(\;x\;+\;c\;t\;)\;+\;\frac{1}{c}\int_{a}^{x+ct} dz\;g(z)\;\right]\\ &+\;\frac{1}{2}\left[\;f(\;x\;-\;c\;t\;)\;-\;\frac{1}{c}\int_{a}^{x-ct} dz\;g(z)\;\right]\end{aligned} \tag{551}$$

where the arbitrary constant of integration cancels. In fact, using this cancellation one can write the solution as

$$\begin{aligned}\phi(x,t) \;&=\; \frac{1}{2}\Big[\;f(\;x\;+\;c\;t\;) + \;f(\;x\;-\;c\;t\;)\;\Big]\\ &+\;\frac{1}{2\;c}\int_{x-ct}^{x+ct} dz\;g(z)\end{aligned} \tag{552}$$

This is D'Alembert's solution of the wave equation and corresponds to a superposition of a backward and forward travelling wave.

6.2 Convolution Theorem

A convolution of two functions $f(x)$ and $g(x)$ is defined as the integral

$$\frac{1}{\sqrt{2\;\pi}}\int_{-\infty}^{\infty} dt\;g(t)\;f(\;x\;-\;t\;) \tag{553}$$

The convolution theorem expresses a convolution as the Fourier Transform of the product of the two functions

$$\begin{aligned}
& \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} dt \; g(t) \; f(\; x \; - \; t \;) \\
& = \; \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} dt \; g(t) \int_{-\infty}^{\infty} dk \; \tilde{f}(k) \; \frac{1}{\sqrt{2\,\pi}} \; \exp \left[\; + \; i \; k \; (\; x \; - \; t \;) \; \right] \\
& = \; \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dt \; g(t) \; \frac{1}{\sqrt{2\,\pi}} \; \exp \left[\; - \; i \; k \; t \; \right] \tilde{f}(k) \; \frac{1}{\sqrt{2\,\pi}} \; \exp \left[\; + \; i \; k \; x \; \right] \\
& = \; \int_{-\infty}^{\infty} dk \; \tilde{g}(k) \; \tilde{f}(k) \; \frac{1}{\sqrt{2\,\pi}} \; \exp \left[\; + \; i \; k \; x \; \right]
\end{aligned} \tag{554}$$

which is the Fourier Transform of the product of Fourier Transforms. Inversely, the inverse Fourier transform of a convolution is merely the product of Fourier transforms.

Example:

The time dependent response of a system $A(t)$ to an applied time dependent field $B(t)$ is given in terms of a response function $\chi(t-t')$ such that

$$A(t) \; = \; \int_{-\infty}^{t} dt' \; \chi(t-t') \; B(t') \tag{555}$$

where the stimulus occurs at a time t' that is earlier than the response time. This expresses causality. The integral over t' in this relation can be extended to ∞ as

$$A(t) \; = \; \int_{-\infty}^{\infty} dt' \; \chi(t-t') \; B(t') \tag{556}$$

if we define

$$\chi(t-t') \; = \; 0 \qquad \text{for } t' \; > \; t \tag{557}$$

Thus, the response has the form of the convolution.

The applied field can be Fourier Transformed into its frequency components, and also the response can be frequency resolved into the components $\tilde{A}(\omega)$. The relation between the frequency components of the response and the applied can be obtained by Fourier Transforming the linear relation, which yields

$$\tilde{A}(\omega) \; = \; \tilde{\chi}(\omega) \; \tilde{B}(\omega) \tag{558}$$

Thus, the response relation simplifies in the frequency domain.

6.3 Parseval's Relation

Parseval's relation is given by

$$\int_{-\infty}^{+\infty} dk \ \tilde{f}(k) \ \tilde{g}(k) \ = \ \int_{-\infty}^{+\infty} dx \ f(x) \ g^*(x) \tag{559}$$

and can be derived using the completeness relation

$$\begin{aligned}
\int_{-\infty}^{+\infty} dx \ f(x) \ g^*(x) \ &= \ \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dk \ \tilde{f}(k) \ \frac{1}{\sqrt{2 \ \pi}} \ \exp \left[\ + \ i \ k \ x \ \right] \ g^*(x) \\
= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dk \ \tilde{f}(k) \ \frac{1}{\sqrt{2 \ \pi}} \ \exp \left[\ + \ i \ k \ x \ \right] & \int_{-\infty}^{+\infty} dk' \ \tilde{g}^*(k') \ \frac{1}{\sqrt{2 \ \pi}} \ \exp \left[\ - \ i \ k' \ x \ \right] \\
= \int_{-\infty}^{+\infty} dk \ \tilde{f}(k) \int_{-\infty}^{+\infty} dk' \ \tilde{g}^*(k') \int_{-\infty}^{+\infty} \frac{dx}{2 \ \pi} \ & \exp \left[\ + \ i \ (\ k \ - \ k' \ ) \ x \ \right] \\
= \int_{-\infty}^{+\infty} dk \ \tilde{f}(k) \int_{-\infty}^{+\infty} dk' \ \tilde{g}^*(k') \ & \delta(\ k \ - \ k' \ ) \\
= \int_{-\infty}^{+\infty} dk \ \tilde{f}(k) \ \tilde{g}^*(k) &
\end{aligned} \tag{560}$$

which is Parseval's relation.

7 Fourier Series

The Stürm-Liouville equation

$$\frac{\partial^2 \phi}{\partial x^2} \; + \; n^2 \; \phi \; = \; 0 \tag{561}$$

with eigenvalue $- \, n^2$ has solutions $\cos nx$ and $\sin nx$ that can be used to form an orthonormal set, as

$$\begin{aligned}
\int_0^{2\pi} dx \; \sin mx \; \sin nx \quad &= \quad \pi \; \delta_{n,m} \qquad\qquad m \; \neq \; 0 \\
\int_0^{2\pi} dx \; \cos mx \; \cos nx \quad &= \quad \pi \; \delta_{n,m} \qquad\qquad m \; \neq \; 0 \\
\int_0^{2\pi} dx \; \sin mx \; \sin nx \quad &= \quad 0
\end{aligned} \tag{562}$$

The basis function corresponding to $n \; = \; 0$ is non-degenerate and can be taken to be

$$\frac{1}{\sqrt{2 \; \pi}} \tag{563}$$

The other basis functions, with $n \; > \; 0$, are degenerate and can be taken to be

$$\begin{aligned}
&\frac{1}{\sqrt{\pi}} \; \sin nx \\
&\frac{1}{\sqrt{\pi}} \; \cos nx
\end{aligned} \tag{564}$$

This set of eigenfunctions generates the finite Fourier series expansion, whereby any well behaved function on the interval $(0, 2\pi)$ can be expanded as

$$f(x) \; = \; a_0 \; \frac{1}{\sqrt{2\pi}} \; + \; \sum_{n=1}^{\infty} \left(\; a_n \; \frac{1}{\sqrt{\pi}} \; \cos nx \; + \; b_n \; \frac{1}{\sqrt{\pi}} \; \sin nx \; \right) \tag{565}$$

where the coefficients $(a_n < b_n)$ are calculated from

$$\begin{aligned}
a_0 \quad &= \quad \int_0^{2\pi} \; dt \; f(t) \; \frac{1}{\sqrt{2 \; \pi}} \\
a_n \quad &= \quad \int_0^{2\pi} \; dt \; f(t) \; \frac{1}{\sqrt{\pi}} \; \cos \; nt \\
b_n \quad &= \quad \int_0^{2\pi} \; dt \; f(t) \; \frac{1}{\sqrt{\pi}} \; \sin \; nt
\end{aligned} \tag{566}$$

This leads to an explicit form of the completeness condition, in which we define the dirac delta function restricted to the interval $(0, 2\pi)$ to be $\Delta(x-t)$ so

$$\begin{aligned}\Delta(x-t) &= \frac{1}{2\,\pi} + \frac{1}{\pi}\sum_{n=1}\left(\cos\,nx\,\cos\,nt\,+\,\sin\,nx\,\sin\,nt\right)\\ &= \frac{1}{2\,\pi} + \frac{1}{\pi}\sum_{n=1}\cos\,n\,(\,x\,-\,t\,)\end{aligned} \tag{567}$$

It can be shown that the set of Fourier expansion coefficients (a_n, b_n) in the expansion of $f(x)$ are the coefficients that minimize the difference

$$\chi(x) \;=\; f(x) \;-\; \frac{a_0}{\sqrt{2\,\pi}} \;-\; \sum_{n=1}^{N}\frac{1}{\sqrt{\pi}}\left(a_n\,\cos\,nx\,+\,b_n\,\sin\,nx\right) \tag{568}$$

as they can be determined from the χ^2 minimization scheme in which

$$I \;=\; \int_0^{2\pi} dx\;\chi^2(x)\;\geq\;0 \tag{569}$$

and

$$\frac{\partial I}{\partial a_n} \;=\; \frac{\partial I}{\partial b_n} \;=\; 0 \qquad \forall\; n\;\leq\;N \tag{570}$$

This leads to the equations

$$\begin{aligned}a_0 &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} dt\;f(t)\\ a_n &= \frac{1}{\sqrt{\pi}}\int_0^{2\pi} dt\;f(t)\;\cos\;nt\\ b_n &= \frac{1}{\sqrt{\pi}}\int_0^{2\pi} dt\;f(t)\;\sin\;nt\end{aligned} \tag{571}$$

For these values of the expansion coefficients, the difference $\chi(x)$ only vanishes for almost all values of x if

$$I \;=\; 0 \tag{572}$$

This condition allows the function to deviate from the Fourier series only at a set of isolated points that contribute zero to the integral. The condition $I\;=\;0$ is equivalent to Bessel's inequality being satisfied, since

$$I \;=\; \int_0^{2\pi} dt\;f^2(t)\;-\;a_0^2\;-\;\sum_{n=1}^{N}\left(\,a_n^2\;+\;b_n^2\,\right) \tag{573}$$

The quantity $a_n^2 + b_n^2$ (which is a function of n) is known as the power spectrum of $f(x)$.

The basis functions $\phi_n(x)$ are continuous at every point in the interval $(0, 2\pi)$ yet, it is possible to expand a square integrable $f(x)$ with a finite number of discontinuities as a Fourier series. If $f(x)$ has a discontinuity at $x = x_0$ it can be proved that the series converges to the value of

$$\lim_{\epsilon \to 0} \frac{1}{2} \left[f(x_0 + \epsilon) + f(x_0 - \epsilon) \right] \tag{574}$$

This can be seen by evaluating the Fourier series expansion of

$$\begin{aligned} f(x) &= x \qquad 0 \leq x < \pi \\ f(x) &= x - 2\pi \qquad \pi < x \leq 2\pi \end{aligned} \tag{575}$$

In this case, it is easily seen that the constant term is zero

$$\begin{aligned} a_0 &= \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} dt \ f(t) \\ &= \frac{1}{\sqrt{2\pi}} \left(\int_0^{\pi} dt \ f(t) + \int_{\pi}^{2\pi} dt \ f(t) \right) \\ &= \frac{1}{\sqrt{2\pi}} \left(\int_0^{\pi} dt \ t + \int_{\pi}^{2\pi} dt \ (t - 2\pi) \right) \\ &= \frac{1}{\sqrt{2\pi}} \left(\frac{\pi^2}{2} + \frac{4\pi^2}{2} - \frac{\pi^2}{2} - 2\pi\pi \right) \\ &= 0 \end{aligned} \tag{576}$$

Using integration by parts one finds that the coefficients of the cosine terms are also zero

$$\begin{aligned} a_n &= \frac{1}{\sqrt{\pi}} \int_0^{2\pi} dt \ f(t) \ \cos nt \\ &= \frac{1}{\sqrt{\pi}} \left(\int_0^{\pi} dt \ f(t) \ \cos nt + \int_{\pi}^{2\pi} dt \ f(t) \ \cos nt \right) \\ &= \frac{1}{\sqrt{\pi}} \left(\int_0^{\pi} dt \ t \ \cos nt + \int_{\pi}^{2\pi} dt \ (t - 2\pi) \ \cos nt \right) \\ &= \frac{1}{\sqrt{\pi}} \left(\frac{\cos n\pi - 1}{n^2} - \frac{\cos n\pi - 1}{n^2} \right) \\ a_n &= 0 \end{aligned} \tag{577}$$

However, the coefficients of the sine terms are evaluated as

$$\begin{aligned}
b_n &= \frac{1}{\sqrt{\pi}} \int_0^{2\pi} dt \ f(t) \ \sin \ nt \\
&= \frac{1}{\sqrt{\pi}} \left(\int_0^{\pi} dt \ f(t) \ \sin \ nt \ + \ \int_{\pi}^{2\pi} dt \ f(t) \ \sin \ nt \right) \\
&= \frac{1}{\sqrt{\pi}} \left(\int_0^{\pi} dt \ t \ \sin \ nt \ + \ \int_{\pi}^{2\pi} dt \ (\ t \ - \ 2 \ \pi \ ) \ \sin \ nt \right) \\
&= \frac{1}{\sqrt{\pi}} \ 2 \ \pi \left(\ - \ \frac{1}{n} \ + \ \frac{1 \ - \ \cos \ n\pi}{n} \right) \\
&= - \ 2 \ \sqrt{\pi} \ \frac{\cos \ n\pi}{n} \\
b_n &= \sqrt{\pi} \ \frac{2}{n} \ (\ - \ 1 \ )^n
\end{aligned} \tag{578}$$

and are non-zero. Hence, we have the Fourier series expansion

$$f(x) \ = \ 2 \ \sum_{n=1}^{\infty} \frac{(\ - \ 1 \ )^n}{n} \ \sin \ nx \tag{579}$$

which just consists of an expansion in terms of the sine functions.

Direct evaluation of the series at $x \ = \ \pi$ yields a sum of zero since $\sin n\pi \ = \ 0$. The original function is undefined at the discontinuity, but has a value of π just below the discontinuity and a value of $- \ \pi$ just above the discontinuity. Thus, we see that

$$0 \ = \ \frac{1}{2} \left[\ \pi \ + \ (\ -\pi \ ) \ \right] \tag{580}$$

as expected.

Homework: 14.1.4

Homework:

Expand x^2 and x^4 in a Fourier series and then evaluate the series at the point $x \ = \ \pi$.

A numerical evaluation of the Fourier series in the vicinity of a discontinuity, shows the Gibbs phenomenon. Consider a square wave train

$$\begin{aligned}
f(x) &= 1 \qquad \text{for} \ 0 \ < \ x \ < \ \pi \\
f(x) &= 0 \qquad \text{for} \ \pi \ < \ x \ < \ 2 \ \pi
\end{aligned} \tag{581}$$

this has a discontinuity at $x = \pi$. The Fourier series expansion is given by

$$f(x) = \frac{1}{2} + \frac{2}{\pi} \sum_{n=0} \frac{\sin(2n+1)x}{2n+1} \tag{582}$$

The Fourier series assigns a value to the function at the discontinuity, which is the mean from just above and below. Furthermore, the Fourier series truncated after N terms, also over-estimates the function or overshoots it just before the discontinuity. This is the Gibbs phenomenon.

7.1 Gibbs Phenomenon

In order to discuss the Gibb's phenomenon, it is necessary to sum the Fourier series. It can be shown that

$$\Delta(x-t) = \frac{1}{2\,\pi} + \frac{1}{\pi} \sum_{n=1}^{\infty} \cos\, n\, (\, x \,-\, t\,) \tag{583}$$

or, equivalently

$$\Delta(x-t) = \frac{1}{2\,\pi} + \frac{1}{\pi}\, \text{Real} \sum_{n=1}^{\infty} \exp\left[\, i\, n\, (\, x \,-\, t\,)\,\right] \tag{584}$$

then, on summing only the first N terms, one has

$$\begin{aligned}
\Delta_N(x-t) &= \;= \frac{1}{2\,\pi} + \frac{1}{\pi}\, \text{Real} \sum_{n=1}^{N} \exp\left[\, i\, n\, (\, x \,-\, t\,)\,\right] \\
&= \frac{1}{2\,\pi} + \frac{1}{\pi}\, \text{Real} \left(\frac{\exp\left[\, i\, (\, N \,+\, 1\,)\, (\, x \,-\, t\,)\,\right] \,-\, \exp\left[\, i\, (\, x \,-\, t\,)\,\right]}{\exp\left[\, i\, (\, x \,-\, t\,)\,\right] \,-\, 1} \right) \\
&= \frac{1}{2\,\pi} + \frac{1}{\pi} \left(\frac{\cos\, \frac{(\, N\, +\, 1\,)\, (\, x\, -\, t\,)}{2}\, \sin\, \frac{N\, (\, x\, -\, t\,)}{2}}{\sin\, \frac{(\, x\, -\, t\,)}{2}} \right) \\
&= \frac{1}{2\,\pi} \left[\frac{\sin\, (\, N \,+\, \frac{1}{2}\,)\, (\, x \,-\, t\,)}{\sin\, \frac{(\, x\, -\, t\,)}{2}} \right]
\end{aligned} \tag{585}$$

Hence, on defining the sum of the first N terms of the Fourier series for $f(x)$ as $f_N(x)$ one has

$$f_N(x) = \int_0^{2\,\pi} dt\; f(t)\; \Delta_N(x-t)$$

$$= \frac{1}{2\pi} \int_0^{2\pi} dt\, f(t) \left[\frac{\sin (N + \frac{1}{2}) (x - t)}{\sin \frac{(x - t)}{2}} \right] \tag{586}$$

The Gibbs phenomenon can be demonstrated by the square wave in which case

$$\begin{aligned} f_N(x) &= \int_0^{\pi} dt\; 1\; \Delta_N(x-t) \\ &= \frac{1}{2\pi} \int_0^{\pi} dt \left[\frac{\sin (N + \frac{1}{2}) (x - t)}{\sin \frac{(x - t)}{2}} \right] \end{aligned} \tag{587}$$

At the discontinuity at $x = \pi$, one has

$$f_N(\pi) = \frac{1}{2\pi} \int_0^{\pi} dt \left[\frac{\sin (N + \frac{1}{2}) (\pi - t)}{\sin \frac{(\pi - t)}{2}} \right] \tag{588}$$

which, on introducing the variable $y = \pi - t$, can be written as

$$f_N(\pi) = \frac{1}{2\pi} \int_0^{\pi} dy \left[\frac{\sin (N + \frac{1}{2}) y}{\sin \frac{y}{2}} \right] \tag{589}$$

The integral can be evaluated in the limit $N \rightarrow \infty$ by writing $z = (N + \frac{1}{2}) y$, so that

$$\begin{aligned} \lim_{N\rightarrow\infty} f_N(\pi) &= \frac{1}{\pi} \int_0^{\infty} dz \left[\frac{\sin z}{z} \right] \\ &= \frac{1}{2} \end{aligned} \tag{590}$$

The over shoot at $x = 0$ can be estimated by rewriting the partial sum, by shifting the variable of integration to $s = x - t$

$$f_N(x) = \frac{1}{2\pi} \int_{x-\pi}^{x} ds \left(\frac{\sin (N + \frac{1}{2}) s}{\sin \frac{s}{2}} \right) \tag{591}$$

The integrand is symmetrical in s and has a maximum value of $\frac{N+\frac{1}{2}}{\pi}$ at $s = 0$ and first falls to zero at $s = \pm \frac{\pi}{N+\frac{1}{2}}$. We shall examine the behavior of the series at the discontinuity at $x = 0$. At $x = 0$ the integral over s starts with a small value of the integrand which oscillates about zero and the integrand then attains its maximum value at the upper limit of integration. However, it is clear to see that the integral will be greater if the range of integration of s covers both positive regions around the central maximum. This occurs when $x \; = \; \frac{\pi}{N \; + \; \frac{1}{2}}$. In this case, one estimates the maximum value of the partial sum is given by

$$\begin{aligned} f_N(x)\Big|_{max} \quad & \sim \quad \frac{1}{2 \, \pi} \int_{-\pi}^{\frac{\pi}{N+\frac{1}{2}}} ds \left[\frac{\sin \, (\, N \; + \; \frac{1}{2} \,) \; s}{\sin \, \frac{s}{2}} \right] \\ & = \quad \frac{1}{2} \; + \; \frac{1}{2 \, \pi} \int_{0}^{\frac{\pi}{N+\frac{1}{2}}} ds \left[\frac{\sin \, (\, N \; + \; \frac{1}{2} \,) \; s}{\sin \, \frac{s}{2}} \right] \\ & \sim \quad \frac{1}{2} \; + \; \frac{1}{\pi} \int_{0}^{\pi} dz \left[\frac{\sin \; z}{z} \right] \end{aligned} \tag{592}$$

where

$$z \; = \; (\; N \; + \; \frac{1}{2} \;) \; s \tag{593}$$

The second integral is greater than 0.5, its' value is 0.588. The truth of this inequality can be seen by plotting the integrand. The integrand when considered as function of s is oscillatory, with a constant period $\sim \; \frac{2\pi}{N}$. As x is increased in steps of $\frac{2\pi}{N}$, the upper limit of s includes one more cycle of the integrand, and the upper limit of the z integration increases by a multiple of 2π. Each successive half cycle yields a contribution of opposite sign and smaller magnitude than the previous half cycle. Thus, when taken in pairs, the contribution from the entire z interval of $(0, \infty)$ [which contributes 0.5] is smaller than the contribution from the first half cycle. Thus, the series over shoots at the discontinuity by 8%.

An alternative formulation of Fourier series makes use of another linear combination of the degenerate eigenfunctions of the Stürm-Liouville equation with periodic boundary conditions

$$\begin{aligned} \phi_m(\varphi) \quad & = \quad \frac{1}{\sqrt{2 \; \pi}} \; \exp \left[\; + \; i \; m \; \varphi \; \right] \\ \phi_{-m}(\varphi) \quad & = \quad \frac{1}{\sqrt{2 \; \pi}} \; \exp \left[\; - \; i \; m \; \varphi \; \right] \end{aligned} \tag{594}$$

and the non degenerate function

$$\phi_0(\varphi) \; = \; \frac{1}{\sqrt{2 \; \pi}} \tag{595}$$

This is the complex representation, in which the eigenfunctions are symmetrically normalized via

$$\int_0^{2\pi} d\varphi \; \phi^*_m(\varphi) \; \phi_n(\varphi) \; = \; \delta_{n,m} \tag{596}$$

and any complex function $\Phi(\varphi)$ on the interval $2\,\pi\ >\ \varphi\ >\ 0$ can be expanded as

$$\Phi(\varphi)\ =\ \sum_m C_m\ \phi_m(\varphi) \tag{597}$$

The complex coefficients C_m are given by

$$C_m\ =\ \frac{1}{\sqrt{2\,\pi}}\ \int_0^{2\,\pi}\ d\varphi\ \exp\left[\ -\ i\ m\ \varphi\ \right]\ \Phi(\varphi) \tag{598}$$

If the function Φ is real, then one must have

$$C_{-m}\ =\ C_m^* \tag{599}$$

These functions often occur as solutions of Stürm-Liouville equations in the azimuthal angle in spherical polar coordinates.

Example:

Consider a cylindrical metal sheet of radius a and infinite length that has been cut across a diameter. The two sheets are almost touching. One half of the cylinder is kept at a potential ϕ_0 and the other half is kept at a potential $-\phi_0$. Determine the potential at an arbitrary point (z, r, φ) inside the cylinder. Assume, that the potential $\phi(z, r, \varphi)$ inside the cylinder is governed by the equation

$$\nabla^2\ \phi\ =\ 0 \tag{600}$$

or in cylindrical coordinates

$$\frac{\partial^2\phi}{\partial z^2}\ +\ \frac{1}{r}\ \frac{\partial}{\partial r}\left(\ r\ \frac{\partial\phi}{\partial r}\ \right)\ +\ \frac{1}{r^2}\ \frac{\partial^2\phi}{\partial\varphi^2}\ =\ 0 \tag{601}$$

Solution:

This can be solved by noting that the problem is invariant under translations along the cylinders axis. Thus, the potential is only a function of (r, φ) alone. Furthermore, one can assume that the potential can be expanded in a discrete Fourier series in φ with arbitrary coefficients that depend on r, since the potential is periodic in φ.

$$\phi(r, \varphi)\ =\ \sum_m\ \frac{C_m(r)}{\sqrt{2\,\pi}}\ \exp\left[\ i\ m\ \varphi\ \right] \tag{602}$$

On substituting the series expansion into Laplace's equation, and on multiplying by the complex conjugate function

$$\frac{1}{\sqrt{2\,\pi}}\ \exp\left[\ -\ i\ n\ \varphi\ \right] \tag{603}$$

and integrating over φ between 0 and $2\,\pi$, one finds that the expansion coefficient $C_n(r)$ satisfies the equation

$$\frac{1}{r}\,\frac{\partial}{\partial r}\left(\,r\,\frac{\partial C_n(r)}{\partial r}\,\right)\;-\;\frac{n^2}{r^2}\,C_n(r)\;=\;0 \tag{604}$$

Thus, we find that

$$C_n(r)\;=\;A_n\,r^n\;+\;B_n\,r^{-n} \tag{605}$$

so that the potential is of the form

$$\phi(r,\varphi)\;=\;\frac{1}{\sqrt{2\,\pi}}\,\sum_{n=-\infty}^{\infty}\left(\,A_n\,r^n\;+\;B_n\,r^{-n}\,\right)\,\exp\left[\,i\,n\,\varphi\,\right] \tag{606}$$

Since, the potential must be finite at the center of the cylinder ($r\;=\;0$) one can set $B_n\;=\;0$. Furthermore, from the boundary condition at $r\;=\;a$ one has

$$\begin{aligned}\phi(a,\varphi)\;&=\;\phi_0 \qquad \text{for}\;\;2\,\pi>\;\varphi\;>\;\pi\\ \phi(a,\varphi)\;&=\;-\,\phi_0 \qquad \text{for}\;\;\pi>\;\varphi\;>\;0\end{aligned} \tag{607}$$

Then, using the Fourier series expansion of $\phi(a,\varphi)$ and the orthogonality condition one has

$$\frac{\phi_0}{\sqrt{2\,\pi}}\left(\,\int_{\pi}^{2\pi}d\varphi\,\exp\left[\,-\,i\,n\,\varphi\,\right]-\int_0^{\pi}d\varphi\,\exp\left[\,-\,i\,n\,\varphi\,\right]\right)\;=\;A_n\,a^n \tag{608}$$

which uniquely determines A_n as

$$A_n\;\;=\;\;-\,\sqrt{2\,\pi}\,\phi_0\,a^{-n}\,\exp\left[\,-\,i\,\frac{n\,\pi}{2}\,\right]\left[\,\frac{\sin\frac{n\,\pi}{2}}{\frac{n\,\pi}{2}}\,\right] \tag{609}$$

Since, for even n one has $\sin\frac{n\pi}{2}\;=\;0$, it is useful to re-write the coefficients as

$$\begin{aligned}A_{2n+1}\;&=\;\frac{4\,i}{\sqrt{2\,\pi}}\,\frac{\phi_0}{2n+1}\,a^{-(2n+1)}\\ A_{2n}\;&=\;0\end{aligned} \tag{610}$$

which are only non-zero for odd n. Thus, the expansion only contains terms that have odd n. The potential is given by

$$\phi(r,\varphi)\;=\;-\,\frac{\phi_0}{2\,\pi}\,\sum_{n=0}^{\infty}\,\frac{8}{2\,n\;+\;1}\left(\frac{r}{a}\right)^{2n+1}\,\sin\;n\,\varphi \tag{611}$$

Example:

An interesting example is given by Laplace's equation for a potential ϕ in a two dimensional region in the shape of a wedge, of angle $\frac{\pi}{b}$, where $b > \frac{1}{2}$. The boundary conditions used will be

$$\Theta(r, \frac{\pi}{b}) = \Theta(r, 0) = 0 \tag{612}$$

Laplace's equation in two dimensions becomes

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} = 0 \tag{613}$$

and this can be solved by separation of variables, and then series expansion. The solutions are sought in the form

$$\phi(r, \theta) = R(r) \, \Theta(\theta) \tag{614}$$

On substitution of this ansatz into Laplace's equation and writing the separation constant as $- \mu^2$, one obtains the two ordinary differential equations. These consist of the differential equation for the angular part

$$\frac{\partial^2 \Theta}{\partial \theta^2} = - \mu^2 \, \Theta \tag{615}$$

and the radial equation

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial R}{\partial r} \right) - \frac{\mu^2}{r^2} R = 0 \tag{616}$$

The angular equation has solutions

$$\begin{aligned} \Theta(\theta) &= A \, \sin \mu \, \theta \\ \Theta(\theta) &= B \, \cos \mu \, \theta \end{aligned} \tag{617}$$

However, due to the boundary conditions, the only allowable solutions are

$$\Theta(\theta) = A \, \sin \mu \, \theta \tag{618}$$

where

$$\mu \frac{\pi}{b} = m \, \pi \tag{619}$$

and m is any positive integer. That is, the allowable values of μ are given by

$$\mu \; = \; m \, b \tag{620}$$

The functions are normalized such that

$$\begin{aligned} A^2 \int_0^{\frac{\pi}{b}} d\theta \, \sin^2 \, m \, \theta \, b \; & = \; \frac{A^2}{b} \int_0^{\pi} dx \, \sin^2 m \, x \\ & = \; \frac{A^2}{2 \, b} \int_0^{\pi} dx \, (\, 1 \; - \; \cos 2 \, m \, x \,) \\ & = \; A^2 \, \frac{\pi}{2 \, b} \\ & = \; 1 \end{aligned} \tag{621}$$

The radial equation becomes

$$r \, \frac{\partial}{\partial r} \left(\, r \, \frac{\partial R}{\partial r} \, \right) \; = \; m^2 \, b^2 \, R \tag{622}$$

The radial equation has solutions

$$\begin{aligned} R(r) \; & = \; C \, r^{\mu} \; + \; D \, r^{-\mu} \\ & = \; C \, r^{mb} \; + \; D \, r^{- \, mb} \end{aligned} \tag{623}$$

As the solution must be regular at $r \; = \; 0$ one has

$$R(r) \; = \; C_m \, r^{mb} \tag{624}$$

and the potential can be expanded as a Fourier series

$$\phi(r, \theta) \; = \; \sum_{m=1}^{\infty} C_m \, r^{mb} \, \sqrt{\frac{2 \, b}{\pi}} \, \sin \, m \, b \, \theta \tag{625}$$

The coefficients C_m have to be determined from additional boundary conditions.

The above solution has the interesting property that when $b \; > \; 1$, which means that the angle between the conducting planes is obtuse, then the radial component of the electric field is given

$$E_r \; = \; - \; \sum_{m=1}^{\infty} m \, b \, C_m \, r^{mb-1} \, \sqrt{\frac{2 \, b}{\pi}} \, \sin \, m \, b \, \theta \tag{626}$$

The Fourier component of the field with $m \; = \; 1$ varies as

$$- \, C_1 \, b \, r^{b-1} \, \sqrt{\frac{2 \, b}{\pi}} \, \sin \, b \, \theta \tag{627}$$

which is unbounded for $b < 1$ as $r \rightarrow 0$. Thus, electric fields can be exceptionally large and have corner singularities close to the edge on a metal object with an acute angle, such as lightning rods.

As an example of the occurrence of a high dimensional eigenvalue equation, consider Laplace's equation in three dimensions

$$\nabla^2 \, \Phi(x,y,z) \; = \; 0 \tag{628}$$

Laplace's equation can be considered as an eigenvalue equation with eigenvalue $\lambda = 0$. The solutions should form a complete set. Since one suspects that all functions can be expanded as polynomials in the variables (x,y,z), one can look for polynomial solutions. Some solutions are easily identified, for example

$$\phi_0(x,y,z) \; = \; 1 \tag{629}$$

or one has the three linearly independent linear functions

$$\begin{aligned} \phi_{1,c}(x,y,z) &= x \\ \phi_{1,s}(x,y,z) &= y \\ \phi_{1,0}(x,y,z) &= z \end{aligned} \tag{630}$$

Although there are six quadratic form there are only five linearly independent quadratic forms which satisfy Laplace's equation. These are

$$\begin{aligned} \phi_{2,s}(x,y,z) &= y\,z \\ \phi_{2,c}(x,y,z) &= x\,z \\ \phi_{2,2s}(x,y,z) &= x\,y \\ \phi_{2,2c}(x,y,z) &= x^2 \, - \, y^2 \\ \phi_{2,0}(x,y,z) &= 2\,z^2 \, - \, x^2 \, - \, y^2 \end{aligned} \tag{631}$$

Thus, the zero eigenvalue of the Laplace operator ∇^2 is highly degenerate. In spherical polar coordinates (r,θ,φ) the eigenfunctions are

$$\phi_0(r,\theta,\varphi) \; = \; 1 \tag{632}$$

and

$$\begin{aligned} \phi_{1,c}(r,\theta,\varphi) &= r\,\sin\theta\,\cos\varphi \\ \phi_{1,s}(r,\theta,\varphi) &= r\,\sin\theta\,\sin\varphi \\ \phi_{1.0}(r,\theta,\varphi) &= r\,\cos\theta \end{aligned} \tag{633}$$

The linear functions, for fixed (r, θ), form a set of orthogonal functions of φ. Likewise, for the set of quadratic functions

$$\begin{aligned}
\phi_{2,s}(r,\theta,\varphi) &= r^2 \ \sin\theta \ \cos\theta \ \sin\varphi \\
\phi_{2,c}(r,\theta,\varphi) &= r^2 \ \sin\theta \ \cos\theta \ \cos\varphi \\
\phi_{2,2s}(r,\theta,\varphi) &= r^2 \ \sin^2\theta \ \cos\varphi \ \sin\varphi \\
\phi_{2,2c}(r,\theta,\varphi) &= r^2 \ \sin^2\theta \ (\ \cos^2\varphi \ - \ \sin^2\varphi \ ) \\
\phi_{2,0}(r,\theta,\varphi) &= r^2 \ (\ 2 \ \cos^2\theta \ - \ \sin^2\theta \ )
\end{aligned} \tag{634}$$

which again form a set orthogonal functions of φ, because the integral over φ vanishes

$$\int_0^{2\pi} d\varphi \ \phi^*_{2,m}(\theta,\varphi) \ \phi_{2,n}(\theta,\varphi) \ = \ 0 \tag{635}$$

if $n \neq m$. Furthermore, even if the eigenfunctions have the same φ dependence, they are orthogonal to the linear functions with weight factor $\sin\theta$ as the integral

$$\int_0^{\pi} d\theta \ \phi^*_{2,m}(\theta,\varphi) \ \sin\theta \ \phi_{1,m}(\theta,\varphi) \ = \ 0 \tag{636}$$

vanishes. For example, when $m = 0$, and on substituting $x = \cos\theta$ our functions are recognized as being orthogonal polynomials which are proportional to the Legendre polynomials $P_n(x)$. Also note that there are only five linearly independent functions $\phi_{2,m}$, since the remaining linear combination is just

$$x^2 \ + \ y^2 \ + \ z^2 \ = \ r^2 \tag{637}$$

which has the same θ and φ dependence as ϕ_0.

Example:

Find all (7) real linearly cubic expressions that are solutions of Laplace's equation, and then express them in terms of spherical polar coordinates.

Hint: Enumerate all cubic mononomials e.g $x^3 \ldots xyz$. Express a general cubic polynomial in terms of these mononomials. Laplace's equation yields a relationship between the coefficients of the mononomials. Use the Gram Schmidt method, to find the linearly independent solutions of Laplace's equation.

Solution.

By substitution of the form

$$\begin{aligned}
\phi \ = \ & \gamma \ x \ y \ z \ + \alpha_1 \ x^3 \ + \ \alpha_2 \ y^3 \ + \ \alpha_3 \ z^3 \\
+ \ & \beta_1 \ x \ y^2 \ + \ \beta_2 \ x \ z^2 \ + \ \beta_3 \ y \ x^2 \ \ \beta_4 \ y \ z^2 \ + \ \beta_5 \ z \ x^2 \ + \ \beta_6 \ z \ y^2
\end{aligned} \tag{638}$$

one finds the seven linearly independent solutions

$$\begin{aligned}
\phi_{3,2s} &= x\ y\ z \\
\phi_{3,2c} &= z\ (\ x^2\ -\ y^2\ ) \\
\phi_{3,0} &= 2\ z^3\ -\ 3\ z\ (\ x^2\ +\ y^2\ ) \\
\phi_{3,3s} &= x^3\ -\ 3\ x\ y^2 \\
\phi_{3,3c} &= y^3\ -\ 3\ y\ x^2 \\
\phi_{3,1s} &= y^3\ +\ y\ x^2\ -\ 4\ y\ z^2 \\
\phi_{3,1c} &= x^3\ +\ x\ y^2\ -\ 4\ x\ z^2
\end{aligned} \tag{639}$$

These combinations are recognized as

$$\begin{aligned}
\phi_{3,2s} &= r^3\ \cos\theta\ \sin^2\theta\ \sin\varphi\ \cos\varphi \\
\phi_{3,2c} &= r^3\ \cos\theta\ \sin^2\theta\ (\ \cos^2\varphi\ -\ \sin^2\varphi\ ) \\
\phi_{3,0} &= r^3\ (\ 2\ \cos^3\theta\ -\ 3\ \cos\theta\ \sin^2\theta\ ) \\
\phi_{3,3s} &= r^3\ \sin^3\theta\ (\ \cos^3\varphi\ -\ \cos\varphi\ \sin^2\varphi\ ) \\
\phi_{3,3c} &= r^3\ \sin^3\theta\ (\ \sin^3\varphi\ -\ \sin\varphi\ \cos^2\varphi\ ) \\
\phi_{3,1s} &= r^3\ (\ \sin^2\theta\ -\ 4\ \cos^2\theta\ )\ \sin\theta\ \sin\varphi \\
\phi_{3,1c} &= r^3\ (\ \sin^2\theta\ -\ 4\ \cos^2\theta\ )\ \sin\theta\ \cos\varphi
\end{aligned} \tag{640}$$

which are orthogonal with each other, when considered as functions of φ.

8 Bessel Functions

Bessel's Differential Equation is

$$x^2 \frac{d^2 y_n(x)}{dx^2} + x \frac{d y_n(x)}{dx} + (x^2 - n^2) y_n = 0 \tag{641}$$

This has a singularity at $x = 0$. This is a regular singular point. The solution either diverges as x^{-n} or x^n. The two solutions are usually determined by the behavior near $x = 0$.

8.0.1 The Generating Function Expansion

The solutions for the different values of n, which are convergent at $x = 0$, can be determined from a generating function $g(x, t)$

$$g(x,t) = \exp \left[\frac{x}{2} (t - t^{-1}) \right] \tag{642}$$

The generating function expansion is given by

$$\exp \left[\frac{x}{2} (t - t^{-1}) \right] = \sum_{n=-\infty}^{n=\infty} y_n(x) \, t^n \tag{643}$$

The generating function is symmetric under the transformation

$$t \rightarrow - t^{-1} \tag{644}$$

which implies that $y_n(x)$ and $y_{-n}(x)$ are related via

$$y_{-n}(x) = (- 1)^n \, y_n(x) \tag{645}$$

On replacing $t = 1$ in the generating function expansion one then finds the sum rule

$$1 = \sum_{n=-\infty}^{n=\infty} y_n(x) \tag{646}$$

or

$$1 = y_0(x) + 2 \sum_{n=1}^{\infty} y_{2n}(x) \tag{647}$$

for all values of x.

8.0.2 Series Expansion

A series expansion (in x) for the functions $y_n(x)$ can be found by writing

$$\begin{aligned} g(x,t) &= \exp\left[\frac{x\,t}{2} \right] \exp\left[- \frac{x}{2\,t} \right] \\ &= \sum_{r=0}^{\infty} \frac{(\,x\,t\,)^r}{2^r\,r!} \sum_{s=0}^{\infty} (\,-\,1\,)^s \frac{x^s\,t^{-s}}{2^s\,s!} \\ &= \sum_{r,s=0}^{\infty} (\,-\,1\,)^s \frac{x^{r+s}\,t^{r-s}}{2^{r+s}\,r!\,s!} \end{aligned} \tag{648}$$

This series expansion can be compared with the generating function expansion

$$g(x,t) = \sum_{n=-\infty}^{\infty} y_n(x)\,t^n \tag{649}$$

if one identifies $n = r - s$ or alternatively

$$r = n + s \tag{650}$$

The function $y_n(x)$, for positive n, is given by the coefficient of t^n and is identified as a polynomial in x where the various powers correspond to the terms in the sum over all values of s. The function is found as

$$\begin{aligned} y_n(x) &= \sum_{s=0}^{\infty} (\,-1\,)^s \frac{x^{n+2s}}{2^{n+2s}\,s!\,(n+s)!} \\ &= \frac{x^n}{2^n} \sum_{s=0}^{\infty} (\,-\,1\,)^s \frac{x^{2s}}{2^{2s}\,s!\,(s+n)!} \end{aligned} \tag{651}$$

which is a series expansion in x which vanishes at the origin for $n > 0$. For negative n, the properties of the generating function yield $y_n(x) = (\,-\,1\,)^n\,y_{-n}(x)$ which also vanishes at the origin.

8.0.3 Recursion Relations

On differentiating the generating function expansion with respect to t the functions $y_n(t)$, for different values of n, are found to satisfy

$$\frac{x}{2}\,(\,1 + t^{-2}\,)\,\exp\left[\frac{x}{2}\,(\,t - t^{-1}\,) \right] = \sum_{n=-\infty}^{n=\infty} y_n(x)\,n\,t^{n-1} \tag{652}$$

On using the generating function expansion in the left hand side

$$\frac{x}{2} \, (\, 1 \, + \, t^{-2} \,) \sum_{n=-\infty}^{n=\infty} y_n(x) \, t^n \; = \; \sum_{n=-\infty}^{n=\infty} y_n(x) \, n \, t^{n-1} \tag{653}$$

and identifying the powers of t^{n-1} one finds the recursion relation

$$y_{n-1}(x) \; + \; y_{n+1}(x) \; = \; \frac{2 \, n}{x} \, y_n(x) \tag{654}$$

This recursion relation can be used to determine $y_{n+1}(x)$ in terms of $y_n(x)$ and $y_{n-1}(x)$. However, since the errors increase with increasing n it is more efficient to use the equation for $y_n(x)$ and $y_{n+1}(x)$ to determine $y_{n-1}(x)$ with lower values of n.

Another recursion relation can be found by taking the derivative of the generating function with respect to x

$$\frac{1}{2} \, (\, t \; - \; t^{-1} \,) \, \exp \left[\, \frac{x}{2} \, (\, t \; - \; t^{-1} \,) \, \right] \; = \; \sum_{n=-\infty}^{n=\infty} \frac{\partial y_n(x)}{\partial x} \, t^n \tag{655}$$

which leads to

$$\frac{\partial y_n(x)}{\partial x} \; = \; \frac{1}{2} \left(\, y_{n-1}(x) \; - \; y_{n+1}(x) \, \right) \tag{656}$$

These two recursion relations can be combined to yield either

$$\frac{n}{x} \, y_n(x) \; + \; \frac{\partial y_n(x)}{\partial x} \; = \; y_{n-1}(x) \tag{657}$$

or

$$\frac{n}{x} \, y_n(x) \; - \; \frac{\partial y_n(x)}{\partial x} \; = \; y_{n+1}(x) \tag{658}$$

respectively, if one eliminates either $y_{n+1}(x)$ or $y_{n-1}(x)$.

Compact alternate forms of the above two recursion relations can be found. For example, starting with

$$\frac{n}{x} \, y_n(x) \; + \; \frac{\partial y_n(x)}{\partial x} \; = \; y_{n-1}(x) \tag{659}$$

one can multiply by x^n and find that

$$\frac{\partial}{\partial x} \left[\, x^n \, y_n(x) \, \right] \; = \; x^n \, y_{n-1}(x) \tag{660}$$

and likewise, starting from the other one of the above pair of relations, one can show that

$$\frac{\partial}{\partial x} \left[x^{-n} \, y_n(x) \right] \; = \; - \, x^{-n} \, y_{n+1}(x) \tag{661}$$

8.0.4 Bessel's Equation

These set of recursion relations can be used to show that the functions $y_n(x)$ satisfy Bessel's equations. On differentiating the recursion relation

$$n \, y_n(x) \; + \; x \, \frac{\partial y_n(x)}{\partial x} \; = \; x \, y_{n-1}(x) \tag{662}$$

one obtains

$$(\, n \; + \; 1 \,) \, \frac{\partial y_n(x)}{\partial x} \; + \; x \, \frac{\partial^2 y_n(x)}{\partial x^2} \; = \; x \, \frac{\partial y_{n-1}(x)}{\partial x} \; + \; y_{n-1}(x) \tag{663}$$

Multiplying the above equation by x and subtracting n times the recurrence relationship for the derivative of $y_n(x)$, one obtains

$$x^2 \, \frac{\partial^2 y_n(x)}{\partial x^2} + x \, \frac{\partial y_n(x)}{\partial x} - n^2 \, y_n(x) \; = \; x^2 \, \frac{\partial y_{n-1}}{\partial x} - (\, n \, - \, 1 \,) \, x \, y_{n-1}(x) \tag{664}$$

The right hand side is identified as $-x^2 \, y_n(x)$, by using the other recursion relation for the derivative of $y_{n-1}(x)$. Thus, we find that $y_n(x)$ does indeed satisfy Bessel's equation

$$x^2 \, \frac{\partial^2 y_n(x)}{\partial x^2} \; + \; x \, \frac{\partial y_n(x)}{\partial x} \; + \; (\, x^2 \; - \; n^2 \,) \, y_n(x) \; = \; 0 \tag{665}$$

As Bessel's equation is a second order differential equation it has two solutions. The two solutions can be found from the Frobenius method as series expansions. The indicial equation yields

$$\alpha^2 \; = \; n^2 \tag{666}$$

The solutions which remain finite or vanish at $x \; = \; 0$, and have the leading term x^n are known as the integer Bessel functions, and are denoted by $J_n(x)$, while the solutions that diverge as x^{-n} at the origin are known as the Neumann functions $N_n(x)$. However, the generating function leads to a unique form of $y_n(x)$, which has been found as an expansion in x. By comparison, one finds that the functions $y_n(x)$ are proportional to the Bessel functions. The normalization is chosen such that

$$y_n(x) \; = \; J_n(x) \tag{667}$$

8.0.5 Integral Representation

The series for the Bessel functions can be expressed in terms of an integral. This can be shown by starting with the generating function expansion

$$\begin{aligned} g(x,t) &= J_0(x) + \sum_{n=1}^{\infty} \left(J_n(x) \, t^n + J_{-n}(x) \, t^{-n} \right) \\ &= J_0(x) + \sum_{n=1}^{\infty} J_n(x) \left(t^n + (- 1)^n \, t^{-n} \right) \end{aligned} \tag{668}$$

Changing variable from t to θ defined by $t = \exp[\, i\theta \,]$ one finds that the expansion takes the form

$$\begin{aligned} g(x, \exp[\, i \, \theta \,]) &= J_0(x) + \sum_{n=1}^{\infty} J_n(x) \left(\exp[+ i \, n \, \theta \,] + (- 1)^n \exp[- i \, n \, \theta \,] \right) \\ &= J_0(x) + \sum_{n=1}^{\infty} J_{2n}(x) \, 2 \, \cos \, 2 \, n \, \theta + \sum_{n=0}^{\infty} J_{2n+1}(x) \, 2 \, i \, \sin \, (\, 2 \, n + 1 \,) \, \theta \end{aligned} \tag{669}$$

where we have separated out the even and odd terms of the series. When expressed in terms of θ, the generating function reduces to

$$g(x, \exp[\, i \, \theta \,]) = \exp \left[\, i \, x \, \sin\theta \, \right] \tag{670}$$

On splitting the complex form of the generating function expansion into equations for the real and imaginary parts one finds the two equations

$$\begin{aligned} \cos \, (\, x \, \sin\theta \,) &= J_0(x) + 2 \sum_{n=1}^{\infty} J_{2n}(x) \, \cos \, 2 \, n \, \theta \\ \sin \, (\, x \, \sin\theta \,) &= 2 \sum_{n=0}^{\infty} J_{2n+1}(x) \, \sin \, (\, 2 \, n + 1 \,) \, \theta \end{aligned} \tag{671}$$

The Bessel functions can be obtained by using the orthogonality properties of the trigonometric function on the interval $(0, \pi)$. That is, we have

$$\begin{aligned} \int_0^{\pi} d\theta \, \cos n\theta \, \cos m\theta &= \frac{\pi}{2} \, \delta_{n,m} \\ \int_0^{\pi} d\theta \, \sin n\theta \, \sin m\theta &= \frac{\pi}{2} \, \delta_{n,m} \end{aligned} \tag{672}$$

Thus, on multiplying the real and imaginary part of the generating function by either $\sin n\theta$ or $\cos n\theta$ and integrating, we have the four equations

$$\begin{aligned}
J_{2n}(x) &= \frac{1}{\pi} \int_0^{2\pi} d\theta \, \cos(\, x \, \sin\theta \,) \, \cos \, 2n\theta \\
J_{2n+1}(x) &= \frac{1}{\pi} \int_0^{2\pi} d\theta \, \sin(\, x \, \sin\theta \,) \, \sin \, (2n+1) \, \theta \\
0 &= \frac{1}{\pi} \int_0^{2\pi} d\theta \, \sin(\, x \, \sin\theta \,) \, \cos \, 2n\theta \\
0 &= \frac{1}{\pi} \int_0^{2\pi} d\theta \, \cos(\, x \, \sin\theta \,) \, \sin \, (2n+1) \, \theta
\end{aligned} \tag{673}$$

depending on whether n is even or odd. Combining these equations in pairs, for odd n and even n, one has

$$\begin{aligned}
J_n(x) &= \frac{1}{\pi} \int_0^{2\pi} d\theta \left[\, \cos(\, x \, \sin\theta \,) \, \cos \, n\theta \, + \, \sin(\, x \, \sin\theta \,) \, \sin \, n\theta \, \right] \\
J_n(x) &= \frac{1}{\pi} \int_0^{2\pi} d\theta \, \cos \, (\, x \, \sin\theta \, - \, n \, \theta \,)
\end{aligned} \tag{674}$$

for non zero n. The above equations are integral representations of the Bessel functions.

8.0.6 Addition Theorem

An addition theorem can be found for the Bessel functions by noting that the generating functions satisfy the relation

$$g(x+y,t) \; = \; g(x,t) \; g(y,t) \tag{675}$$

so

$$\sum_{n=-\infty}^{\infty} J_n(x+y) \; t^n \; = \; \sum_{m=-\infty}^{\infty} J_m(x) \; t^m \; \sum_{l=-\infty}^{\infty} J_l(y) \; t^l \tag{676}$$

or

$$\sum_{n=-\infty}^{\infty} J_n(x+y) \; t^n \; = \; \sum_{n=-\infty}^{\infty} \; \sum_{m=-\infty}^{\infty} J_m(x) \; J_{n-m}(y) \; t^n \tag{677}$$

Hence, on equating the coefficients of t^n, one has the Bessel function addition theorem

$$J_n(x+y) \; = \; \sum_{m=-\infty}^{\infty} J_m(x) \; J_{n-m}(y) \tag{678}$$

The Bessel functions often occur in problems that involve circular planar symmetry, like a vibrating drum head. In this case, one describes the location of a point on the circular surface of the drum by planar polar coordinates (r, φ). Another application occurs in the theory of diffraction.

Example:

Consider a light wave falling incident normally on a screen with a circular opening of radius a. It will be seen that the intensity of the transmitted light falling on a distant screen will form a circular pattern. The intensity of the transmitted light may fall to zero on concentric circles. The strength of the electric field passing through the circular aperture and arriving at a distant point on the other side of the aperture, directed an angle α normal to the aperture is given by

$$E \sim \int_0^a dr \; r \int_0^{2\pi} d\varphi \; \exp \left[\; i \; \frac{2\pi}{\lambda} \; r \; \sin\alpha \; \cos\varphi \; \right] \tag{679}$$

This electric field is the sum of the amplitudes of the light originating from the points (r, φ) inside the circular aperture, weighted by the phase from their differences in optical path length $r \; \cos\varphi \; \sin\alpha$. The integration over φ can be performed using the integral representation of the Bessel function

$$E \sim \int_0^a dr \; r \; 2 \; \pi \; J_0 \left(\; \frac{2\pi}{\lambda} \; r \; \sin\alpha \; \right) \tag{680}$$

The integration over r can be performed by using the recursion relations, leading to

$$E \sim \frac{\lambda \; a}{\sin\alpha} \; J_1 \left(\; \frac{2 \; \pi \; a}{\lambda} \; \sin\alpha \; \right) \tag{681}$$

The intensity of the light, I, arriving at the distant screen is proportional to $| \; E \; |^2$, so

$$I \sim \left(\; \frac{\lambda \; a}{\sin\alpha} \; \right)^2 \; J_1^2 \left(\; \frac{2 \; \pi \; a}{\lambda} \; \sin\alpha \; \right) \tag{682}$$

The angle α lies between 0 and $\frac{\pi}{2}$ so the factor $\sin\alpha$ vanishes at 0. Thus, the denominator vanishes for light transmitted in the normal direction, but fortunately so does the Bessel function J_1, as can be seen from the Frobenius series. Thus, on using l'Hopital's rule, the intensity is non-vanishing for a point directly in front of the aperture, as expected. However, the intensity falls to zero in specific directions α determined by the vanishing of the Bessel function J_1

$$J_1 \left(\; \frac{2 \; \pi \; a}{\lambda} \; \sin\alpha \; \right) \; = \; 0 \tag{683}$$

For a sufficiently large aperture, $a \gg \lambda$, the intensity falls to zero at the angles. The first zero is found at the angle α determined by

$$\frac{2\pi\ a}{\lambda}\ \sin\alpha\ =\ 3.8137 \tag{684}$$

For a macroscopic opening $a\ =\ 0.5\ \times\ 10^{-2}$ m and $\lambda\ \sim\ 10^{-7}$ m one has

$$\alpha\ \sim\ 10^{-5}\ rad \tag{685}$$

Thus, the first circle of zero intensity makes has an extremely small angular spread. The outer circles are determined by the higher order zeroes of the Bessel function , and for large n are approximated by

$$\frac{2\ \pi\ a}{\lambda}\ \sin\alpha\ \sim\ n\ \pi \tag{686}$$

which is similar to the Bragg condition. The outer dark rings are hard to observe as the intensity between the rings is very low.

Example:

A particle of mass m is confined within a cylinder of radius a and length l. The particle is in an energy eigenstate described by the equation

$$-\ \frac{\hbar^2}{2\ m}\ \nabla^2\Psi\ =\ E\ \Psi \tag{687}$$

where the allowed value of the energy is denoted by E. The wave function $\Psi(r,\theta,z)$ expressed in terms of cylindrical coordinates satisfies the boundary conditions

$$\begin{aligned}\Psi(a,\theta,z)\ &=\ 0\\ \Psi(r,\theta,0)\ &=\ \Psi(r,\theta,l)\ =\ 0\end{aligned} \tag{688}$$

Find an expression for the wave functions and the allowed energies.

The eigenvalue equation can be written in the form

$$\frac{1}{r}\ \frac{\partial}{\partial r}\left(\ r\ \frac{\partial\Psi}{\partial r}\ \right)\ +\ \frac{1}{r^2}\ \frac{\partial^2\Psi}{\partial\theta^2}\ +\ \frac{\partial^2\Psi}{\partial z^2}\ =\ -\ \frac{2\ m\ E}{\hbar^2}\ \Psi \tag{689}$$

On substituting the ansatz for the eigenfunction

$$\Psi(r,\theta,z)\ =\ R(r)\ \Theta(\theta)\ Z(z) \tag{690}$$

into the equation and diving by Ψ one finds

$$\frac{1}{r\,R}\,\frac{\partial}{\partial r}\left(\,r\,\frac{\partial R}{\partial r}\,\right)\;+\;\frac{1}{r^2\,\Theta}\,\frac{\partial^2\Theta}{\partial\theta^2}\;=\;-\;\frac{2\,m\,E}{\hbar^2}\;-\;\frac{1}{Z}\,\frac{\partial^2 Z}{\partial z^2} \tag{691}$$

Since the z dependence is entirely contained in the right hand side, and the left hand side is constant as the independent variable z is changed, we must have

$$\frac{\partial^2 Z}{\partial z^2}\;=\;-\;\kappa^2\;Z \tag{692}$$

where $-\;\kappa^2$ is an arbitrary constant. This equation has a general solution

$$Z(z) = \;A\;\cos\kappa z\;+\;B\;\sin\kappa z \tag{693}$$

Since Ψ must vanish on the two surfaces $z\;=\;0$ and $z\;=\;l$ one determines the constants as

$$\begin{aligned} A\;&=\;0\\ B\;\sin\kappa l\;&=\;0 \end{aligned} \tag{694}$$

Hence, we have the allowed solutions

$$Z(z)\;=\;B\;\sin\frac{n_z\;\pi\;z}{l} \tag{695}$$

where n_z is an arbitrary positive integer, and $\kappa\;=\;\frac{n_z\pi}{l}$. On substituting $Z(z)$ back into the differential equation, and multiplying by r^2 one has

$$\frac{r}{R}\,\frac{\partial}{\partial r}\left(\,r\,\frac{\partial R}{\partial r}\,\right)\;+\;\frac{1}{\Theta}\,\frac{\partial^2\Theta}{\partial\theta^2}\;=\;-\;r^2\left(\frac{2\,m\,E}{\hbar^2}\;-\;\frac{n_z^2\pi^2}{l^2}\right) \tag{696}$$

From the above equation one can recognize that the θ dependent term must also be a constant, say $-\;m^2$, and therefore satisfies the differential equation

$$\frac{\partial^2\Theta(\theta)}{\partial\theta^2}\;=\;-\;m^2\;\Theta \tag{697}$$

which has solutions of the form

$$\Theta(\theta)\;=\;\exp\left[\;i\;m\;\theta\;\right] \tag{698}$$

Since the wave function has a unique value at any point, one must have

$$\Theta(\theta\;+\;2\;\pi)\;=\;\Theta(\theta) \tag{699}$$

which implies that m must be a positive or negative integer.
Finally, we find that the radial function satisfies the equation

$$r\,\frac{\partial}{\partial r}\left(\,r\,\frac{\partial R}{\partial r}\,\right)\;-\;m^2\;R\;=\;-\;r^2\left(\,\frac{2\,m\,E}{\hbar^2}\;-\;\frac{n_z^2\pi^2}{l^2}\,\right)\,R \tag{700}$$

We shall put this equation into a dimensionless form by introducing the variable $x = k\ r$, where k is to be determined. The differential equation of $R(x/k)$ becomes

$$x \frac{\partial}{\partial x} \left(x \frac{\partial R}{\partial x} \right) - m^2 R = - \frac{x^2}{k^2} \left(\frac{2\ m\ E}{\hbar^2} - \frac{n_z^2 \pi^2}{l^2} \right) R \qquad (701)$$

If we choose the value of k to be given by

$$k^2 = \left(\frac{2\ m\ E}{\hbar^2} - \frac{n_z^2 \pi^2}{l^2} \right) \qquad (702)$$

the differential equation has the form of Bessel's equation

$$x \frac{\partial}{\partial x} \left(x \frac{\partial R}{\partial x} \right) + (\ x^2 - m^2\ )\ R = 0 \qquad (703)$$

and has the solutions

$$R(r) = J_m(kr) \qquad (704)$$

which are regular at the origin. Since, the wave function must vanish at the walls of the cylinder, the value k must satisfy

$$J_m(ka) = 0 \qquad (705)$$

and so the allowed values of k are given by

$$k_{m,n} = \frac{z_{m,n}}{a} \qquad (706)$$

where $z_{m,n}$ is the n-th zero of the m-th Bessel function, i.e.

$$J_m(z_{m,n}) = 0 \qquad (707)$$

Thus we have shown that the eigenfunctions are of the form of

$$\Psi(r, \theta, z) = \sin \frac{n_z\ \pi\ z}{l}\ \exp \left[\ i\ m\ \theta\ \right]\ J_m(\frac{z_{m,n}\ r}{a}) \qquad (708)$$

and the allowed energy eigenvalues are simply given by

$$E = \frac{\hbar^2}{2\ m} \left(\frac{z_{m,n}^2}{a^2} + \frac{n_z^2\ \pi^2}{l^2} \right) \qquad (709)$$

Example:

Consider the electromagnetic field inside a cylindrical metal cavity of radius a and length l. Maxwell's equations are given by

$$\vec{\nabla} \wedge \vec{E} = - \frac{1}{c} \frac{\partial \vec{B}}{\partial t} \tag{710}$$

and

$$\vec{\nabla} \wedge \vec{B} = + \frac{1}{c} \frac{\partial \vec{E}}{\partial t} \tag{711}$$

Maxwell's equations can be combined to yield the wave equation governing the electric field

$$\vec{\nabla} \wedge \left(\vec{\nabla} \wedge \vec{E} \right) = - \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} \tag{712}$$

and since Gauss's law holds

$$\vec{\nabla} . \vec{E} = 0 \tag{713}$$

one has

$$- \nabla^2 \vec{E} = - \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} \tag{714}$$

On representing the time dependence of the electric field as a wave of frequency ω via

$$\vec{E}(\underline{r}, t) = \vec{E}(\underline{r}) \text{ Real} \left[\exp[\, i \, \omega \, t \,] \right] \tag{715}$$

then one finds that the spatial dependence of the field satisfies

$$- \nabla^2 \vec{E}(\underline{r}) = \frac{\omega^2}{c^2} \vec{E}(\underline{r}) \tag{716}$$

In cylindrical coordinates the z component of the electric field satisfies the Laplacian eigenvalue equation

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial E_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 E_z}{\partial \theta^2} + \frac{\partial^2 E_z}{\partial z^2} = - \frac{\omega^2}{c^2} E_z \tag{717}$$

On using the method of separation of variables we assume that the z component of the electric field can be written as the product

$$E_z = R(r) \, \Theta(\theta) \, Z(z) \tag{718}$$

On substituting this ansatz into the partial differential equation one finds that it separates into three ordinary differential equations. The z dependent function $Z(z)$ satisfies

$$\frac{\partial^2 Z(z)}{\partial z^2} = - k_z^2 \, Z(z) \tag{719}$$

and $\Theta(\theta)$ satisfies

$$\frac{\partial^2 \Theta(\theta)}{\partial \theta^2} = - m^2 \, \Theta(\theta) \tag{720}$$

Using the values of the separation constants, one finds that the Radial function $R(r)$ has to satisfy

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial R}{\partial r} \right) - \frac{m^2}{r^2} R = - \left(\frac{\omega^2}{c^2} - k_z^2 \right) R \tag{721}$$

which is Bessel's equation. Thus, the general solution of the partial differential equation has been found to be of the form

$$E_z(\underline{r}) = \sum_{m,k_r} J_m(k_r r) \exp \left[i \, m \, \theta \right] \left(a_{m,k_r} \sin k_z z + b_{m,k_r} \cos k_z z \right) \tag{722}$$

where the constants of separation are related by

$$\frac{\omega^2}{c^2} = k_z^2 + k_r^2 \tag{723}$$

The boundary condition at the cylindrical walls is that the component of the electric field parallel to the axis vanishes. This implies that

$$J_m(k_r \, a) = 0 \tag{724}$$

Hence, the allowed values of k_r are given in terms of the zeros of the m-th Bessel function. The allowed k values are given by

$$k_r = \frac{z_{m,n}}{a} \tag{725}$$

where z_{mn} stands for the n-th zero of the m-th Bessel function, i.e. $J_m(z_{m,n}) = 0$. The electromagnetic field must also satisfy boundary conditions at the two ends of the cylinder. The boundary conditions at the ends of the cylinder $z = 0$ and $z = l$ are satisfied by setting $a_{m,k_r} = 0$ and $k_z = \frac{n_z \, \pi}{l}$ for integer and zero values of n_z. In this case, the tangential components of the field E_r and E_θ vanish at $z = 0$ and $z = l$. This leads to the magnetic induction field being purely transverse. The allowed values of the frequencies are given by

$$\omega = c \sqrt{\frac{z_{m,n}^2}{a^2} + \frac{n_z^2 \, \pi^2}{l^2}} \tag{726}$$

8.0.7 Orthonormality

The orthonormality relations for the Bessel functions can be proved by starting from Bessel's equation

$$x^2 \frac{\partial^2 \phi_\nu(x)}{\partial x^2} + x \frac{\partial \phi_\nu(x)}{\partial x} + (x^2 - \nu^2) \phi_\nu(x) = 0 \tag{727}$$

Due to physical reasons, we shall write $x = k\,r$ and use zero boundary conditions at the center and edge of the circular area $r = 0$ and at $r = a$. Thus, we demand that our solution must satisfy

$$\phi_\nu(0) = \phi_\nu(ka) = 0 \tag{728}$$

In this case, Bessel's equation has the form

$$\begin{aligned} \frac{\partial^2}{\partial r^2}\,\phi_\nu(kr) + \frac{1}{r}\,\frac{\partial}{\partial r}\,\phi_\nu(kr) + \left(k^2 - \frac{\nu^2}{r^2} \right) \phi_\nu(kr) &= 0 \\ \frac{1}{r}\,\frac{\partial}{\partial r}\left(r\,\frac{\partial}{\partial r}\,\phi_\nu(kr) \right) + \left(k^2 - \frac{\nu^2}{r^2} \right) \phi_\nu(kr) &= 0 \end{aligned} \tag{729}$$

where k^2 can be regarded as the eigenvalue. The eigenvalue, or rather the value k_m, is determined by demanding that the solution of Bessel's equation $\phi_\nu(k_m r)$ satisfies the boundary condition

$$\phi_\nu(k_m a) = 0 \tag{730}$$

The orthogonality of $\phi_\nu(k_m a)$ and $\phi_\nu(k_n a)$ can be proved by multiplying the equation for $\phi_\nu(k_m a)$ by $\phi_\nu(k_n a)$ and subtracting this from the analogous equation with m and n interchanged

$$\begin{aligned} \phi_\nu(k_m r)\,\frac{1}{r}\,\frac{\partial}{\partial r}\left(r\,\frac{\partial}{\partial r}\,\phi_\nu(k_n r) \right) - \phi_\nu(k_n r)\,\frac{1}{r}\,\frac{\partial}{\partial r}\left(r\,\frac{\partial}{\partial r}\,\phi_\nu(k_m r) \right) \\ = \phi_\nu(k_n r)\,(\,k_m^2 - k_n^2\,)\,\phi_\nu(k_m r) \end{aligned} \tag{731}$$

On multiplying by the weighting factor r (which, due to the two dimensional circular symmetry, is related to the infinitesimal area element given by $dr\;r\;d\varphi$) and integrating by parts, one finds that

$$\begin{aligned} \phi_\nu(k_m r)\;r\,\frac{\partial}{\partial r}\,\phi_\nu(k_n r)\,\Big|_0^a - \phi_\nu(k_n r)\;r\,\frac{\partial}{\partial r}\,\phi_\nu(k_m r)\,\Big|_0^a \\ = (\,k_m^2 - k_n^2\,)\int_0^a dr\;r\;\phi_\nu(k_n r)\;\phi_\nu(k_m r) \end{aligned} \tag{732}$$

Using the boundary conditions at $r = a$ and noting that the solutions are finite at $r = 0$, one finds that the eigenfunctions corresponding to different eigenvalues are orthogonal, as

$$(\,k_m^2 - k_n^2\,)\int_0^a dr\;r\;\phi_\nu(k_n r)\;\phi_\nu(k_m r) = 0 \tag{733}$$

The normalization can be found by setting $k_m = k_n + \epsilon$, hence, on using the boundary condition at $r = 0$ one has

$$\phi_\nu(k_n a + \epsilon a) \; a \; \phi'_\nu(k_n a) \; - \; \phi_\nu(k_n a) \; a \; \phi'_\nu(k_n a + \epsilon a) \Big|_0^a$$
$$= 2 \, \epsilon \int_0^a dr \; r \; \phi_\nu(k_n r) \; \phi_\nu(k_n r) \tag{734}$$

and using the boundary conditions one finds

$$2 \, \epsilon \int_0^a dr \; r \; \phi_\nu(k_n r) \; \phi_\nu(k_n r) \; = \; a^2 \; k_n \; \epsilon \; \phi'^2_\nu(k_n a) \tag{735}$$

Furthermore, since

$$\phi_{\nu+1}(k_n a) \; = \; \frac{\nu}{k_n a} \; \phi_\nu(k_n a) \; - \; \phi'_\nu(k_n a) \tag{736}$$

one has

$$\int_0^a dr \; r \; \phi^2_\nu(k_n r) \; = \; \frac{a^2}{2} \left[\; \phi^2_{\nu+1}(k_n a) \; \right] \tag{737}$$

In the limit $a \to \infty$, the normalization condition becomes

$$\int_0^\infty dr \; \phi_\nu(kr) \; r \; \phi_\nu(k' r) \; = \; \frac{1}{k} \; \delta(k' - k) \tag{738}$$

8.0.8 Bessel Series

Since the set of Bessel functions $\phi_\nu(k_n a)$ for fixed ν and different k_m values form a complete set, then an arbitrary function $\Phi(r)$ can be expanded as a Bessel Series

$$\Phi(r) \; = \; \sum_m \; C_m \; \phi_\nu(k_m r) \tag{739}$$

for $a > r > 0$. The expansion coefficients C_m can be found via

$$C_m \; = \; \frac{2}{a^2 \; \phi^2_{\nu+1}(k_m a)} \int_0^a dr \; \Phi(r) \; r \; \phi_\nu(k_m r) \tag{740}$$

Example:

The amplitude $u(r, \theta, t)$ of the vertical displacements of a circular drumhead of radius a satisfies the wave equation

$$\nabla^2 u \ - \ \frac{1}{c^2} \ \frac{\partial^2 \ u}{\partial t^2} \ = \ 0 \qquad (741)$$

where c is the velocity of the sound waves on the drumhead. Since the drumhead is fixed tightly to the circular rim, the boundary conditions is that there is no vertical displacement so

$$u(a, \theta, t) \ = \ 0 \qquad (742)$$

In circular coordinates one has

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\ r \ \frac{\partial u}{\partial r} \right) \ + \ \frac{1}{r^2} \ \frac{\partial^2 u}{\partial \theta^2} \ = \ \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} \qquad (743)$$

This partial differential equation can be solved by assuming that the solution can be expressed as a Fourier series in the time variable. For any fixed time t, the solution can be considered to be a function of (r, θ). The θ dependence can be expressed as a series in Legendre polynomials, where the coefficients are functions of r. The undetermined coefficients which are functions of r can then be expanded as a Bessel series. The general term in this multiple expansion is given by the ansatz

$$u(r, \theta, t) \ = \ R(r) \ \Theta(\theta) \ \exp \left[\ i \ \omega \ t \ \right] \qquad (744)$$

On substituting this ansatz into the equation, cancelling the common time dependent terms, the equation reduces to

$$\Theta(\theta) \ \frac{1}{r} \frac{\partial}{\partial r} \left(\ r \ \frac{\partial R(r)}{\partial r} \right) \ + \ \frac{R(r)}{r^2} \ \frac{\partial^2 \Theta(\theta)}{\partial \theta^2} \ = \ - \ \frac{\omega^2}{c^2} \ R(r) \ \Theta(\theta) \qquad (745)$$

On multiplying by $r^2 \ R^{-1}(r) \ \Theta^{-1}(\theta)$ one has

$$\frac{r}{R(r)} \frac{\partial}{\partial r} \left(\ r \ \frac{\partial R(r)}{\partial r} \right) \ + \ \frac{1}{\Theta(\theta)} \ \frac{\partial^2 \Theta(\theta)}{\partial \theta^2} \ = \ - \ \frac{\omega^2}{c^2} \ r^2 \qquad (746)$$

This equation can be written such that one side depends on r alone and another side which depends on θ alone

$$\frac{r}{R(r)} \frac{\partial}{\partial r} \left(\ r \ \frac{\partial R(r)}{\partial r} \right) + \ \frac{\omega^2}{c^2} \ r^2 \ = \ - \ \frac{1}{\Theta(\theta)} \ \frac{\partial^2 \Theta(\theta)}{\partial \theta^2} \qquad (747)$$

Thus, the solution can be obtained by the method of separation of variables. It can be seen that, since the left hand side is independent of θ and the right hand side is independent of r, they must be equal to a constant, (say $- m^2$). Thus, we have

$$\frac{\partial^2 \Theta(\theta)}{\partial \theta^2} = - m^2 \Theta(\theta) \tag{748}$$

which has solutions of the form

$$\Theta(\theta) = A \cos m\theta + B \sin m\theta \tag{749}$$

Since, one can identify the point (r, θ) as $(r, \theta + 2\pi)$, then one requires that

$$\Theta(\theta + 2\pi) = \Theta(\theta) \tag{750}$$

which requires that m is an integer. Furthermore, the other side of the equation is equal to the same constant

$$r \frac{\partial}{\partial r} \left(r \frac{\partial R(r)}{\partial r} \right) + \frac{\omega^2}{c^2} r^2 R(r) = m^2 R(r) \tag{751}$$

which can be recognized as Bessel's equation of integer order

$$x^2 \frac{\partial^2 J_m(x)}{\partial x^2} + x \frac{\partial J_m(x)}{\partial x} + (x^2 - m^2) J_m(x) = 0 \tag{752}$$

if the variable $x = \frac{\omega}{c} r$. The solutions $J_m(x)$ are retained and the Neumann functions are discarded as the amplitude is expected to not diverge at $r = 0$. Thus, for a fixed Fourier component ω, the solution can be written as

$$u_\omega(r, \theta, t) = \sum_{m=0}^{\infty} \exp \left[i \omega t \right] J_m \left(\frac{\omega}{c} r \right) (A_m(\omega) \cos m\theta + B_m(\omega) \sin m\theta) \tag{753}$$

The allowed values of ω, ω_n, are determined by the boundary condition, which becomes

$$J_m \left(\frac{\omega_n}{c} a \right) = 0 \tag{754}$$

Thus, the frequencies of the normal modes of the drum head are determined by the zeroes of the Bessel functions $J_m(x)$. The general solution, is a sum over the different frequencies ω_n, and thus is in the form of a Bessel series

$$u(r, \theta, t) = \sum_{m=0}^{\infty} \sum_{\omega_n} \exp \left[i \omega_n t \right] (A_m(\omega_n) \cos m\theta + B_m(\omega_n) \sin m\theta) J_m \left(\frac{\omega_n}{c} r \right) \tag{755}$$

The expansion coefficients have to be determined from the initial conditions. This can be done, as an arbitrary initial condition can always be expanded in terms of a Bessel series.

Example:

A disk of radius R in the x-y plane ($z = 0$) is kept at a constant potential ϕ_0 and the rest of the plane $z = 0$ is kept at zero potential. Find the potential for $z > 0$.

The potential satisfies Laplace's equation

$$\nabla^2 \phi = 0 \tag{756}$$

which in cylindrical symmetry, where the potential is independent of θ, becomes

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) + \frac{\partial^2 \phi}{\partial z^2} = 0 \tag{757}$$

Using the method of separation of variables one seeks solutions of the homogeneous equation in the form

$$\phi(r, z) = R(r) \, Z(z) \tag{758}$$

On substitution of the ansatz for the solution, one finds that R and Z must satisfy

$$\frac{1}{r \, R} \frac{\partial}{\partial r} \left(r \frac{\partial R}{\partial r} \right) = - \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} \tag{759}$$

Since the left and right hand side are functions of independent variables r and z, they must be equal to a constant (say $- k^2$). Then the differential equation is equivalent to the pair of ordinary differential equations

$$\frac{\partial^2 Z}{\partial z^2} = k^2 \, Z \tag{760}$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial R}{\partial r} \right) + k^2 \, R = 0 \tag{761}$$

The equation for $Z(z)$ has the solution

$$Z(z) = A \exp \left[- k \, z \right] + B \exp \left[+ k \, z \right] \tag{762}$$

but since the potential must vanish as $z \to \infty$ one has $B = 0$. Likewise, the radial part of the potential is given by

$$R(r) = J_0(kr) \tag{763}$$

as the potential remains finite at the center of the disk, $r = 0$. Thus, we find the general solution of the partial differential equation is of the form of the linear superposition

$$\phi(r,z) = \int_0^\infty dk \; A(k) \; J_0(kr) \; \exp\left[- \; k \; z \right] \tag{764}$$

where $A(k)$ has to be determined by the boundary condition at $z = 0$.

Imposing the boundary condition at $z = 0$ yields

$$\phi(r,0) = \int_0^\infty dk \; A(k) \; J_0(kr) \tag{765}$$

On multiplying by $J_0(k'r)$ and integrating over r with a weight factor of r one has

$$\int_0^\infty dr \; r \; J_0(k'r) \; \phi(r,0) = \int_0^\infty dr \; r \; J_0(k'r) \int_0^\infty dk \; A(k) \; J_0(kr) \tag{766}$$

On interchanging the order of integration and using the continuum form of the orthonormality relation

$$\int_0^\infty dr \; r \; J_0(kr) \; J_0(k'r) = \frac{1}{k} \, \delta(\, k \; - \; k' \,) \tag{767}$$

one determines the coefficients $A(k')$, as the integral

$$\frac{1}{k'} \; A(k') = \phi_0 \int_0^R dr \; r \; J_0(k'r) \tag{768}$$

However, due to the Bessel function recursion relation

$$\frac{\partial}{\partial r} \left(\; r \; J_1(k'r) \; \right) = k' \; r \; J_0(k'r) \tag{769}$$

one can perform the integration and find

$$A(k') = \phi_0 \; R \; J_1(k'R) \tag{770}$$

Hence, we have the potential as

$$\phi(r,z) = \phi_0 \; R \int_0^\infty dk \; J_1(kR) \; J_0(kr) \; \exp\left[- \; k \; z \right] \tag{771}$$

The potential above the center of the disk ($r = 0$) is given by the integral

$$\begin{aligned} \phi(0,z) &= \phi_0 \; R \int_0^\infty dk \; J_1(kR) \; \exp \Bigg[- \; k \; z \Bigg] \\ &= \phi_0 \left[1 \; - \; \frac{z}{\sqrt{z^2 \; + \; R^2}} \right] \end{aligned} \tag{772}$$

This can be seen by noting the special case of the Bessel function recurrence relations yields

$$J_1(x) \;=\; - \; \frac{\partial J_0(x)}{\partial x} \tag{773}$$

This relation can be used in the integration of the expression for the potential. On integrating by parts with respect to k, one finds the equation

$$\begin{aligned} \phi(0,z) &= \phi_0 \Bigg(\; - \; J_0(kR) \; \exp \Bigg[\; - \; k \; z \Bigg] \Bigg|_{k=0}^{k=\infty} \; - \; z \int_0^\infty dk \; J_0(kR) \; \exp \Bigg[\; - \; k \; z \Bigg] \Bigg) \\ \phi(0,z) &= \phi_0 \Bigg(\; 1 \; - \; z \int_0^\infty dk \; J_0(kR) \; \exp \Bigg[\; - \; k \; z \Bigg] \Bigg) \end{aligned} \tag{774}$$

The last integral can be evaluated by using the integral representation of the Bessel function.

$$\begin{aligned} \int_0^\infty dk \; J_0(kR) \; \exp \Bigg[\; - \; k \; z \Bigg] &= \int_0^\infty dk \; \left(\frac{2}{\pi} \right) \int_0^{\frac{\pi}{2}} d\varphi \; \cos(\; kR \; \sin\varphi \;) \; \exp \Bigg[\; - \; k \; z \Bigg] \\ &= \left(\frac{2}{\pi} \right) \int_0^{\frac{\pi}{2}} d\varphi \int_0^\infty dk \; \cos(\; kR \; \sin\varphi \;) \; \exp \Bigg[\; - \; k \; z \Bigg] \\ &= \left(\frac{2}{\pi} \right) \int_0^{\frac{\pi}{2}} d\varphi \; \frac{z}{z^2 \; + \; R^2 \; \sin^2\varphi} \\ &= \frac{1}{\sqrt{z^2 \; + \; R^2}} \end{aligned} \tag{775}$$

Thus, the potential on the axis is given by

$$\phi(0,z) \;=\; \phi_0 \left[1 \; - \; \frac{z}{\sqrt{z^2 \; + \; R^2}} \right] \tag{776}$$

Example:

A cylinder, of length l and radius a, has the top plate held at a potential $\phi(l,r)$ and the bottom plate is held at a potential $\phi(0,r)$. The potential between the plates is given by

$$\nabla^2 \phi = 0 \tag{777}$$

which reduces to

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) + \frac{\partial^2 \phi}{\partial z^2} = 0 \tag{778}$$

From separation of variables one finds the solutions of the homogeneous equation in the form

$$\phi(z,r) = R(r) \, Z(z) \tag{779}$$

On substituting this form into the partial differential equation, one finds that

$$\frac{1}{r \, R} \frac{\partial}{\partial r} \left(r \frac{\partial R}{\partial r} \right) = - \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} \tag{780}$$

Thus, the equations for the r dependence and z dependence separates. On assuming a separation constant of $- \,^2$, one finds that the differential equation for R and Z is equivalent to the pair of ordinary differential equations

$$\frac{\partial^2 Z}{\partial z^2} = k^2 \, Z \tag{781}$$

and

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial R}{\partial r} \right) + k^2 \, R = 0 \tag{782}$$

The equation for $Z(z)$ has a general solution of the form

$$Z(z) = A_k \cosh[\, k \, z \,] + B_k \sinh[\, k \, z \,] \tag{783}$$

while the solution of the radial equation which is regular at the center of the cylinder, $r = 0$, is given by

$$R(r) = J_0(kr) \tag{784}$$

The Bessel function of zero-th order occurs since the potential is invariant under arbitrary rotations about the cylinders axis. The boundary condition at the surface of the cylinder is equivalent to requiring

$$J_0(ka) = 0 \tag{785}$$

which yields the allowed values of k, in terms of the zeroes of the zeroth order Bessel function, $k_n = \frac{z_n}{a}$. The solution can be expressed as

$$\phi(z,r) = \sum_k \left(A_k \cosh[\, k \, z \,] + B_k \sinh[\, k \, z \,] \right) J_0(kr) \tag{786}$$

The coefficients A_k and B_k can be obtained, by first finding the coefficients in the Bessel expansion of $\phi(0,r)$ and $\phi(l,r)$. At the top plate, ($z \; = \; l$), we expand the boundary value as a Bessel series

$$\phi(l,r) \; = \; \sum_k \tilde{\phi}_k(l) \; J_0(kr) \tag{787}$$

where the expansion coefficients are found from

$$\tilde{\phi}_k(l) \; = \; \frac{2}{a^2 \; J_1^2(ka)} \int_0^a dr \; r \; \phi(l,r) \; J_0(kr) \tag{788}$$

and likewise at $z \; = \; 0$ one can also expand $\phi(0,r)$. Then, at the bottom plate, ($z \; = \; 0$), we have

$$\phi(0,r) \; = \; \sum_k \tilde{\phi}_k(0) \; J_0(kr) \tag{789}$$

where the coefficients are found from

$$\tilde{\phi}_k(0) \; = \; \frac{2}{a^2 \; J_1^2(ka)} \int_0^a dr \; r \; \phi(0,r) \; J_0(kr) \tag{790}$$

Then finally, we have the solution in the form of a sum

$$\phi(z,r) \; = \; \sum_k \left[\; \tilde{\phi}_k(0) \; \frac{\sinh \; k \; (l \; - \; z \;)}{\sinh \; k \; l} \; + \; \tilde{\phi}_k(l) \; \frac{\sinh \; k \; z}{\sinh \; k \; l} \; \right] J_0(kr) \tag{791}$$

where the allowed values of k are given by the zeroes of the Bessel function.

Homework: 11.2.3

Homework: 11.2.9

8.1 Neumann Functions

The Neumann functions $N_n(x)$ are also solutions of Bessel's equation, and are known as Bessel functions of the second kind. They are distinguished from the Bessel functions of the first kind $J_n(x)$ in that they diverge as x^{-n} in the limit $x \; \rightarrow \; 0$. In particular, for non-integer ν they are defined in terms of $J_\nu(x)$ and $J_{-\nu}(x)$ via

$$N_\nu(x) \; = \; \frac{\cos \nu\pi \; J_\nu(x) \; - \; J_\nu(x)}{\sin \nu\pi} \tag{792}$$

Thus, the Neumann functions are particular linear combinations of the Bessel functions. On substituting the power series expansion for $J_\nu(x)$ one finds

$$N_\nu(x) \; = \; - \; \frac{(\nu-1)!}{\pi} \left(\frac{2}{x} \right)^\nu \; + \; \ldots \tag{793}$$

for $\nu \; > \; 0$.

Example:

An example which involves Neumann functions is the co-axial wave guide. The co-axial wave guide or cable is composed of two metal cylinders, with the same axis. The radius of the outer cylinder is b and the radius of the inner cylinder is a. The electromagnetic field is confined in the region enclosed between the two cylinders. We shall consider the component of the electric field E_z, along the direction of the axis, $\hat{e}_z$. This satisfies

$$\overrightarrow{\nabla} \wedge \left(\overrightarrow{\nabla} \wedge \overrightarrow{E} \right) \; = \; - \; \frac{1}{c^2} \, \frac{\partial^2 \overrightarrow{E}}{\partial t^2} \tag{794}$$

or on Fourier Transforming with respect to time

$$\overrightarrow{\nabla} \wedge \left(\overrightarrow{\nabla} \wedge \overrightarrow{E} \right) \; = \; \frac{\omega^2}{c^2} \, \overrightarrow{E} \tag{795}$$

However, one has the identity

$$\overrightarrow{\nabla} \wedge \left(\overrightarrow{\nabla} \wedge \overrightarrow{E} \right) \; = \; - \, \nabla^2 \, \overrightarrow{E} \; + \; \overrightarrow{\nabla} \, (\, \overrightarrow{\nabla} \, . \, \overrightarrow{E} \,) \tag{796}$$

and Gauss's law reduces to $\overrightarrow{\nabla} \, . \, \overrightarrow{E} \; = \; 0$ in vacuum with no charges present. Thus, the z component of the electric field is governed by

$$\nabla^2 \, E_z \; + \; \left(\frac{\omega}{c} \right)^2 \, E_z \; = \; 0 \tag{797}$$

In cylindrical coordinates this partial differential equation has the form

$$\frac{1}{r} \, \frac{\partial}{\partial r} \left(r \, \frac{\partial E_z}{\partial r} \right) \; + \; \frac{1}{r^2} \, \frac{\partial^2 E_z}{\partial \theta^2} \; + \; \frac{\partial^2 E_z}{\partial z^2} \; + \; \left(\frac{\omega}{c} \right)^2 \, E_z \; = \; 0 \tag{798}$$

On using separation of variables one assumes that the E.M. waves have the form

$$E_z(r, \theta, z, t) \; = \; \sum_{m,k} \, A_m(k) \; R_m(r) \; \Theta(\theta) \; Z(z) \; \exp \left[\; - \; i \; \omega \; t \; \right] \tag{799}$$

On solving for the (θ, z) dependence, and using the condition that E_z is $2\,\pi$ periodic in θ one has travelling waves of the form

$$E_z(r, \theta, z, t) \; = \; \sum_{m,k} C_m(k) \, R_m(r) \, \exp \left[\, - \, i \, m \, \theta \, \right] \, \exp \left[\, i \, (\, k \, z \, - \, \omega \, t \,) \, \right] \quad (800)$$

where the radial function satisfies

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\, r \, \frac{\partial R_m}{\partial r} \, \right) \; - \; \frac{m^2}{r^2} \, R_m \; + \; \left(\, \frac{\omega^2}{c^2} \; - \; k^2 \, \right) R_m \; = \; 0 \quad (801)$$

The radial equation has a solution for $b \; > \; r \; > \; a$ given by

$$R_m(r) \; = \; A_m \; J_m(\alpha r) \; + \; B_m \; N_m(\alpha r) \quad (802)$$

where $\alpha^2 \; = \; \frac{\omega^2}{c^2} \; - \; k^2$. The Neumann functions are allowed since the region where they diverge, ($r \; = \; 0$), has been excluded. The allowed values of α are determined by the boundary conditions at $r \; = \; a$ and $r \; = \; b$ where the tangential field E_z must vanish. Hence, the ratio of the two coefficients and α are determined from the boundary conditions

$$R_m(a) \; = \; A_m \; J_m(\alpha a) \; + \; B_m \; N_m(\alpha a) \; = \; 0 \quad (803)$$

and

$$R_m(b) \; = \; A_m \; J_m(\alpha b) \; + \; B_m \; N_m(\alpha b) \; = \; 0 \quad (804)$$

The allowed values of α are determined from the transcendental equation

$$N_m(\alpha a) \; J_m(\alpha b) \; = \; N_m(\alpha b) \; J_m(\alpha a) \quad (805)$$

The frequencies of the E.M. waves are given by

$$\frac{\omega^2}{c^2} \; = \; \alpha^2 \; + \; k^2 \quad (806)$$

Since k^2 must be positive if the wave is to be transmitted, the minimum frequency is given by $\omega_{min} \; = \; c \, \alpha$.

The Hankel functions are defined as solutions of Bessel's equation which are the superpositions

$$H^+_\nu(x) \; = \; J_\nu(x) \; + \; i \; N_\nu(x) \quad (807)$$

and

$$H^-_\nu(x) \; = \; J_\nu(x) \; - \; i \; N_\nu(x) \quad (808)$$

The Hankel functions have the asymptotic forms of

$$\lim_{x \to \infty} \; H^\pm_\nu(x) \; \to \; \exp \left[\; \pm \; i \; x \; \right] \quad (809)$$

and since they diverge at the origin has a natural interpretation in terms of outgoing cylindrical waves or incoming cylindrical waves.

Example:

Consider the diffraction of an electromagnetic plane wave E_0 with frequency ω, by a metal wire of radius a. The electric vector is parallel to the cylindrical axis, and the direction of propagation is perpendicular to the cylindrical axis. The incident field is

$$\hat{e}_z \; E_0 \; \exp \left[\; i \; (\; k \; r \; \cos\theta \; - \; \omega \; t \;) \; \right] \tag{810}$$

The amplitude of the diffracted electric field satisfies Helmholtz's equation

$$\frac{1}{r} \; \frac{\partial}{\partial r} \left(\; r \; \frac{\partial E_{sc}}{\partial r} \; \right) \; + \; \frac{1}{r^2} \; \frac{\partial^2 E_{sc}}{\partial \theta^2} \; + \; k^2 \; E_{sc} \; = \; 0 \tag{811}$$

The amplitude must also satisfy the boundary condition that the tangential field vanishes at the surface of the conductor

$$E_{sc}(a, \theta) \; + \; E_0 \; \exp \left[\; i \; k \; a \; \cos\theta \; \right] \; = \; 0 \tag{812}$$

The boundary condition at infinity is given by the radiation condition

$$\lim_{r \to \infty} \left(\; \frac{\partial E_{sc}}{\partial r} \; + \; i \; k \; E_{sc} \; \right) \; = \; 0 \tag{813}$$

On applying the method of separation of variables one finds the solution as a series

$$E_{sc}(r, \theta) \; = \; \sum_{m=0}^{\infty} \left(\; A_m \; \cos m \, \theta + B_m \; \sin m \, \theta \; \right) \left[\; C_m \; H^{+}_{m}(kr) + D_m \; H^{-}_{m}(kr) \; \right] \tag{814}$$

On examining the boundary condition at $r \; \rightarrow \; \infty$ one finds that the expansion coefficient $D_m \; = \; 0$. From the symmetry condition $\theta \; \rightarrow \; - \; \theta$, the solution must be an even function of θ so one has $B_m \; = \; 0$. Thus, the solution is of the form

$$E_{sc}(r, \theta) \; = \; \sum_{m=0}^{\infty} \; C_m \; \cos m \; \theta \; H^{+}_{m}(kr) \tag{815}$$

From the boundary condition at $r \; = \; a$ one has

$$\sum_{m=0}^{\infty} \; C_m \; \cos m \; \theta \; H^{+}_{m}(ka) \; + \; E_0 \; \exp \left[\; i \; k \; a \; \cos\theta \; \right] \; = \; 0 \tag{816}$$

Furthermore, as

$$\exp \left[\, i \, k \, a \, \cos\theta \, \right] \; = \; J_0(ka) \; + \; 2 \, \sum_{m=1}^{\infty} \, (\, i \,)^m \, J_m(ka) \, \cos m \, \theta \tag{817}$$

one can determine the coefficients C_m uniquely. In particular

$$C_0 \, H_0^+(ka) \; = \; - \, E_0 \, J_0(ka) \tag{818}$$

and

$$C_m \, H_0^+(ka) \; = \; - \, 2 \, (\, i \,)^m \, E_0 \, J_m(ka) \tag{819}$$

Thus, the scattered wave is given by

$$E_{sc} \; = \; - \, E_0 \, \left[\, \frac{J_0(ka)}{H_0^+(ka)} \, H_0^+(kr) \; + \; 2 \, \sum_{m=1}^{\infty} \, (\, i \,)^m \, \frac{J_m(ka)}{H_m^+(ka)} \, H_m^+(kr) \, \cos m \, \theta \, \right] \tag{820}$$

8.2 Spherical Bessel Functions

The spherical Bessel Functions $j_n(x)$ are related to Bessel functions of half integer order. The spherical Bessel functions occur in three dimensional problems with spherical symmetry. For example, in three dimensions the radial part of the solution of Laplace's equation can be written as

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(\, r^2 \, \frac{\partial R(r)}{\partial r} \, \right) \; + \; \left(\, k^2 \; - \; \frac{l \, (\, l \; + \; 1 \,)}{r^2} \, \right) \, R(r) \; = \; 0 \tag{821}$$

On substituting the form of the radial function as

$$R(r) \; = \; \frac{\phi(kr)}{(\, k \, r \,)^{\frac{1}{2}}} \tag{822}$$

one obtains Bessel's equation of half integer order

$$r^2 \, \frac{\partial^2 \phi}{\partial r^2} \; + \; r \, \frac{\partial \phi}{\partial r} \; + \; \left[\, k^2 \, r^2 \; - \; (\, l \; + \frac{1}{2} \,)^2 \, \right] \, \phi \; = \; 0 \tag{823}$$

Thus one has a solution for the radial function of the form

$$R(r) \; = \; \frac{J_{l+\frac{1}{2}}(kr)}{\sqrt{k \, r}} \tag{824}$$

The spherical Bessel functions are defined as the solution

$$j_m(x) \; = \; \sqrt{\frac{\pi}{2 \, x}} \, J_{m+\frac{1}{2}}(x) \tag{825}$$

incorporating a specific constant of proportionality. The spherical Neumann functions are defined analogously by

$$\eta_m(x) \;=\; \sqrt{\frac{\pi}{2\,x}}\;N_{m+\frac{1}{2}}(x) \tag{826}$$

8.2.1 Recursion Relations

It can be seen that the zeroth order spherical Bessel function $j_0(x)$ is given by

$$j_0(x) \;=\; \frac{\sin x}{x} \tag{827}$$

The recurrence relations for the spherical Bessel functions are given by

$$\begin{aligned} j_{n-1}(x) \;+\; j_{n+1}(x) \;&=\; \frac{2\,n\;+\;1}{x}\;j_n(x) \\ n\;j_{n-1}(x)\;-\;(\;n\;+\;1\;)\;j_{n+1}(x) \;&=\; (\;2\,n\;+\;1\;)\;j'_n(x) \end{aligned} \tag{828}$$

The recurrence relations can be used to evaluate the low order spherical Bessel functions

$$\begin{aligned} j_1(x) \;&=\; \frac{\sin x}{x^2}\;-\;\frac{\cos x}{x} \\ j_2(x) \;&=\; \left(\frac{3\;-\;x^2}{x^3}\right)\;\sin x\;-\;\frac{3}{x^2}\;\cos x \end{aligned} \tag{829}$$

The general form of the spherical Bessel functions can be obtained from the recursion relations by combining them into the form

$$\begin{aligned} \frac{\partial}{\partial x}\left(\;x^{n+1}\;j_n(x)\;\right) \;&=\; x^{n+1}\;j_{n-1}(x) \\ \frac{\partial}{\partial x}\left(\;x^{-n}\;j_n(x)\;\right) \;&=\; -\;x^{-n}\;j_{n+1}(x) \end{aligned} \tag{830}$$

By induction one can establish the Rayleigh formula

$$j_n(x) \;=\; (\;-\;1\;)^n\;x^n\;\left(\;\frac{1}{x}\;\frac{\partial}{\partial x}\;\right)^n\;j_0(x) \tag{831}$$

for the spherical Bessel function of order n. The asymptotic, large x, behavior is given by

$$j_n(x) \; = \; \frac{1}{x} \; \sin \left(\; x \; - \; n \; \frac{\pi}{2} \; \right) \tag{832}$$

This follows as the asymptotic large x behavior is governed by the terms of lowest power in $\frac{1}{x}$. The derivatives present in the Rayleigh formula produce a faster decay and hence negligible contributions when they act on the powers of x. Thus the leading term of the large x behavior is determined by the term where the n derivatives in the Rayleigh formula for $j_0(x)$ all act on the factor $\sin x$.

8.2.2 Orthogonality Relations

The orthogonality relations for the spherical Bessel functions can be expressed as

$$\int_0^a dr \; j_n(kr) \; r^2 \; j_n(k'r) \; = \; \frac{a^3}{3} \; \left[\; j_{n+1}(ka) \; \right]^2 \; \delta_{k,k'} \tag{833}$$

where k and k' are solutions of the equation

$$j_n(ka) \; = \; 0 \tag{834}$$

expressing the boundary condition.

8.2.3 Spherical Neumann Functions

The spherical Neumann functions can also be evaluated explicitly as

$$\begin{aligned} \eta_0(x) \; &= \; - \; \frac{\cos x}{x} \\ \eta_1(x) \; &= \; - \; \frac{\cos x}{x^2} \; - \; \frac{\sin x}{x} \\ \eta_2(x) \; &= \; - \; \left(\; \frac{3 \; - \; x^2}{x^3} \; \right) \; \cos x \; - \; \frac{3}{x^2} \; \sin x \end{aligned} \tag{835}$$

etc. It can be seen that the spherical Neumann functions diverge at the origin.

Example:

The free particle energy eigenvalue equation in three dimensions

$$- \; \frac{\hbar^2}{2 \; m} \; \nabla^2 \; \Psi \; = \; E \; \Psi \tag{836}$$

has an energy eigenfunction Ψ that can be expressed as

$$\Psi(r,\theta,\varphi) \ = \ R(r) \ \Theta(\theta) \ \Phi(\varphi) \tag{837}$$

The wave function $\Psi(r,\theta,\varphi)$ with angular momentum l has a radial wave function $R_l(kr)$ which satisfies the differential equation

$$\frac{\partial R(r)}{\partial r^2} \ + \ \frac{2}{r} \ \frac{\partial R(r)}{\partial r} \ = \ \left(\ k^2 \ - \ \frac{l \ (\ l \ + \ 1 \ )}{r^2} \ \right) R(r) \ = \ 0 \tag{838}$$

where the energy eigenvalue is given by $E \ = \ \frac{\hbar^2 \ k^2}{2 \ m}$. The radial function has the general solution

$$R_l(r) \ = \ A_l \ j_l(kr) \ + \ B_l \ \eta_l(kr) \tag{839}$$

The solution which is regular at $r \ = \ 0$ corresponds to the case where $B_l \ = \ 0$.

Example:

The energy eigenfunction for a particle, of angular momentum l, moving in a short ranged potential $V(r)$ such that $V(r) \ = \ 0$ for $r \ > \ a$ has a radial wave function

$$R_l(r) \ = \ A_l \ j_l(kr) \ + \ B_l \ \eta_l(kr) \tag{840}$$

for $r \ > \ a$. The wave functions have the asymptotic form

$$\begin{aligned} j_l(kr) \ &\sim \ \frac{1}{k \ r} \ \sin\left(\ k \ r \ - \ l \ \frac{\pi}{2} \ \right) \\ \eta_l(kr) \ &\sim \ - \ \frac{1}{k \ r} \ \cos\left(\ k \ r \ - \ l \ \frac{\pi}{2} \ \right) \end{aligned} \tag{841}$$

On writing $\frac{B_l}{A_l} \ = \ - \tan \delta_l(k)$, one finds that

$$R_l(r) \ = \ A_l \ \frac{1}{k \ r} \ \sin\left(\ k \ r \ - \ l \ \frac{\pi}{2} \ + \ \delta_l(k) \ \right) \tag{842}$$

for $r \ > \ a$. The energy eigenfunction is of the form of a standing spherical wave, in which the effect of the potential is contained in the phase shift $\delta_l(k)$.

Example:

A quantum mechanical particle in a stationary state experiences a strong repulsive potential $V(r)$ from a nucleus which prevents the particle from entering the nucleus. The potential $V(r)$ is spherically symmetric and can be represented by

$$V(r) = \left\{ \begin{array}{ccc} \infty & r < a \\ 0 & r > a \end{array} \right\} \tag{843}$$

The wave function Ψ, which expresses the state of the particle, satisfies the energy eigenvalue equation

$$- \frac{\hbar^2}{2\ m} \nabla^2 \Psi + V(r) \Psi = E \Psi \tag{844}$$

The effect of the potential is to demand that the wave function $\Psi(r, \theta, \varphi)$ satisfies the boundary condition

$$\Psi(a, \theta, \varphi) = 0 \tag{845}$$

at $r = a$. This corresponds to the condition that the particle does not enter the nucleus. Due to the spherical symmetry of the potential, we have a solution of the form

$$\Psi_{l,m}(r, \theta, \varphi) = R_l(r)\ Y_l^m(\theta, \varphi) \tag{846}$$

The radial function $R_l(r)$ is given by

$$R_l(r) = A_l\ j_l(kr) + B_l\ \eta_l(kr) \tag{847}$$

where A_l and B_l are arbitrary constants, and the energy eigenvalue is given by $E = \frac{\hbar^2\ k^2}{2\ m}$. The boundary condition at the surface of the spherical nucleus determines the ratio of the constants

$$0 = A_l\ j_l(ka) + B_l\ \eta_l(ka) \tag{848}$$

Thus, one has

$$\frac{B_l}{A_l} = - \frac{j_l(ka)}{\eta_l(ka)} \tag{849}$$

In this case, the phase shift $\delta_l(k)$ is determined by the energy and the radius of the nucleus

$$\tan \delta_l(k) = \frac{j_l(ka)}{\eta_l(ka)} \tag{850}$$

Thus, determination of the angle and energy dependence of the scattering cross-section can be used to determine the phase shift, which can then be used to determine the characteristic properties of the scattering potential.

Homework: 11.7.22

An important example is given by the expansion of a plane wave in terms of spherical Bessel functions

$$\exp \left[\, i \; k \; r \; \cos \theta \, \right] \; = \; \sum_{n=0}^{\infty} \, C_n \; j_n(kr) \tag{851}$$

The coefficient C_n is evaluated as

$$C_n \;\; = \; i^n \; (\; 2 \; n \; + \; 1 \;) \; P_n(\cos \theta) \tag{852}$$

where $P_n(x)$are the Legendre Polynomials. It should be expected that plane waves can be expressed in terms of spherical Bessel functions with the same k values as both the spherical Bessel functions and the plane wave are both free particle energy eigenfunctions.

9 Legendre Polynomials

9.0.4 Generating Function Expansion

The generating function $g(x,t)$ yields an expansion for the Legendre polynomials $P_n(x)$. The generating function expansion is simply

$$\begin{aligned} g(x,t) &= \left(1 - 2\,x\,t + t^2 \right)^{-\frac{1}{2}} \\ &= \sum_{n=0}^{\infty} P_n(x)\ t^n \end{aligned} \tag{853}$$

This has direct application in electrostatics, where the potential $\phi(\vec{r})$ due to a charge distribution $\rho(\vec{r})$ is given by the solution of Poisson's equation. The solution can be expressed in terms of the Green's function and the charge density, and the Green's function can be expanded using the generating function expansion

$$\begin{aligned} \phi(\vec{r}) &= \int d^3\vec{r'}\ \frac{\rho(\vec{r'})}{|\ \vec{r} - \vec{r'}\ |} \\ &= \int_0^\infty dr'\ r'^2 \int_0^\pi d\theta\ \sin\theta \int_0^{2\pi} d\varphi\ \frac{\rho(\vec{r'})}{\sqrt{r^2 - 2\,r\,r'\ \cos\theta + r'^2}} \\ &= \int_0^\infty dr'\ r'^2 \int_0^\pi d\theta\ \sin\theta \int_0^{2\pi} d\varphi\ \rho(\vec{r'}) \sum_{n=0}^{\infty} \frac{1}{r_>} \left(\frac{r_<}{r_>} \right)^n P_n(\cos\theta) \end{aligned} \tag{854}$$

where θ is the angle between $\vec{r}$ and $\vec{r'}$, and $r_<$ and $r_>$ are, respectively, the smaller and large values of (r, r').

Homework:

Evaluate the potential due to a spherically symmetric charge density

$$\begin{aligned} \rho(r) &= 0 \qquad \text{for } r > a \\ \rho(r) &= \rho_0 \qquad \text{for } r < a \end{aligned} \tag{855}$$

Assume that the Legendre polynomials $P_l(\cos\theta)$ are orthogonal, with weight factor $\sin\theta$.

9.0.5 Series Expansion

The generating function can be used to find the series expansion of the Legendre polynomials. First we expand in powers of $2\,x\,t\;-\;t^2$, via

$$\begin{aligned} g(x,t) &= \frac{1}{\sqrt{1\;-\;2\,x\,t\;+\;t^2}} \\ &= \sum_{s=0}^{\infty} \frac{(2s)!}{2^{2s}\,(s!)^2}\,(\,2\,x\,t\;-\;t^2\,)^s \end{aligned} \tag{856}$$

and then expand in powers of t

$$\begin{aligned} g(x,t) &= \sum_{s=0}^{\infty} \frac{(2s)!}{2^{2s}\,(s!)^2}\,t^s\,(\,2\,x\;-\;t\,)^s \\ &= \sum_{s=0}^{\infty} \frac{(2s)!}{2^{2s}\,(s!)^2}\,t^s \sum_{r=0}^{\infty} (\,-\,1\,)^r\,\frac{s!}{r!\,(s-r)!}\,(\,2\,x\,)^{s-r}\,t^r \end{aligned} \tag{857}$$

On writing $n\;=\;s\;+\;r$ and keeping n fixed $s\;=\;n\;-\;r$, so

$$\begin{aligned} g(x,t) &= \sum_{n=0}^{\infty} \sum_{r=0}^{[\frac{n}{2}]} \frac{(2n-2r)!}{2^{2n-2r}\,r!\,(n-r)!\,(n-2r)!}\,t^n\,(\,-\,1\,)^r\,(\,2\,x\,)^{n-2r} \\ &= \sum_{n=0}^{\infty} \sum_{r=0}^{[\frac{n}{2}]} \frac{(2n-2r)!}{2^{n}\,r!\,(n-r)!\,(n-2r)!}\,t^n\,(\,-\,1\,)^r\,(\,x\,)^{n-2r} \end{aligned} \tag{858}$$

Thus, the Legendre polynomials are given by

$$P_n(x)\;=\;\sum_{r=0}^{[\frac{n}{2}]} \frac{(2n-2r)!}{2^{n}\,r!\,(n-r)!\,(n-2r)!}\,(\,-\,1\,)^r\,(\,x\,)^{n-2r} \tag{859}$$

Hence, the Legendre polynomials have the highest power of x^n, and terms which decrease in powers of x^2. Thus, for odd n the series only contains odd terms in x, whereas for even n the series is even in x. The series in decreasing powers of x^{-2} terminates when $n\;=\;2\,r$ for even n and when $n\;=\;2\,r+1$ for odd n.

9.0.6 Recursion Relations

Recursion relations for the Legendre polynomials can be found by taking the derivative of the generating function with respect to t. Thus, starting from

$$\begin{aligned} g(x,t) &= \left(1 - 2\,x\,t + t^2 \right)^{-\frac{1}{2}} \\ &= \sum_{n=0}^{\infty} P_n(x)\; t^n \end{aligned} \tag{860}$$

one obtains

$$\begin{aligned} \frac{\partial}{\partial t}\; g(x,t) &= \frac{x - t}{(\;1 - 2\,x\,t + t^2\;)^{\frac{3}{2}}} \\ &= \sum_{n=0}^{\infty} P_n(x)\; n\; t^{n-1} \end{aligned} \tag{861}$$

The above equation can be written as

$$\begin{aligned} (\;x - t\;)\; g(x,t) &= (\;1 - 2\,x\,t + t^2\;) \sum_{n=0}^{\infty} n\; P_n(x)\; t^{n-1} \\ (\;x - t\;) \sum_{m=0}^{\infty} P_m(x)\; t^m &= (\;1 - 2\,x\,t + t^2\;) \sum_{n=0}^{\infty} n\; P_n(x)\; t^{n-1} \end{aligned} \tag{862}$$

On equating like powers of t one has

$$(\;2\,n + 1\;)\; x\; P_n(x) = (\;n + 1\;)\;\; P_{n+1}(x) + n\; P_{n-1}(x) \tag{863}$$

This recursion relation can be used to construct the higher order Legendre polynomials starting from $P_0(x) = 1$ and $P_1(x) = x$.

An alternate form of the recursion relation can be obtained by taking the derivative of the generating function expansion with respect to x

$$\begin{aligned} \frac{\partial}{\partial x}\; g(x,t) &= \frac{t}{(\;1 - 2\,x\,t + t^2\;)^{\frac{3}{2}}} \\ &= \sum_{n=0}^{\infty} \frac{\partial}{\partial x} P_n(x)\; t^n \end{aligned} \tag{864}$$

or

$$
\begin{aligned}
t\ g(x,t) \ &= \ (\ 1 \ - \ 2 \ x \ t \ + \ t^2 \ ) \ \sum_{n=0}^{\infty} \ \frac{\partial}{\partial x} \ P_n(x) \ t^n \\
t \ \sum_{n=0}^{\infty} \ P_n(x) \ t^n \ &= \ (\ 1 \ - \ 2 \ x \ t \ + \ t^2 \ ) \ \sum_{n=0}^{\infty} \ \frac{\partial}{\partial x} \ P_n(x) \ t^n
\end{aligned}
\tag{865}
$$

Equating like powers of t we obtain the recursion relation

$$
\left(\ 2 \ x \ \frac{\partial}{\partial x} \ P_n(x) \ + \ P_n \ \right) \ = \ \frac{\partial}{\partial x} \ P_{n+1}(x) \ + \ \frac{\partial}{\partial x} \ P_{n-1}(x) \tag{866}
$$

This is not very useful.

A more useful relation can be obtained, if one takes the derivative of

$$
(\ 2 \ n \ + \ 1 \ ) \ x \ P_n(x) \ = \ (\ n \ + \ 1 \ ) \ P_{n+1}(x) \ + \ n \ P_{n-1}(x) \tag{867}
$$

to give

$$
(\ 2 \ n \ + \ 1 \ ) \left(\ x \ \frac{\partial}{\partial x} \ P_n(x) + P_n(x) \ \right) \ = \ (\ n \ + \ 1 \ ) \ \frac{\partial}{\partial x} \ P_{n+1}(x) + n \ \frac{\partial}{\partial x} \ P_{n-1}(x) \tag{868}
$$

This relation can be used to eliminate the derivative of $P_n(x)$ in the previous equation, by multiplying by 2 and subtracting ($2 \ n \ + \ 1$) times the previous equation, leading to

$$
(\ 2 \ n \ + \ 1 \ ) \ P_n(x) \ = \ \frac{\partial}{\partial x} \ P_{n+1}(x) \ - \ \frac{\partial}{\partial x} \ P_{n-1}(x) \tag{869}
$$

On eliminating the derivative of $P_{n-1}(x)$, by multiplying by n and subtracting, one obtains

$$
x \ \frac{\partial}{\partial x} \ P_n(x) \ + \ (\ n \ + \ 1 \ ) \ P_n(x) \ = \ \frac{\partial}{\partial x} \ P_{n+1}(x) \tag{870}
$$

Alternatively, on eliminating the derivative of $P_{n+1}(x)$ by multiplying by $(n+1)$ and subtracting, one obtains

$$
x \ \frac{\partial}{\partial x} \ P_n(x) \ - \ n \ P_n(x) \ = \ \frac{\partial}{\partial x} \ P_{n-1}(x) \tag{871}
$$

The above two equations are to be combined. One is first put in the form $n \rightarrow n - 1$ so it becomes

$$x \frac{\partial}{\partial x} P_{n-1}(x) + n P_{n-1}(x) = \frac{\partial}{\partial x} P_n(x) \tag{872}$$

and this is combined with x times the relation

$$x \frac{\partial}{\partial x} P_n(x) - n P_n(x) = \frac{\partial}{\partial x} P_{n-1}(x) \tag{873}$$

so as to eliminate $\frac{\partial}{\partial x} P_{n-1}(x)$. On performing these manipulations one obtains the recursion relation

$$(1 - x^2) \frac{\partial}{\partial x} P_n(x) = n P_{n-1}(x) - n x P_n(x) \tag{874}$$

Finally, if one uses the above recursion relation together with

$$(2 n + 1) x P_n(x) = (n + 1) P_{n+1}(x) + n P_{n-1}(x) \tag{875}$$

one obtains a recursion relation in the form

$$(1 - x^2) \frac{\partial}{\partial x} P_n(x) = (n + 1) x P_n(x) - (n + 1) P_{n+1}(x) \tag{876}$$

Example:

The multi-pole expansion can be derived, using spherical polar coordinates where $z = r \cos\theta$, from the properties of Legendre polynomials. The mathematical basis for this expansion is found in the identity

$$\frac{\partial}{\partial z} \left[\frac{P_n(\cos\theta)}{r^{(n+1)}} \right] = - (n + 1) \frac{P_{n+1}(\cos\theta)}{r^{(n+2)}} \tag{877}$$

This can be proved starting with the expression

$$\left(\frac{\partial}{\partial z} \right)_{x,y} = \left(\frac{\partial r}{\partial z} \right) \frac{\partial}{\partial r} + \left(\frac{\partial \cos\theta}{\partial z} \right) \frac{\partial}{\partial \cos\theta} \tag{878}$$

and with $r = \sqrt{x^2 + y^2 + z^2}$ and $\cos\theta = \frac{z}{\sqrt{x^2 + y^2 + z^2}}$ one has

$$\left(\frac{\partial}{\partial z} \right)_{x,y} = \left(\frac{z}{r} \right) \frac{\partial}{\partial r} + \left(\frac{r^2 - z^2}{r^3} \right) \frac{\partial}{\partial \cos\theta} \tag{879}$$

Hence,

$$\frac{\partial}{\partial z} \left[\frac{P_n(\cos\theta)}{r^{(n+1)}} \right] = - (n + 1) \cos\theta \left[\frac{P_n(\cos\theta)}{r^{(n+2)}} \right] + \sin^2\theta \frac{\partial}{\partial \cos\theta} \left[\frac{P_n(\cos\theta)}{r^{(n+2)}} \right] \tag{880}$$

but one has the recursion relation

$$\sin^2\theta \frac{\partial P_n(\cos\theta)}{\partial \cos\theta} = (n + 1) \cos\theta \, P_n(\cos\theta) - (n + 1) P_{(n+1)}(\cos\theta) \tag{881}$$

Thus, one has proved the identity

$$\frac{\partial}{\partial z} \left[\frac{P_n(\cos\theta)}{r^{(n+1)}} \right] = - (n + 1) \frac{P_{n+1}(\cos\theta)}{r^{(n+2)}} \tag{882}$$

Alternatively, this identity can be shown to be true by starting from the generating function expansion

$$g(\cos\theta, r) = \frac{1}{\sqrt{1 + r^2 - 2 r \cos\theta}} = \sum_{n=0}^{\infty} \frac{P_n(\cos\theta)}{r^{(n+1)}} \tag{883}$$

On taking the derivative with respect to z, keeping (x, y) fixed, one has

$$\begin{aligned} \frac{\partial}{\partial z} \frac{1}{\sqrt{1 + x^2 + y^2 + z^2 - 2 z}} &= \frac{1 - z}{(1 + x^2 + y^2 + z^2 - 2 z)^{\frac{3}{2}}} \\ &= \frac{(1 - r \cos\theta)}{(1 + r^2 - 2 r \cos\theta)^{\frac{3}{2}}} \end{aligned} \tag{884}$$

Hence, we have

$$\frac{\partial}{\partial z} \left(\sum_{n=0}^{\infty} \frac{P_n(\cos\theta)}{r^{(n+1)}} \right) = \frac{(1 - r \cos\theta)}{(1 + r^2 - 2 r \cos\theta)^{\frac{3}{2}}} \tag{885}$$

which can be written as

$$\begin{aligned} (1 + r^2 - 2 r \cos\theta) \frac{\partial}{\partial z} \left(\sum_{n=0}^{\infty} \frac{P_n(\cos\theta)}{r^{(n+1)}} \right) &= \frac{(1 - r \cos\theta)}{\sqrt{(1 + r^2 - 2 r \cos\theta)}} \\ &= (1 - r \cos\theta) \sum_{n=0}^{\infty} \frac{P_n(\cos\theta)}{r^{(n+1)}} \end{aligned} \tag{886}$$

On substituting the identity that is being verified, we find

$$\sum_{n=0}^{\infty} (1 + r^2 - 2 r \cos\theta) (n + 1) \frac{P_{(n+1)}(\cos\theta)}{r^{(n+2)}} = \sum_{n=0}^{\infty} \frac{\cos\theta \, P_n(\cos\theta)}{r^n} - \sum_{n=0}^{\infty} \frac{P_n(\cos\theta)}{r^{(n+1)}} \tag{887}$$

or on changing the index of summation

$$\sum_{n=0}^{\infty} n \, \frac{P_{(n-1)}(\cos\theta)}{r^n} + \sum_{n=0}^{\infty} (n + 1) \frac{P_{(n+1)}(\cos\theta)}{r^n} = \sum_{n=0}^{\infty} (2 n + 1) \frac{\cos\theta \, P_n(\cos\theta)}{r^n} \tag{888}$$

which is satisfied identically, because of the recursion relation

$$(2 n + 1) \cos\theta \, P_n(\cos\theta) = n \, P_{(n-1)}(\cos\theta) + (n + 1) \, P_{(n+1)}(\cos\theta) \tag{889}$$

Thus, we have verified the identity in question.

9.0.7 Legendre's Equation

The Legendre polynomials satisfy Legendre's equation. Legendre's equation can be derived starting with the recursion relation

$$(1 - x^2) \frac{\partial}{\partial x} P_n(x) = n \, P_{n-1}(x) - n \, x \, P_n(x) \tag{890}$$

Differentiating the recursion relation with respect to x one obtains

$$(1 - x^2) \frac{\partial^2}{\partial x^2} P_n(x) - 2 x \frac{\partial}{\partial x} P_n(x) = n \frac{\partial}{\partial x} P_{n-1}(x) - n \, x \frac{\partial}{\partial x} P_n(x) - n \, P_n(x) \tag{891}$$

and then using

$$x \frac{\partial}{\partial x} P_n(x) - n \, P_n(x) = \frac{\partial}{\partial x} P_{n-1}(x) \tag{892}$$

to eliminate the derivative of $P_{n-1}(x)$ one obtains Legendre's equation

$$(1 - x^2) \frac{\partial^2}{\partial x^2} P_n(x) - 2 x \frac{\partial}{\partial x} P_n(x) + n (n + 1) P_n(x) = 0 \tag{893}$$

Legendre's differential equation has singular points at $x = \pm 1$, where the solution $P_n(x)$ may become infinite. The value of n must be an integer if the solution is to remain finite. If n is integer the Frobenius series expansion terminates and the solution becomes a polynomial.

If the solution is assumed to be of the form

$$P_n(x) \; = \; x^{\alpha} \sum_{n=0}^{\infty} C_n \; x^n \tag{894}$$

then it can be shown that the indicial equation yields

$$\alpha \; = \; 0 \tag{895}$$

and the coefficient of x^m satisfies the recursion relation

$$\begin{aligned} (\, m \; + \; 2 \,) (\, m \; + \; 1 \,) \, C_{m+2} \; &= \; \left[\, m \, (\, m \; - \; 1 \,) \; + \; 2 \, m \; - \; n \, (\, n \; + \; 1 \,) \, \right] C_m \\ &= \; \left[\, m \, (\, m \; + \; 1 \,) \; - \; n \, (\, n \; + \; 1 \,) \, \right] C_m \end{aligned} \tag{896}$$

which terminates after n terms when n is an integer.

Legendre's equation is most frequently seen in a form where the independent variable is in the form $x \; = \; \cos\theta$. In this case, the first order derivative with respect to x is given by

$$\frac{\partial}{\partial x} \; = \; - \; \frac{1}{\sin\theta} \, \frac{\partial}{\partial\theta} \tag{897}$$

and the second order derivative is evaluated as

$$\begin{aligned} \frac{\partial^2}{\partial x^2} \; &= \; \frac{1}{\sin\theta} \, \frac{\partial}{\partial\theta} \left(\, \frac{1}{\sin\theta} \, \frac{\partial}{\partial\theta} \, \right) \\ &= \; \frac{1}{\sin^2\theta} \, \frac{\partial^2}{\partial\theta^2} \; - \; \frac{\cos\theta}{\sin^3\theta} \, \frac{\partial}{\partial\theta} \end{aligned} \tag{898}$$

Thus, Legendre's equation takes the form

$$\begin{aligned} \frac{\partial^2}{\partial\theta^2} \, P_n(\cos\theta) \; + \; \frac{\cos\theta}{\sin\theta} \, \frac{\partial}{\partial\theta} \, P_n(\cos\theta) \; + \; n \, (\, n \; + \; 1 \,) \, P_n(\cos\theta) \; &= \; 0 \\ \frac{1}{\sin\theta} \, \frac{\partial}{\partial\theta} \left(\, \sin\theta \, \frac{\partial}{\partial\theta} \, P_n(\cos\theta) \, \right) \; + \; n \, (\, n \; + \; 1 \,) \, P_n(\cos\theta) \; &= \; 0 \end{aligned} \tag{899}$$

9.0.8 Orthogonality

Legendre's differential equation in the variable x can be written as

$$\frac{\partial}{\partial x} \left[(1 - x^2) \frac{\partial}{\partial x} P_n(x) \right] + n (n + 1) P_n(x) = 0 \tag{900}$$

which is a Stürm-Liouville equation, with eigenvalue $n (n + 1)$ and weighting factor unity. The boundary conditions are imposed at $x = \pm 1$, which are regular singular points as $(1 - x^2) = 0$ at the ends of the interval.

The orthogonality condition is found by multiplying by $P_m(x)$ as the weight factor is unity, and subtracting this from the equation with n and m interchanged. After integrating over x between $+1$ and -1 one obtains

$$\int_{-1}^{+1} dx \left[P_m(x) \frac{\partial}{\partial x} \left((1 - x^2) \frac{\partial}{\partial x} P_n(x) \right) - P_n(x) \frac{\partial}{\partial x} \left((1 - x^2) \frac{\partial}{\partial x} P_m(x) \right) \right]$$
$$= \left(n (n + 1) - m (m + 1) \right) \int_{-1}^{+1} dx \, P_m(x) \, P_n(x) \tag{901}$$

On integrating by parts, and noting that the factor $(1 - x^2)$ vanishes at both the boundaries, then as long as $P_n(\pm 1)$ is not infinite one has

$$\left(n (n + 1) - m (m + 1) \right) \int_{-1}^{+1} dx \, P_m(x) \, P_n(x) = 0 \tag{902}$$

Thus, the Legendre functions are orthogonal as long as the eigenvalues are not equal $n (n + 1) \neq m (m + 1)$.

The Legendre functions are defined such that $P_n(1) = 1$. The normalization integral can be evaluated from the square of the generating function expansion

$$(1 - 2 x t + t^2)^{-1} = \left(\sum_{n=0}^{n=\infty} P_n(x) \, t^n \right)^2 \tag{903}$$

On integrating over x from -1 to $+1$ one has

$$\int_{-1}^{+1} dx \, \frac{1}{1 - 2 x t + t^2} = \sum_{n=0}^{n=\infty} t^{2n} \int_{-1}^{+1} dx \, P_n^2(x) \tag{904}$$

where we have used the orthogonality of the Legendre functions. The integral can be evaluated as

$$- \frac{1}{2 t} \ln \frac{1 - 2 t + t^2}{1 + 2 t + t^2} = \sum_{n=0}^{n=\infty} t^{2n} \int_{-1}^{+1} dx \, P_n^2(x) \tag{905}$$

The left hand side can be expanded in powers of t as

$$\frac{1}{t} \ \ln \frac{1 \ + \ t}{1 \ - \ t} \ = \ 2 \sum_{n=0}^{n=\infty} \frac{t^{2n}}{2 \ n \ + \ 1} \tag{906}$$

On equating like coefficients of t^{2n} one has

$$\int_{-1}^{+1} dx \ P_n^2(x) \ = \ \frac{2}{2 \ n \ + \ 1} \tag{907}$$

Hence, we can write the orthonormality condition as

$$\int_{-1}^{+1} dx \ P_n(x) \ P_m(x) \ = \ \delta_{n,m} \ \frac{2}{2 \ n \ + \ 1} \tag{908}$$

9.0.9 Legendre Expansions

Due to the orthogonality conditions and the completeness of the eigenfunctions of a Stürm-Liouville equation, any function can be expanded on the interval $(-1,+1)$ as a Legendre series

$$f(x) \ = \ \sum_{n=0}^{n=\infty} C_n \ P_n(x) \tag{909}$$

where the coefficients C_m can be evaluated from

$$\frac{2}{2 \ m \ + \ 1} \ C_m \ = \ \int_{-1}^{+1} dt \ P_m(t) \ f(t) \tag{910}$$

The completeness condition can be expressed as

$$\begin{aligned} f(x) \ &= \ \sum_{n=0}^{n=\infty} \frac{2 \ n \ + \ 1}{2} \ P_n(x) \int_{-1}^{+1} dt \ \ P_n(t) \ f(t) \\ &= \ \int_{-1}^{+1} dt \ f(t) \ \sum_{n=0}^{n=\infty} \frac{2 \ n \ + \ 1}{2} \ P_n(x) \ P_n(t) \end{aligned} \tag{911}$$

Hence, we may expand the delta function, on the interval $(-1,+1)$ as

$$\delta(\ x \ - \ t \ ) \ = \ \sum_{n=0}^{n=\infty} \frac{2 \ n \ + \ 1}{2} \ P_n(x) \ P_n(t) \tag{912}$$

Example:

Find the electrostatic potential for a point charge with charge q, located at a distance a from the center, inside a uniform conducting spherical shell or radius R.

The potential inside the sphere satisfies Poisson's equation

$$- \nabla^2 \phi \; = \; 4 \pi \rho \tag{913}$$

where ρ is only non-zero at the position of the point charge. Elsewhere, Poisson's equation simplifies to

$$\nabla^2 \phi \; = \; 0 \tag{914}$$

We shall assume that the polar axis, ($\theta \; = \; 0$) , runs through the center and the charge q. Then the potential is invariant under changes of the azimuthal angle φ, and so ϕ is independent of φ. Laplace's equation takes the form

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \phi}{\partial \theta} \right) \; = \; 0 \tag{915}$$

This has solutions of the form

$$\phi(r, \theta) \; = \; \sum_{l=0}^{\infty} \left(A_l \, r^l \; + \; B_l \, r^{-(l+1)} \right) P_l(\cos\theta) \tag{916}$$

where A_l and B_l are arbitrary constants that are to be determined by the boundary conditions.

In order for the shell to be at constant potential one must have

$$\phi(R, \theta) \; = \; \sum_{l=0}^{\infty} \left(A_l \, R^l \; + \; B_l \, R^{-(l+1)} \right) P_l(\cos\theta) \; = \; \phi_0 \tag{917}$$

Hence, for $l \; \neq \; 0$ one finds the relation between the expansion coefficients

$$A_l \; = \; - \, B_l \, R^{-(2l+1)} \tag{918}$$

and for $l \; = \; 0$ one has

$$A_0 \; + \; \frac{B_0}{R} \; = \; \phi_0 \tag{919}$$

Thus, one can express the potential in terms of the coefficients B_l via

$$\phi(r, \theta) \; = \; \phi_0 \; + \; B_0 \left(\frac{1}{r} \; - \; \frac{1}{R} \right) \; + \; \sum_{l=1}^{\infty} B_l \, R^{-(l+1)} \left(\frac{R^{(l+1)}}{r^{(l+1)}} \; - \; \frac{r^l}{R^l} \right) P_l(\cos\theta) \tag{920}$$

for $r > a$. The coefficients B_l can be found from the boundary condition at the point $(r = a, \theta = 0)$. Near this point, the potential should be dominated by the singular behavior of the point charge

$$\lim_{r \to a} \phi(r, \theta) \sim \frac{q}{(r - a)} = \frac{q}{r} \sum_{l=0}^{\infty} \frac{a^l}{r^l} \tag{921}$$

Hence, one finds the coefficients as

$$\begin{aligned} B_0 &= q \\ B_l &= q \, a^l \end{aligned} \tag{922}$$

Thus, we have we have identified the contribution from the point charge q as

$$\phi_q(r, \theta) = \frac{q}{\sqrt{r^2 + a^2 - 2 \, r \, a \, \cos\theta}} = \frac{q}{r} \sum_{l=0}^{\infty} \frac{a^l}{r^l} \, P_l(\cos\theta) \tag{923}$$

The induced contribution to the potential from the charge on the conducting surface is found, from the principle of linear superposition, as

$$\begin{aligned} \phi_{ind}(r, \theta) &= - \frac{q}{R} \sum_{l=0}^{\infty} \left(\frac{a \, r}{R^2} \right)^l P_l(\cos\theta) \\ &= - \frac{q}{R} \frac{1}{\sqrt{1 - 2 \, \frac{r \, a}{R^2} \, \cos\theta + \left(\frac{r \, a}{R^2} \right)^2}} \\ &= - \frac{q \, R}{a} \frac{1}{\sqrt{r^2 + \left(\frac{R^2}{a} \right)^2 - 2 \, r \left(\frac{R^2}{a} \right) \cos\theta}} \end{aligned} \tag{924}$$

which is just the contribution from a point image charge of magnitude $q' = - \, q \, \frac{R}{a}$ located outside the shell at a distance $\frac{R^2}{a}$ from the center. Since the expansions converge, we have found the solution.

Example:

Consider a metallic sphere of radius a in a uniform electric field, E_0. The potential ϕ in the vacuum satisfies Laplace's equation

$$\nabla^2 \, \phi = 0 \tag{925}$$

The electric field is chosen to be oriented along the polar axis, so the problem has azimuthal symmetry and the potential is independent of φ. We shall use the method of separation of variables and assume that the potential can be found in the form of a series expansion

$$\phi(r,\theta) \ = \ \sum_l \ C_l \ R_l(r) \ \Theta_l(\theta) \tag{926}$$

which satisfies the partial differential equation

$$\frac{1}{r^2} \ \frac{\partial}{\partial r} \left(\ r^2 \ \frac{\partial \ \phi}{\partial r} \ \right) \ + \ \frac{1}{r^2 \ \sin\theta} \ \frac{\partial}{\partial \theta} \left(\ \sin\theta \ \frac{\partial \phi}{\partial \theta} \ \right) \ = \ 0 \tag{927}$$

On writing the separation constant as $l \ (\ l \ + \ 1 \ )$ one has the radial function $R_l(r)$ satisfying the equation

$$\frac{\partial}{\partial r} \left(\ r^2 \ \frac{\partial R}{\partial r} \ \right) \ = \ l \ (\ l \ + \ 1 \ ) \ R \tag{928}$$

which has the solution

$$R_l(r) \ = A_l \ r^l \ + \ B_l \ r^{-(l+1)} \tag{929}$$

The angular dependence is given by

$$\Theta_l(\theta) \ = \ P_l(\cos\theta) \tag{930}$$

where l is an integer, for $\Theta_l(\theta)$ to be non-singular along the poles.

Thus one has the solution in the form of a series expansion

$$\phi(r,\theta) \ = \ \sum_{l=0}^{\infty} \left(\ A_l \ r^l \ + \ B_l \ r^{-(l+1)} \ \right) P_l(\cos\theta) \tag{931}$$

The coefficients A_l and B_l are to be determined from the boundary conditions.

As $r \ \rightarrow \ \infty$, the potential has to reduce to the potential of the uniform electric field

$$\begin{aligned} \lim_{r\to\infty} \ \phi(r,\theta) \quad & \rightarrow \quad - \ E_0 \ r \ \cos\theta \\ & = \quad - \ E_0 \ r \ P_1(\cos\theta) \end{aligned} \tag{932}$$

Thus, only the two A_L coefficients A_0 and A_1 can be non-zero. The potential has the form

$$\phi(r,\theta) \ = \ A_0 \ - \ E_0 \ r \ P_1(\cos\theta) \ + \ \sum_{l=0}^{\infty} \ B_l \ r^{-(l+1)} \ P_l(\cos\theta) \tag{933}$$

The metallic sphere is held at a constant potential so

$$\phi(a,\theta) \; = \; const \tag{934}$$

As the Legendre polynomials are linearly independent, the coefficients of the Legendre polynomials must vanish at the surface of the sphere. Hence, we have the set of equations

$$\begin{aligned} 0 \; &= \; - \, E_0 \; a \; + \; B_1 \; a^{-2} \\ 0 \; &= \; B_l \qquad \text{for } l \; > \; 1 \end{aligned} \tag{935}$$

which leads to the potential having the form

$$\phi(r,\theta) \; = \; A_0 \; + \; \frac{B_0}{r} \; - \; E_0 \; r \; P_1(\cos\theta) \left(1 \; - \; \frac{a^3}{r^3} \right) \tag{936}$$

If the sphere is assumed to be uncharged we can set $B_0 \; = \; 0$.

Example:

Consider the solution of Poisson's equation

$$\nabla^2 \; \phi \; = \; - \, 4 \; \pi \; \rho(\overrightarrow{r}) \tag{937}$$

in which the charge density is distributed uniformly on a circle of radius a centered on the origin, and in the plane $z \; = \; 0$. The total charge on the ring is q. We shall solve Poisson's equation in a region that does not include the charge distribution. The effect of the charge distribution, is to be included by specifying a boundary condition.

For points not in the plane $z \; = \; 0$, the charge density is zero, and so one has Laplace's equation

$$\nabla^2 \; \phi \; = \; 0 \tag{938}$$

Since, the geometry has an axial symmetry, the potential ϕ is only a function of (r,θ). In spherical polar coordinates, one has

$$\frac{1}{r^2} \; \frac{\partial}{\partial r} \left(\; r^2 \; \frac{\partial \phi}{\partial r} \; \right) \; + \; \frac{1}{r^2 \; \sin\theta} \; \frac{\partial}{\partial \theta} \left(\; \sin\theta \; \frac{\partial \phi}{\partial \theta} \; \right) \; + \; \frac{1}{r^2 \; \sin^2\theta} \; \frac{\partial^2 \phi}{\partial \varphi^2} \; = \; 0 \tag{939}$$

if $\theta \; = \; \frac{\pi}{2}$. Due to the axial symmetry, this reduces to

$$\frac{1}{r^2} \; \frac{\partial}{\partial r} \left(\; r^2 \; \frac{\partial \phi}{\partial r} \; \right) \; + \; \frac{1}{r^2 \; \sin\theta} \; \frac{\partial}{\partial \theta} \left(\; \sin\theta \; \frac{\partial \phi}{\partial \theta} \; \right) \; = \; 0 \tag{940}$$

This partial differential equation can be solved by the method of separation of variables,

$$\phi(r,\theta) \;=\; R(r)\;\Theta(\theta) \tag{941}$$

which, on dividing by ϕ, leads to the equation

$$\frac{1}{R}\,\frac{\partial}{\partial r}\left(\;r^2\;\frac{\partial R}{\partial r}\;\right) \;=\; -\;\frac{1}{\Theta\;\sin\theta}\;\frac{\partial}{\partial\theta}\left(\;\sin\theta\;\frac{\partial\Theta}{\partial\theta}\;\right) \tag{942}$$

Then since one side of the equation is a function of r alone, and the other side is a function of θ alone, both sides of the equation must be equal to a constant C

$$\begin{aligned} \frac{\partial}{\partial r}\left(\;r^2\;\frac{\partial R}{\partial r}\;\right) \;&=\; C\;R(r) \\ \frac{\partial}{\partial\theta}\left(\;\sin\theta\;\frac{\partial\Theta}{\partial\theta}\;\right) \;&=\; -\;C\;\sin\theta\;\Theta(\theta) \end{aligned} \tag{943}$$

On writing $C \;=\; n\;(\;n\;+\;1\;)$, we find that

$$R_n(r) \;=\; A_n\;r^n \;+\; B_n\;r^{-(n+1)} \tag{944}$$

and $\Theta(\theta)$ is given by

$$\Theta_n(\theta) \;=\; P_n(\cos\theta) \tag{945}$$

Thus a general solution, that does not diverge at infinity, is given by the series

$$\phi(r,\theta) \;=\; \sum_n \;A_n\;r^{-(n+1)}\;P_n(\cos\theta) \tag{946}$$

This series is unique and the coefficients A_n can be determined from the appropriate boundary condition.

A boundary condition that can be easily determined is given by the potential along the z axis. Since all the elemental charges are located at equal distances d from the point on the z axis

$$d \;=\; \sqrt{\;z^2\;+\;a^2} \tag{947}$$

and in spherical polar coordinates $r = z, \theta = 0$. The potential at a point on the z axis $(r, 0)$ is just given by the sum of the contributions from each elemental charge, the sum is just

$$\phi(r,0) \;=\; q\;\frac{1}{\sqrt{r^2\;+\;a^2}} \tag{948}$$

where q is the total charge on the ring. The potential has the expansion

$$\phi(r,0) \;=\; q \sum_{n=0}^{\infty} (\,-\,1\,)^n \, \frac{(2n)!}{2^{2n}\,(n!)^2} \, \frac{a^{2n}}{r^{(2n+1)}} \tag{949}$$

On noting that $P(\cos 0) \;=\; 1$, one can uniquely identify the coefficients A_n by comparing the expansions in inverse powers of r as

$$A_{2n} \;=\; q\,(\,-\,1\,)^n \, \frac{(2n)!}{2^{2n}\,(n!)^2} \, a^{2n} \tag{950}$$

while

$$A_{2n+1} \;=\; 0 \tag{951}$$

Hence, we obtain the potential $\phi(r,\theta)$ as an expansion

$$\phi(r,\theta) \;=\; \frac{q}{r} \sum_{n=0}^{\infty} (\,-\,1\,)^n \, \frac{(2n)!}{2^{2n}\,(n!)^2} \left(\frac{a}{r}\right)^{2n} P_n(\cos\theta) \tag{952}$$

Example:

As another example consider a sphere that is cut into two hemispheres of radius a. The hemisphere at $r \;=\; a$ and with $\pi \;>\; \theta \;>\; \frac{\pi}{2}$ is held at a potential ϕ_0, while the other hemisphere at $r \;=\; a$ and $\frac{\pi}{2} \;>\; \theta \;>\; 0$ is held at a potential $-\,\phi_0$.

Since the problem is symmetric under rotations around the z axis, the potential $\phi(r,\theta)$ is independent of φ. The potential inside the sphere satisfies Laplace's equation

$$\nabla^2\,\phi \;=\; 0 \tag{953}$$

which in spherical polar coordinates, and using the azimuthal symmetry, becomes

$$\frac{1}{r^2}\,\frac{\partial}{\partial r}\left(\,r^2\,\frac{\partial\phi}{\partial r}\,\right) \;+\; \frac{1}{r^2\,\sin\theta}\,\frac{\partial}{\partial\theta}\left(\,\sin\theta\,\frac{\partial\phi}{\partial\theta}\,\right) \;=\; 0 \tag{954}$$

The solution is found by the method of separation of variables

$$\phi(r,\theta) \;=\; R(r)\;\Theta(\theta) \tag{955}$$

after which it is found that the radial function $R(r)$ must satisfy an eigenvalue equation

$$\frac{\partial}{\partial r}\left(\,r^2\,\frac{\partial R}{\partial r}\,\right) \;=\; n\,(\,n\,+\,1\,)\,R \tag{956}$$

Then, for fixed n we have the solution

$$R_n(r) \; = \; \bigg(\, A_n \, r^n \; + \; B_n \, r^{-(n+1)} \, \bigg) \tag{957}$$

The angular part must satisfy Legendre's equation

$$\frac{\partial}{\partial \theta} \left(\; \sin \theta \, \frac{\partial \Theta(\theta)}{\partial \theta} \; \right) \; + \; n \; (\; n \; + \; 1 \;) \; \Theta(\theta) \; = \; 0 \tag{958}$$

which forces n to be an integer. The solution is given by the Legendre polynomial in $\cos \theta$

$$\Theta_n(\theta) \; = \; P_n(\cos \theta) \tag{959}$$

Thus, we can form a general solution as a series expansion

$$\phi(r, \theta) \; = \; \sum_{n=0}^{\infty} \; \bigg(\; A_n \, r^n \; + \; B_n \, r^{-(n+1)} \; \bigg) \, P_n(\cos \theta) \tag{960}$$

The coefficients B_n are zero as the potential $\phi(0, \theta)$ is expected to be finite. The coefficients A_n can be obtained from the boundary condition at $r \; = \; a$. That is, since one has

$$\phi(a, \theta) \; = \; \sum_{n=0}^{\infty} \; A_n \, a^n \, P_n(\cos \theta) \tag{961}$$

then, on using the orthogonality of the Legendre polynomials one has

$$\begin{aligned} \frac{2}{2 \, n \; + \; 1} \, A_n \, a^n \; & = \; \int_0^{\pi} \; d\theta \; \sin \theta \; \phi(a, \theta) \; P_n(\cos \theta) \\ & = \; \phi_0 \, \left(\; \int_{\frac{\pi}{2}}^{\pi} \; d\theta \; \sin \theta \; \; P_n(\cos \theta) \; - \; \int_0^{\frac{\pi}{2}} \; d\theta \; \sin \theta \; P_n(\cos \theta) \; \right) \end{aligned} \tag{962}$$

When this integral is evaluated, since the function $\phi(a, \theta)$ is odd only the Legendre polynomials with odd values of n survive, as $P_{2n}(\cos \theta)$ is an even function of $\cos \theta$. Then

$$A_{2n+1} \, a^{2n+1} \; = \; \phi_0 \, \sum_{n=0}^{\infty} \; (\, - \, 1 \,)^{n+1} \, \frac{(4n+3) \; (2n-1)!!}{(2n+2)!!} \tag{963}$$

Thus, we have the potential as an expansion

$$\phi(r, \theta) \; = \; \phi_0 \, \sum_{n=0}^{\infty} (\, - \, 1 \,)^{n+1} \, \frac{(4n+3) \; (2n-1)!!}{(2n+2)!!} \, \left(\, \frac{r}{a} \, \right)^{2n+1} \, P_{2n+1}(\cos \theta) \tag{964}$$

Example:

A plane wave can be expanded as

$$\exp\left[i \vec{k} . \vec{r} \right] = \sum_{l=0}^{\infty} C_l \; j_l(kr) \; P_l(\cos\theta) \tag{965}$$

where θ is the angle between the position and the direction of the momentum. This form of the expansion is to be expected as both the Bessel function expansion and the plane wave are eigenstates of the Laplacian, with eigenvalue $- k^2$. It can be shown that $C_l = i^l \; (2 \, l + 1)$.

On differentiating the expansion with respect to kr, one obtains

$$i \cos\theta \exp\left[i \vec{k} . \vec{r} \right] = \sum_{l=0}^{\infty} C_l \; j'_l(kr) \; P_l(\cos\theta) \tag{966}$$

or on using the expansion again

$$i \cos\theta \sum_{l=0}^{\infty} C_l \; j_l(kr) \; P_l(\cos\theta) = \sum_{l=0}^{\infty} C_l \; j'_l(kr) \; P_l(\cos\theta) \tag{967}$$

The recurrence relation can be used to express $\cos\theta \; P_n(\cos\theta)$ entirely in terms of the Legendre polynomials via

$$(2 \, l + 1) \cos\theta \; P_l(\cos\theta) = (l + 1) \; P_{l+1}(\cos\theta) + l \; P_{l-1}(\cos\theta) \tag{968}$$

On multiplying by $P_m(\cos\theta) \; \sin\theta$ and integrating one obtains

$$i \left(\frac{m}{2 \, m - 1} C_{m-1} \; j_{m-1}(kr) + \frac{(m + 1)}{2 \, m + 3} C_{m+1} \; j_{m+1}(kr) \right) = C_m \; j'_m(kr) \tag{969}$$

Then on using the recurrence relations for the derivative of the spherical Bessel functions

$$j'_m(kr) = \frac{m}{2 \, m + 1} \; j_{m-1}(kr) - \frac{(m + 1)}{2 \, m + 1} \; j_{m+1}(kr) \tag{970}$$

one finds

$$\begin{aligned} i & \left(\frac{m}{2 \, m - 1} C_{m-1} \; j_{m-1}(kr) + \frac{(m + 1)}{2 \, m + 3} C_{m+1} \; j_{m+1}(kr) \right) \\ & = C_m \left(\frac{m}{2 \, m + 1} \; j_{m-1}(kr) - \frac{(m + 1)}{2 \, m + 1} \; j_{m+1}(kr) \right) \end{aligned} \tag{971}$$

Since the two Bessel functions, of order $m-1$ and $m+1$, can be considered to be linearly independent, one can equate the coefficients to yield the recursion relation

$$C_m \;=\; i\,\frac{(\,2\,m\;+\;1\,)}{(\,2\,m\;-\;1\,)}\,C_{m-1} \tag{972}$$

The first coefficient can be obtained by examining the limit $k\;\rightarrow\;0$ since in this case only $j_0(0)$ survives, and has a magnitude of unity. Hence,

$$C_0 \;=\; 1 \tag{973}$$

and we have the expansion coefficients as

$$C_l \;=\; i^l\;(\,2\,l\;+\;1\,) \tag{974}$$

Thus, we have found the expansion of the plane wave in terms of the spherical Bessel functions.

Example:

In quantum mechanics, the wave function in a scattering experiment is given by

$$\psi(\overrightarrow{r}) \;=\; \exp\left[\,i\,\overrightarrow{k}\,.\,\overrightarrow{r}\,\right]\;+\;\frac{f(k,\theta)}{r}\;\exp\left[\,i\,k\,r\,\right] \tag{975}$$

which is a superposition of the incident or unscattered wave of momentum $\hbar\,\overrightarrow{k}$, with a spherical outgoing scattered wave. The amplitude of the scattered wave, with a central scattering potential, is given by

$$f(k,\theta) \;=\; \frac{1}{k}\,\sum_{l=0}^{\infty}\,(\,2\,l\;+\;1\,)\exp\left[\,i\,\delta_l(k)\,\right]\;\sin\delta_l(k)\;P_l(\cos\theta) \tag{976}$$

where θ is the scattering angle, $\hbar\,k$ is the magnitude of the incident momentum, and $\delta_l(k)$ is the phase shift produced by the short ranged scattering potential. The differential scattering cross-section, $\frac{d\sigma}{d\Omega}$ multiplied by the solid angle subtended by the detector $d\Omega$ governs the relative probability that a particle of momentum k will be scattered through an angle θ into a detector that subtends a solid angle $d\Omega$ to the target. The dependence on the size of the detector is given by the factor $d\Omega$. The differential scattering cross-section can be shown to be given by the scattering amplitude through

$$\frac{d\sigma}{d\Omega}(k,\theta) \;=\; |\;f(k,\theta)\;|^2 \tag{977}$$

The total scattering cross-section is determined as an integration over all solid angles of the differential scattering cross-section

$$\begin{aligned}\sigma_T(k) &= \int d\Omega \, \frac{d\sigma}{d\Omega}(k,\theta) \\ &= \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \, \sin\theta \mid f(k,\theta) \mid^2\end{aligned} \tag{978}$$

On substituting, the expansion in terms of the Legendre series, and integrating, one can use the orthogonality relations and obtain the total scattering cross-section as

$$\sigma_T(k) = \frac{4\,\pi}{k^2} \sum_{l=0}^{\infty} (\, 2\, l \, + \, 1 \,) \, \sin^2\delta_l(k) \tag{979}$$

9.1 Associated Legendre Functions

The Asssociated Legendre functions, $P_n^m(\cos\theta)$, satisfy the associated Legendre differential equation

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \, \frac{\partial}{\partial\theta} \, P_n^m(\cos\theta) \right) + \left[n\,(\,n\,+\,1\,) \, - \, \frac{m^2}{\sin^2\theta} \right] P_n^m(\cos\theta) \, = \, 0 \tag{980}$$

or with the substitution $x = \cos\theta$ one has

$$(\,1\,-\,x^2\,)\,\frac{\partial^2}{\partial x^2}\,P_n^m(x) \, - \, 2\,x\,P_n^m(x) \, + \, \left[n\,(\,n\,+\,1\,) \, - \, \frac{m^2}{1\,-\,x^2} \right] P_n^m(x) \, = \, 0 \tag{981}$$

This also has regular singular points at $x \pm 1$. When $m^2 = 0$, the associated Legendre differential equation reduces to Legendre's differential equation.

The associated Legendre functions are given by the expression

$$P_n^m(x) \, = \, (\,1\,-\,x^2\,)^{\frac{m}{2}} \, \frac{\partial^m}{\partial x^m} \, P_n(x) \tag{982}$$

where $P_n(x)$ are the Legendre polynomials. It can be proved that these functions satisfy the associated Legendre differential equation. Let us note that the associated Legendre functions are zero if $m > n$, since the polynomial $P_n(x)$ is a polynomial of order n.

9.1.1 The Associated Legendre Equation

The associated Legendre functions satisfy the associated Legendre equation, as can be shown by by starting from Legendre's equation

$$(1 - x^2) \frac{\partial^2}{\partial x^2} P_n(x) - 2 x \frac{\partial}{\partial x} P_n(x) + n (n + 1) P_n(x) = 0 \quad (983)$$

and then differentiating m times. On using the formula

$$\frac{\partial^m}{\partial x^m} \bigg(A(x) \, B(x) \bigg) = \sum_{n=0}^{n=m} C(m,n) \frac{\partial^{m-n}}{\partial x^{m-n}} A(x) \frac{\partial^n}{\partial x^n} B(x) \quad (984)$$

one obtains

$$\begin{aligned} (1 - x^2) \frac{\partial^{2+m}}{\partial x^{2+m}} P_n(x) - 2 x (m + 1) \frac{\partial^{1+m}}{\partial x^{1+m}} P_n(x) \\ + (n - m) (n + m + 1) \frac{\partial^m}{\partial x^m} P_n(x) = 0 \end{aligned} \quad (985)$$

since $(1 - x^2)$ only has two non-vanishing orders of derivatives.

On setting

$$\frac{\partial^m}{\partial x^m} P_n(x) = (1 - x^2)^{-\frac{m}{2}} P_n^m(x) \quad (986)$$

and then differentiating, one obtains

$$\frac{\partial^{m+1}}{\partial x^{m+1}} P_n(x) = (1 - x^2)^{-\frac{m}{2}} \frac{\partial}{\partial x} P_n^m(x) + \frac{m \, x}{1 - x^2} (1 - x^2)^{-\frac{m}{2}} P_n^m(x) \quad (987)$$

On differentiating a second time, one obtains

$$\begin{aligned} \frac{\partial^{m+2}}{\partial x^{m+2}} P_n(x) &= (1 - x^2)^{-\frac{m}{2}} \frac{\partial^2}{\partial x^2} P_n^m(x) \\ &+ 2 \frac{m \, x}{1 - x^2} (1 - x^2)^{-\frac{m}{2}} \frac{\partial}{\partial x} P_n^m(x) \\ &+ \frac{m (m + 2) x^2}{(1 - x^2)^2} (1 - x^2)^{-\frac{m}{2}} P_n^m(x) \\ &+ \frac{m}{(1 - x^2)} (1 - x^2)^{-\frac{m}{2}} P_n^m(x) \end{aligned} \quad (988)$$

These expressions are substituted into the m-th order differential relation, and after cancelling the common factor of $(1 - x^2)^{-\frac{m}{2}}$ one has

$$(1 - x^2) \frac{\partial^2}{\partial x^2} P_n^m(x) - 2 x \frac{\partial}{\partial x} P_n^m(x) + \bigg(n (n + 1) - \frac{m^2}{1 - x^2} \bigg) P_n^m(x) = 0 \quad (989)$$

Expressing the variable x in terms of the variable appropriate to the polar angle $x = \cos\theta$, the Associated Legendre equation becomes

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\,P_n^m(\cos\theta)\right) + \left(n\,(\,n+1\,) - \frac{m^2}{\sin^2\theta}\right) P_n^m(x) \;=\; 0 \tag{990}$$

This equation reduces to Legendre's differential equation when $m = 0$ and the associated Legendre function of order m equal to zero is the Legendre polynomial.

The Legendre polynomial are non zero for the range of n values such that $n \geq m \geq 0$, but can also be defined for negative m values in which case

$$n \;\geq\; m \;\geq\; -\,n \tag{991}$$

and

$$P_n^{-m}(x) \;=\; (\,-\,1\,)^m\,\frac{(n-m)!}{(n+m)!}\,P_n^m(x) \tag{992}$$

since the differential equation only involves m^2 and does not depend on the sign of m.

The associated Legendre equation is often encountered in three dimensional situations which involve the Laplacian, in which the azimuthal dependence does not vanish. In this case, one has

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\,\frac{\partial\psi}{\partial r}\right) \;+\; \frac{1}{r^2\,\sin\theta}\,\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial\psi}{\partial\theta}\right) \;+\; \frac{1}{r^2\sin^2\theta}\,\frac{\partial^2\psi}{\partial\varphi^2} \;=\; -\,k^2\,\psi \tag{993}$$

On using the ansatz for separation of variables

$$\psi(r,\theta,\varphi) \;=\; R(r)\;\Theta(\theta)\;\Phi(\varphi) \tag{994}$$

and diving by ψ one obtains

$$\frac{1}{r^2\,R}\frac{\partial}{\partial r}\left(r^2\,\frac{\partial R}{\partial r}\right) + \frac{1}{r^2\,\sin\theta\;\Theta}\,\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial\Theta}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta\;\Phi}\,\frac{\partial^2\Phi}{\partial\varphi^2} \;=\; -\,k^2 \tag{995}$$

On multiplying by $r^2\,\sin^2\theta$, one recognizes that since all the φ dependence is contained in the term

$$\frac{1}{\Phi}\,\frac{\partial^2\Phi}{\partial\varphi^2} \tag{996}$$

this must be a constant. That is, the azimuthal dependence must satisfy

$$\frac{\partial^2\Phi}{\partial\varphi^2} \;=\; -\,m^2\;\Phi \tag{997}$$

where m^2 is an arbitrary constant, (not necessarily integer). The above equation has solutions of the form

$$\Phi_m(\varphi) \; = \; \frac{1}{\sqrt{2\,\pi}} \; \exp \left[\; i \; m \; \varphi \; \right] \tag{998}$$

Since, with fixed (r, θ), the values of φ and $\varphi \; + \; 2 \; \pi$ represent the same physical point, one must have

$$\Phi_m(\varphi) \; = \; \Phi_m(\varphi + 2\pi) \tag{999}$$

which implies that m satisfies the condition

$$\exp \left[\; i \; m \; 2 \; \pi \; \right] \; = \; 1 \tag{1000}$$

and therefore m must be an integer. On substituting the constant back into the original equation one obtains

$$\frac{1}{r^2 \; R} \frac{\partial}{\partial r} \left(\; r^2 \; \frac{\partial R}{\partial r} \; \right) + \frac{1}{r^2 \; \sin\theta \; \Theta} \; \frac{\partial}{\partial \theta} \left(\; \sin\theta \; \frac{\partial \Theta}{\partial \theta} \; \right) - \frac{m^2}{r^2 \sin^2\theta} \; = \; - \; k^2 \tag{1001}$$

This equation can be rewritten as

$$\frac{1}{R} \frac{\partial}{\partial r} \left(\; r^2 \; \frac{\partial R}{\partial r} \; \right) \; + \; k^2 \; r^2 \; = \; - \; \frac{1}{\sin\theta \; \Theta} \; \frac{\partial}{\partial \theta} \left(\; \sin\theta \; \frac{\partial \Theta}{\partial \theta} \; \right) \; + \; \frac{m^2}{\sin^2\theta} \tag{1002}$$

The two sides of the equation depend on the different independent variables (r, θ), and therefore must be constants, say, $l \; (\; l \; + \; 1 \;)$. Then it can be seen that the θ dependence is given by the $\Theta_l^m(\theta)$ which satisfy the equation

$$\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\; \sin\theta \frac{\partial \Theta_l^m}{\partial \theta} \; \right) \; + \; \left[\; l \; (\; l \; + \; 1 \;) \; - \; \frac{m^2}{\sin^2\theta} \; \right] \; \Theta_l^m(\theta) \; = \; 0 \tag{1003}$$

The above equation is related to the equation for the associated Legendre functions. That is, the solution is given by

$$\Theta_l^m(\theta) \; = \; P_l^m(\cos\theta) \tag{1004}$$

and l must be integer.

9.1.2 Generating Function Expansion

The generating function expansion for the associated Legendre functions can be obtained from the generating function expansion of the Legendre polynomials

$$\frac{1}{\sqrt{1 \; - \; 2 \; x \; t \; + \; t^2}} \; = \; \sum_{n=0}^{\infty} \; P_n(x) \; t^n \tag{1005}$$

and the definition

$$P_n^m(x) \; = \; (\; 1 \; - \; x^2 \;)^{\frac{m}{2}} \; \frac{\partial^m}{\partial x^m} \; P_n(x) \tag{1006}$$

By differentiating the recursion relation m times, and multiplying by $(\, 1 - x^2 \,)^{\frac{m}{2}}$ one obtains

$$\frac{(2m)!}{2^m \; m!} \; \frac{(\; 1 \; - \; x^2 \;)^{\frac{m}{2}} \; t^m}{(\; 1 \; - \; 2 \; x \; t \; + \; t^2 \;)^{m+\frac{1}{2}}} \; = \; \sum_{n=0}^{\infty} \; P_n^m(x) \; t^n \tag{1007}$$

However, the first $m - 1$ associated Legendre functions in the sum are zero. Hence we have

$$\begin{aligned} \frac{(2m)!}{2^m \; m!} \; \frac{(\; 1 \; - \; x^2 \;)^{\frac{m}{2}}}{(\; 1 \; - \; 2 \; x \; t \; + \; t^2 \;)^{m+\frac{1}{2}}} \; &= \; \sum_{n=m}^{\infty} \; P_n^m(x) \; t^{n-m} \\ \frac{(2m)!}{2^m \; m!} \; \frac{(\; 1 \; - \; x^2 \;)^{\frac{m}{2}}}{(\; 1 \; - \; 2 \; x \; t \; + \; t^2 \;)^{m+\frac{1}{2}}} \; &= \; \sum_{s=0}^{\infty} \; P_{m+s}^m(x) \; t^s \end{aligned} \tag{1008}$$

9.1.3 Recursion Relations

The associated Legendre functions also satisfy recursion relations. The recursion relations become identical to the recursion relations of the Legendre polynomials when $m \; = \; 0$. The recursion relations for the associated Legendre functions can be derived from the recursion relations of the Legendre polynomials, by differentiating with respect to x, m times. For example, consider the recursion relation for the polynomial, $P_n(x)$,

$$(\; 2 \; n \; + \; 1 \;) \; x \; P_n(x) \; = \; (\; n \; + \; 1 \;) \; P_{n+1}(x) \; + \; n \; P_{n-1}(x) \tag{1009}$$

and differentiate with respect to x m times

$$\begin{aligned} (\; 2 \; n \; + \; 1 \;) \; x \; \frac{\partial^m}{\partial x^m} \; P_n(x) \; + \; m \; (\; 2 \; n \; + \; 1 \;) \; \frac{\partial^{m-1}}{\partial x^{m-1}} \; P_n(x) \\ = \; (\; n \; + \; 1 \;) \; \frac{\partial^m}{\partial x^m} \; P_{n+1}(x) \; + \; n \; \frac{\partial^m}{\partial x^m} \; P_{n-1}(x) \end{aligned} \tag{1010}$$

On identifying the associated Legendre polynomial as

$$\frac{\partial^m}{\partial x^m} \; P_n(x) \; = \; (\; 1 \; - \; x^2 \;)^{-\frac{m}{2}} \; P_n^m(x) \tag{1011}$$

the above relation reduces to

$$(\, 2 \, n + 1 \,) \, x \, P_n^m(x) + m \, (\, 2 \, n + 1 \,) \, (\, 1 - x^2 \,)^{\frac{1}{2}} \, P_n^{m-1}(x) \; = \; (\, n + 1 \,) \, P_{n+1}^m(x) + n \, P_{n-1}^m(x) \tag{1012}$$

Likewise, on starting with

$$(2 n + 1) P_n(x) = \frac{\partial}{\partial x} P_{n+1}(x) - \frac{\partial}{\partial x} P_{n-1}(x) \quad (1013)$$

and differentiating m times, one obtains

$$(2 n + 1) \frac{\partial^m}{\partial x^m} P_n(x) = \frac{\partial^{m+1}}{\partial x^{m+1}} P_{n+1}(x) - \frac{\partial^{m+1}}{\partial x^{m+1}} P_{n-1}(x) \quad (1014)$$

or

$$(2 n + 1) (1 - x^2)^{\frac{1}{2}} P_n^m(x) = P_{n+1}^{m+1}(x) - P_{n-1}^{m+1}(x) \quad (1015)$$

If m is replaced by $m - 1$ in the above equation, it can be combined with the previous recursion relation to yield the recursion relation

$$(2 n + 1) x P_n^m(x) = (n + 1 - m) P_{n+1}^m(x) + (n + m) P_{n-1}^m(x) \quad (1016)$$

The above recurrence relation for the Associated Legendre functions reduces to the corresponding recursion relation for the Legendre polynomials when $m = 0$.

Example:

The above recursion relation has an important application in quantum mechanics. The probability for an electron in an atom to undergo a transition between a state of orbital angular momentum (l, m) to an electronic state orbital angular momentum (l', m') is proportional to the modulus squared of the integrals

$$\begin{gathered} \int_0^\pi d\theta \, \sin\theta \, P_{l'}^m(\cos\theta) \, (\cos\theta) \, P_l^m(\cos\theta) \\ \int_0^\pi d\theta \, \sin\theta \, P_{l'}^{m+1}(\cos\theta) \, (\sin\theta) \, P_l^m(\cos\theta) \\ \int_0^\pi d\theta \, \sin\theta \, P_{l'}^{m-1}(\cos\theta) \, (\sin\theta) \, P_l^m(\cos\theta) \end{gathered} \quad (1017)$$

for the case $m' = m$ and $m' = m \pm 1$ respectively. Basically, in the dipole approximation, the electromagnetic field is represented by a complex time dependent vector

$$\propto \overrightarrow{r} \exp \left[i \omega t \right] \quad (1018)$$

In a non-relativistic approximation one would expect that the electromagnetic field would be represented by a vector, with three linearly independent basis vectors, or three polarizations. The three components of this complex vector are

$$\begin{aligned} r\ \sin\theta\ \cos\varphi & \left[\ i\ \omega\ t\ \right] \\ r\ \sin\theta\ \sin\varphi & \left[\ i\ \omega\ t\ \right] \\ r\ \cos\theta & \left[\ i\ \omega\ t\ \right] \end{aligned} \tag{1019}$$

The θ dependence of the vector is responsible for the factors in parenthesis sandwiched between the Legendre functions. It can be seen, that the first pair of these integrals can be expressed as

$$\begin{aligned} \frac{1}{2\,l\,+\,1}\int_0^\pi d\theta\ \sin\theta\ P_{l'}^m(\cos\theta)\left(\ (\ l\ +\ m\ )\ P_{l-1}^m(\cos\theta)\ +(\ l\ -\ m\ +\ 1\ )\ P_{l+1}^m(\cos\theta)\ \right) \\ \frac{1}{2\,l\,+\,1}\int_0^\pi d\theta\ \sin\theta\ P_{l'}^{m+1}(\cos\theta)\left(\ P_{l+1}^{m+1}(\cos\theta)\ -\ P_{l-1}^{m+1}(\cos\theta)\ \right) \end{aligned} \tag{1020}$$

by using the above two recursion relations. As the associated Legendre functions are expected to be orthogonal, since they are eigenvalues of a Stürm-Liouville equation, these integrals are only non-zero if $l'\,\pm\,1=\,l$. This condition is called a selection rule. The vanishing of the integral means that the only transitions which are allowed are those in which the magnitude of the electrons angular momentum is not conserved! The resolution of this apparent paradox is that the electromagnetic field carries a unit of angular momentum. The photon, which is the quantum particle representing an electromagnetic field has a quantized angular momentum, or spin of magnitude $1\,\hbar$. Likewise, a similar consideration of the superscript, m, also yields a selection rule of $m'\ -\ m\ =\ \pm\,1$, or 0. The index m corresponds to the z component of the angular momentum. The m selection rule corresponds to the statement that the angular momentum of the photon may be oriented in three directions, or have three polarizations. In the non-relativistic limit, the three polarizations correspond to the three possible values of m for which $P_1^m(\cos\theta)$ is non-vanishing.

Homework:

Derive a recursion relation which will reduce the last expression to the sums of integrals which only consist of the product of associated Legendre functions with index $m-1$, and the weighting factor $\sin\theta$.

9.1.4 Orthogonality

Associated Legendre functions with the same fixed m value are orthogonal, for different values of n. This can easily be proved from the differential equation

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}P_n^m(\cos\theta)\right)+\left(n\,(\,n\,+\,1\,)\,-\,\frac{m^2}{\sin^2\theta}\right)P_n^m(\cos\theta)\;=\;0 \tag{1021}$$

by multiplying by $P_{n'}^m(\cos\theta)$ and subtracting the analogous equation with n and n' interchanged. Since m is fixed, the terms involving $m^2\sin^{-2}\theta$ identically cancel, and on multiplying by the weight factor, one is left with

$$\left[\,P_{n'}^m(\cos\theta)\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}P_n^m(\cos\theta)\right)\,-\,P_n^m(\cos\theta)\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}P_{n'}^m(\cos\theta)\right)\right]$$
$$=\;\left(n'\,(\,n'\,+\,1\,)\,-\,n\,(\,n\,+\,1\,)\right)P_{n'}^m(\cos\theta)\;\sin\theta\;P_n^m(\cos\theta) \tag{1022}$$

which on integrating over θ from 0 to π, one obtains

$$\left(n'\,(\,n'+1\,)-n\,(\,n+1\,)\right)\int_0^\pi d\theta\;P_{n'}^m(\cos\theta)\;\sin\theta\;P_n^m(\cos\theta)\;=\;0 \tag{1023}$$

since the boundary terms vanish identically, if the associated Legendre functions and their derivatives are finite at the boundaries.

One finds that the associated Legendre functions have the normalization integrals given by the value

$$\int_0^\pi d\theta\;P_{n'}^m(\cos\theta)\;\sin\theta\;P_n^m(\cos\theta)\;=\;\delta_{n,n'}\,\frac{2}{2\,n\,+\,1}\,\frac{(n+m)!}{(n-m)!} \tag{1024}$$

Homework:

Evaluate the normalization integral for the case $n\;=\;n'$.

12.5.16

Example:

One example of the occurrence of the associated Legendre functions occurs in the vector potential $\vec{A}$ from a current loop.

Consider a circular current carrying loop of radius a in the equatorial plane ($\theta = \frac{\pi}{2}$), in which the current is constant and has a value I. The magnetic induction field, $\overrightarrow{B}$ is given by the solution of

$$\overrightarrow{\nabla} \wedge \overrightarrow{B} = \frac{4\,\pi}{c} \overrightarrow{j} \tag{1025}$$

where $\overrightarrow{j}$ is the current density. Together with the definition of the vector potential

$$\overrightarrow{B} = \overrightarrow{\nabla} \wedge \overrightarrow{A} \tag{1026}$$

one has

$$\overrightarrow{\nabla} \wedge \left(\overrightarrow{\nabla} \wedge \overrightarrow{A} \right) = \frac{4\,\pi}{c} \overrightarrow{j} \tag{1027}$$

Since, the problem has azimuthal symmetry $\overrightarrow{B}$ should be independent of φ and have no component in the direction $\hat{e}_\varphi$. The vector potential, therefore, is entirely in the direction $\hat{e}_\varphi$

$$\overrightarrow{A} = A_\varphi \, \hat{e}_\varphi \tag{1028}$$

Hence, one finds that the magnetic induction is given by

$$\overrightarrow{B} = \frac{1}{r^2 \, \sin\theta} \left| \begin{array}{ccc} \hat{e}_r & r\,\hat{e}_\theta & r\,\sin\theta\,\hat{e}_\varphi \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \theta} & \frac{\partial}{\partial \varphi} \\ 0 & 0 & r\,\sin\theta\,A_\varphi \end{array} \right| \tag{1029}$$

Then, the magnetic induction is given by

$$\overrightarrow{B} = \frac{1}{r^2\,\sin\theta} \left[\hat{e}_r \frac{\partial}{\partial\theta} \left(r\,\sin\theta\,A_\varphi \right) - \hat{e}_\theta\, r \frac{\partial}{\partial r} \left(r\,\sin\theta\,A_\varphi \right) \right] \tag{1030}$$

which is independent of φ.

$$\begin{aligned} \overrightarrow{\nabla} \wedge \overrightarrow{B} &= \frac{1}{r^2\,\sin\theta} \left| \begin{array}{ccc} \hat{e}_r & r\,\hat{e}_\theta & r\,\sin\theta\,\hat{e}_\varphi \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \theta} & \frac{\partial}{\partial \varphi} \\ \frac{1}{r\,\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,A_\varphi\right) & -\frac{\partial}{\partial r}\left(r\,A_\varphi\right) & 0 \end{array} \right| \\ &= -\,\hat{e}_\varphi \left[\frac{1}{r}\frac{\partial^2}{\partial r^2}\left(r\,A_\varphi \right) + \frac{1}{r^2}\frac{\partial}{\partial\theta}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,A_\varphi \right)\right)\right] \end{aligned} \tag{1031}$$

Thus, we have the equation

$$-\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}\left(r\,A_\varphi \right) + \frac{1}{r^2}\frac{\partial}{\partial\theta}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,A_\varphi \right)\right)\right] = \frac{4\,\pi}{c}\,j_\varphi \tag{1032}$$

which off the $\theta = \frac{\pi}{2}$ plane becomes

$$\left[\frac{1}{r} \frac{\partial^2}{\partial r^2} \left(r A_\varphi \right) + \frac{1}{r^2} \frac{\partial}{\partial \theta} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta A_\varphi \right) \right) \right] = 0 \qquad (1033)$$

On separating variables using

$$A_\varphi = R(r) \, \Theta(\theta) \qquad (1034)$$

one has

$$\frac{r}{R(r)} \frac{\partial^2}{\partial r^2} \left(r R(r) \right) = - \frac{1}{\Theta(\theta)} \frac{\partial}{\partial \theta} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \, \Theta(\theta) \right) \right) \qquad (1035)$$

On writing the separation constant as equal to $n (n + 1)$ one has

$$R_n(r) = A_n \, r^n + B_n \, r^{-(n+1)} \qquad (1036)$$

and the angular dependence is given by the solution of the equation

$$\frac{\partial}{\partial \theta} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \, \Theta(\theta) \right) \right) + n (n + 1) \, \Theta(\theta) = 0 \qquad (1037)$$

or

$$\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \Theta(\theta) \right) + \left[n (n + 1) - \frac{1}{\sin^2\theta} \right] \Theta(\theta) = 0 \qquad (1038)$$

which has the solution

$$\Theta(\theta) = P^1_n(\cos\theta) \qquad (1039)$$

Thus, the solution is of the general form

$$A_\varphi(r, \theta) = \sum_{n=0}^{\infty} \left(A_n \, r^n + B_n \, r^{-(n+1)} \right) P^1_n(\cos\theta) \qquad (1040)$$

The expansion coefficient $A_n = 0$ for $r > a$ as the vector potential must fall to zero as $r \rightarrow \infty$.

The coefficients B_n are determined from the boundary condition on the z axis where it is easy to calculate $\overrightarrow{B}$ as

$$B_z(r, \frac{\pi}{2}) = \frac{2 \pi}{c} I \frac{a^2}{(a^2 + r^2)^{\frac{3}{2}}} \qquad (1041)$$

Using

$$\begin{aligned} \overrightarrow{B} &= \frac{1}{r^2 \sin\theta} \left[\hat{e}_r \frac{\partial}{\partial \theta} \left(r \sin\theta A_\varphi \right) - \hat{e}_\theta \, r \frac{\partial}{\partial r} \left(r \sin\theta A_\varphi \right) \right] \\ &= \hat{e}_r \left(\frac{\cot\theta}{r} A_\varphi + \frac{1}{r} \frac{\partial A_\varphi}{\partial \theta} \right) - \hat{e}_\theta \left(\frac{1}{r} \frac{\partial r A_\varphi}{r} \right) \end{aligned} \qquad (1042)$$

one finds the general expression for the induction field. Since the derivative of the associated Legendre function can be expressed as

$$\frac{\partial}{\partial\theta} \, P_n^1(\cos\theta) \; = \; - \, \sin\theta \, \frac{\partial}{\partial\cos\theta} \, P_n^1(\cos\theta) \tag{1043}$$

and on using the recursion relation

$$(\, 1 - x^2 \,)^{\frac{1}{2}} \, \frac{\partial}{\partial x} \, P_n^m(x) \; = \; \frac{1}{2} \, P_n^{m+1}(x) - \frac{1}{2} \, (n+m) \, (n-m+1) \, P_n^{m-1}(x) \tag{1044}$$

and also

$$P_n^{m+1}(x) \; = \; \frac{2 \, m \, x}{\sqrt{1 \, - \, x^2}} \, P_n^m(x) \, + \, \Bigg(\, m \, (\, m \, - \, 1 \,) \, - \, n \, (\, n \, + \, 1 \,) \, \Bigg) \, P_n^{m-1}(x) \tag{1045}$$

one has

$$\frac{m \, x}{\sqrt{1 \, - \, x^2}} \, P_n^m(x) - (\, 1 - x^2 \,)^{\frac{1}{2}} \, \frac{\partial}{\partial x} \, P_n^m(x) \; = \; (\, n + m \,) \, (\, n - m + 1 \,) \, P_n^{m-1}(x) \tag{1046}$$

On substituting $m \; = \; 1$ one finds that

$$B_r(r,\theta) \; = \; \frac{1}{r^2} \, \sum_{n=0}^{\infty} \, A_n \, n \, (\, n \, + \, 1 \,) \, r^{-n} \, P_n(\cos\theta) \tag{1047}$$

and

$$B_\theta(r,\theta) \; = \; \frac{1}{r^2} \, \sum_{n=0}^{\infty} \, n \, A_n \, r^{-n} \, P_n^1(\cos\theta) \tag{1048}$$

On substituting $\theta \; = \; 0$ one has $P_m(1) \; = \; 1$ and $P_n^1(1) \; = \; 0$, thus the field on the z axis takes both the forms

$$\begin{aligned} B_r(r,0) \; &= \; \frac{1}{r^2} \, \sum_{n=0}^{\infty} \, A_n \, n \, (\, n \, + \, 1 \,) \, r^{-n} \\ &= \; \frac{2 \, \pi}{c} \, I \, \frac{a^2}{(\, a^2 \, + \, r^2 \,)^{\frac{3}{2}}} \end{aligned} \tag{1049}$$

From this one finds that, on expanding in powers of r^{-1} only the terms odd in r^{-n} and thus only the odd n coefficients (A_{2n+1}) are finite and are uniquely given by

$$A_{2n+1} \; = \; (\, - \, 1 \,)^n \, \frac{2 \, \pi \, I}{c \, 2^{(2n+1)}} \, \frac{(2n)!}{n! \, (n+1)!} \tag{1050}$$

This completes the solution for the vector potential.

9.2 Spherical Harmonics

The spherical harmonics are solutions for the angular part of Laplace's equation. They are composed of a product of an azimuthal function $\Phi(\phi)$ and a polar part $\Theta(\theta)$ and are normalized to unity.

The azimuthal part is given by the solution of

$$\frac{\partial^2}{\partial\varphi^2} \, \Phi(\varphi) \;=\; - \, m^2 \, \Phi(\varphi) \tag{1051}$$

which has solutions

$$\Phi_m(\varphi) \;=\; \frac{1}{\sqrt{2\,\pi}} \, \exp\left[\, i \, m \, \varphi \, \right] \tag{1052}$$

The value of m is integer since the function $\Phi_m(\varphi)$ is periodic in φ with period $2\,\pi$.

The polar angle dependence is given by

$$\Theta_n^m(\theta) \;=\; \sqrt{\frac{2n+1}{2} \, \frac{(n-m)!}{n+m)!}} \; P_n^m(\cos\theta) \tag{1053}$$

where, $n \; > \; m \; > \; - \, n$.

The spherical harmonics are defined by the product

$$\begin{aligned} Y_n^m(\theta,\varphi) \;&=\; (\, - \, 1 \,)^n \; \Theta_n^m(\theta) \; \Phi_m(\varphi) \\ &=\; (\, - \, 1 \,)^n \; \sqrt{\frac{2n+1}{2} \, \frac{(n-m)!}{(n+m)!}} \; P_n^m(\cos\theta) \; \frac{1}{\sqrt{2\,\pi}} \; \exp\left[\, i \, m \, \varphi \, \right] \\ &=\; (\, - \, 1 \,)^n \; \sqrt{\frac{2n+1}{4\,\pi} \, \frac{(n-m)!}{(n+m)!}} \; P_n^m(\cos\theta) \; \exp\left[\, i \, m \, \varphi \, \right] \end{aligned} \tag{1054}$$

The phase factor $(\, - \, 1 \,)^n$ is purely conventional and is known as the Condon - Shortley phase factor.

9.2.1 Expansion in Spherical Harmonics

Any function of the direction (θ,φ) can be expanded as a double series of the spherical harmonics

$$f(\theta,\varphi) \;=\; \sum_{l,m} C_l^m \; Y_l^m(\theta,\varphi) \tag{1055}$$

as the spherical harmonics form a complete set. Furthermore, the expansion coefficients can be obtained from

$$C_l^m \; = \; \int_0^\pi \, d\theta \, \int_0^{2\pi} \, d\varphi \; \sin\theta \; Y_l^m(\theta,\varphi)^* \; f(\theta,\varphi) \tag{1056}$$

The completeness relation can be expressed as

$$\delta(\; \Omega_1 \; - \; \Omega_2 \;) \; = \; \sum_{l=0}^{l=\infty} \; \sum_{m=-l}^{m=l} \; Y_l^m(\theta_1,\varphi_1)^* \; Y_l^m(\theta_2,\varphi_2) \tag{1057}$$

where

$$\delta(\; \Omega \; - \; \Omega' \;) \; = \; \delta(\; \varphi \; - \; \varphi' \;) \; \delta(\; \cos\theta \; - \; \cos\theta' \;) \tag{1058}$$

since this is equal to unity on integrating over all solid angles $d\Omega \; = \; d\varphi \; d\theta \; \sin\theta$ and θ is uniquely specified by the value of $\cos\theta$ for $\pi \; > \; \theta \; > \; 0$.

Alternately one can re-write the completeness relation as

$$\delta(\; \Omega_1 \; - \; \Omega_2 \;) \; = \; \sum_{l=0}^{\infty} \; \frac{2 \; l \; + \; 1}{4 \; \pi} \; P_l(\cos\gamma) \tag{1059}$$

where γ is the angle between (θ_1,φ_1) and (θ_2,φ_2). This can be proved by choosing the spherical polar coordinate system such that (θ_2,φ_2) is directed along the polar axis. In this case $\theta_2 \; = \; 0$, and so $\sin\theta_2 \; = \; 0$, therefore, the only non-zero associated Legendre functions and hence non-zero spherical harmonics, $Y_l^m(\theta_2,\varphi_2)$, are those corresponding to $m \; = \; 0$. Then as we have $P_l^0(1) \; = \; 1$, the completeness relation simply takes the form

$$\delta(\; \Omega_1 \;) \; = \; \sum_{l=0}^{l=\infty} \; \frac{1}{2 \; \pi} \; \frac{(2 \; l \; + \; 1 \;)}{2} \; P_l^0(\cos\theta_1) \tag{1060}$$

where $\cos\theta_1 \; = \; \cos\gamma$.

If these equivalent forms of the completeness relations can be identified for each term in the sum over l we have the spherical harmonic addition theorem.

9.2.2 Addition Theorem

Given two vectors with directions (θ_1,φ_1) and (θ_2,φ_2) have an angle γ between them. The angle is given by the vector product

$$\cos\gamma \; = \; \cos\theta_1 \; \cos\theta_2 \; + \; \sin\theta_1 \; \sin\theta_2 \; \cos(\varphi_1 \; - \; \varphi_2 \;) \tag{1061}$$

The addition theorem states

$$P_l(\cos\gamma) \; = \; \frac{4\,\pi}{2\,l\,+\,1} \sum_{m=-l}^{m=l} Y_l^m(\theta_1,\varphi_1)^* \; Y_l^m(\theta_2,\varphi_2) \tag{1062}$$

Example:

The multi-pole expansion of a potential $\phi(\underline{r})$ obtained for a charge distribution $\rho(\underline{r}')$, can be obtained from the generating function

$$\frac{1}{|\,\underline{r}\,-\,\underline{r}'\,|} \; = \; \sum_{l=0}^{\infty} \frac{r'^l}{r^{l+1}} \; P_l(\cos\theta) \tag{1063}$$

for $r' \; < \; r$. Using the addition theorem one has

$$\frac{1}{|\,\underline{r}\,-\,\underline{r}'\,|} \; = \; \sum_{l,m} \frac{r'^l}{r^{l+1}} \, \frac{4\,\pi}{2\,l\,+\,1} \; Y_l^{m*}(\theta',\varphi') \; Y_l^m(\theta,\varphi) \tag{1064}$$

Hence, one may write

$$\phi(\underline{r}) \; = \; \sum_{l,m} \frac{4\,\pi}{2\,l\,+\,1} \; q_l^m \; \frac{Y_l^m(\theta,\varphi)}{r^{l+1}} \tag{1065}$$

where

$$q_l^m \; = \; \int d^3\underline{r}' \; Y_l^{m*}(\theta',\varphi') \; r'^l \; \rho(\underline{r}') \tag{1066}$$

One has the symmetry

$$q_l^{-m} \; = \; (\,-\,1\,)^m \; q_l^{m*} \tag{1067}$$

The multipole expansion provides a nice separation of the potential into pieces, each of which has a unique angular dependence and a dependence on r.

The multipole moments q_l^m characterize the charge distribution $\rho(\underline{r}')$. The low order moments are given by

$$q_0^0 \; = \; \frac{1}{\sqrt{4\,\pi}} \int d^3\underline{r}' \; \rho(\underline{r}') \; = \; \frac{q}{\sqrt{4\,\pi}} \tag{1068}$$

where q is the total charge. Also

$$\begin{aligned} q_1^1 \; &= \; - \sqrt{\frac{3}{8\,\pi}} \int d^3\underline{r}' \; r' \; \sin\theta' \; \exp\left[\;-\;i\;\varphi\;\right] \rho(\underline{r}') \\ &= \; - \sqrt{\frac{3}{8\,\pi}} \int d^3\underline{r}' \left(\; x' \;-\; i\;y' \;\right) \rho(\underline{r}') \\ &= \; - \sqrt{\frac{3}{8\,\pi}} \left(\; p_x \;-\; i\;p_y \;\right) \end{aligned} \tag{1069}$$

and

$$\begin{aligned} q_1^0 &= - \sqrt{\frac{3}{4\,\pi}} \int d^3\underline{r}' \; r' \; \cos\theta' \; \rho(\underline{r}') \\ &= - \sqrt{\frac{3}{4\,\pi}} \; p_z \end{aligned} \tag{1070}$$

where the dipole moment is given by

$$\overrightarrow{p} = \int d^3\underline{r}' \; \overrightarrow{r}' \; \rho(\underline{r}') \tag{1071}$$

The next order contributions are given by

$$\begin{aligned} q_2^2 &= \frac{1}{4} \sqrt{\frac{15}{2\,\pi}} \int d^3\underline{r}' \; r'^2 \; \sin^2\theta' \; \exp\left[- \, i \; 2 \; \varphi' \right] \rho(\underline{r}') \\ &= \frac{1}{4} \sqrt{\frac{15}{2\,\pi}} \int d^3\underline{r}' \left(x' \; - \; i \; y' \right)^2 \rho(\underline{r}') \\ &= \frac{1}{12} \sqrt{\frac{15}{2\,\pi}} \left(Q_{1,1} \; - \; 2 \; i \; Q_{1,2} + \; Q_{2,2} \right) \end{aligned} \tag{1072}$$

where we are introducing the notation which labels the (x, y, z) components by (x_1, x_2, x_3), and have introduced a tensor $Q_{i,j}$ win which the components are labeled by the subscripts corresponding to (x_i, x_j). The multi-pole moment corresponding to $l \; = \; 2$ and $m \; = \; 1$ is given by

$$\begin{aligned} q_2^1 &= - \sqrt{\frac{15}{8\,\pi}} \int d^3\underline{r}' \; r'^2 \; \sin\theta' \; \cos\theta' \; \exp\left[- \, i \; \varphi' \right] \rho(\underline{r}') \\ &= - \sqrt{\frac{15}{8\,\pi}} \int d^3\underline{r}' \left(x' \; - \; i \; y' \right) z' \; \rho(\underline{r}') \\ &= - \frac{1}{3} \sqrt{\frac{15}{8\,\pi}} \left(Q_{1,3} \; - \; i \; Q_{2,3} \right) \end{aligned} \tag{1073}$$

and finally the $l \; = \; 2$, $m \; = \; 0$ component is given by

$$\begin{aligned} q_2^0 &= \frac{1}{2} \sqrt{\frac{5}{4\,\pi}} \int d^3\underline{r}' \; r'^2 \left(3 \; \cos^2\theta' \; - \; 1 \right) \rho(\underline{r}') \\ &= \frac{1}{2} \sqrt{\frac{5}{4\,\pi}} \int d^3\underline{r}' \left(3 \; z'^2 \; - \; r'^2 \right) \rho(\underline{r}') \end{aligned}$$

$$= \frac{1}{2} \sqrt{\frac{5}{4 \pi}} Q_{3,3} \tag{1074}$$

in which the quadrupole moment is represented by the traceless tensor

$$Q_{i,j} = \int d^3\underline{r}' \left(3 \, x'_i \, x'_j - {r'}^2 \right) \rho(\underline{r}') \tag{1075}$$

where $\underline{r}'$ is a position variable associated with the charge distribution.

In terms of the multi-pole moments, the potential at a position $\underline{r}$ far away from the charge distribution is given by

$$\phi(\underline{r}) = \frac{q}{r} + \frac{\overrightarrow{p} \, . \, \overrightarrow{r}}{r^3} + \sum_{i,j} Q_{i,j} \frac{x_i \, x_j}{r^5} + \ldots \tag{1076}$$

This series is expected to converge rapidly if the $\underline{r}$ is far away from the charges.

10 Hermite Polynomials

The generating function expansion for the Hermite Polynomials is given by

$$g(x,t) \;=\; \exp\left[\;-\;t^2\;+\;2\;x\;t\;\right] \;=\; \sum_{n=0}^{\infty} H_n(x)\,\frac{t^n}{n!} \tag{1077}$$

10.0.3 Recursion Relations

The generating function can be used to develop the recurrence relations

$$H_{n+1}(x) \;=\; 2\;x\;H_n(x) \;-\; 2\;n\;H_{n-1}(x) \tag{1078}$$

and

$$\frac{\partial}{\partial x}\;H_n(x) \;=\; 2\;n\;H_{n-1}(x) \tag{1079}$$

10.0.4 Hermite's Differential Equation

Also one can use the recurrence relations to establish the differential equation for the Hermite polynomials. First on using

$$\frac{\partial}{\partial x}\;H_n(x) \;=\; 2\;n\;H_{n-1}(x) \tag{1080}$$

combined with

$$2\;n\;H_{n-1}(x) \;=\; 2\;x\;H_n(x) \;-\; H_{n+1}(x) \tag{1081}$$

one has

$$\frac{\partial}{\partial x}\;H_n(x) \;=\; 2\;x\;H_n(x) \;-\; H_{n+1}(x) \tag{1082}$$

Differentiating this with respect to x yields

$$\frac{\partial^2}{\partial x^2}\;H_n(x) \;=\; 2\;H_n(x) \;+\; 2\;x\;\frac{\partial H_n(x)}{\partial x} \;-\; \frac{\partial H_{n+1}(x)}{\partial x} \tag{1083}$$

Finally, on increasing the index by unity one has

$$\frac{\partial}{\partial x}\;H_{n+1}(x) \;=\; 2\;(\;n\;+\;1\;)\;H_n(x) \tag{1084}$$

which can be used to eliminate the derivative of $H_{n+1}(x)$. This leads to the Hermite's differential equation

$$\frac{\partial^2}{\partial x^2}H_n(x) \;-\; 2\;x\;\frac{\partial}{\partial x}H_n(x) \;+\; 2\;n\;H_n(x) \;=\; 0 \tag{1085}$$

This is not of the form of a Stürm-Liouville equation, unless one introduces a weighting function

$$w(x) \; = \; \exp \left[\; - \; x^2 \; \right] \tag{1086}$$

This is found by examining the ratio's of the first two coefficients in the Stürm-Liouville form

$$p(x) \; \frac{\partial^2 \phi}{\partial x^2} \; + \; \frac{\partial p(x)}{\partial x} \; \frac{\partial \phi}{\partial x} \; + \; q(x) \; \phi(x) \; = \; \lambda \; w(x) \; \phi(x) \tag{1087}$$

in which case one identifies the ratio

$$\frac{\frac{\partial p(x)}{\partial x}}{p(x)} \; = \; - \; 2 \; x \tag{1088}$$

or on integrating

$$\ln p(x) \; = \; - \; x^2 \tag{1089}$$

Since the integrating factor is

$$p(x) \; = \; \exp \left[\; - \; x^2 \; \right] \tag{1090}$$

one finds the above weighting factor and the differential equation has the form

$$\frac{\partial}{\partial x} \bigg(\; \exp \left[\; - \; x^2 \; \right] \; \frac{\partial}{\partial x} H_n(x) \bigg) \; + \; 2 \; n \; \exp \left[\; - \; x^2 \; \right] \; H_n(x) \; = \; 0 \tag{1091}$$

10.0.5 Orthogonality

The Hermite polynomials form an orthogonal set

$$\int_{-\infty}^{\infty} dx \; H_n(x) \; \exp \left[\; - \; x^2 \; \right] \; H_m(x) \; = \; 0 \tag{1092}$$

if $n \; \neq \; m$. For $n \; = \; m$, one can obtain the normalization by use of the generating function. Integrating the product of two generating functions multiplied by the weight function

$$\begin{aligned} & \int_{-\infty}^{\infty} dx \; g(x,s) \; \exp \left[\; - \; x^2 \; \right] \; g(x,t) \\ = & \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \int_{-\infty}^{\infty} dx \; \exp \left[\; - \; x^2 \; \right] \; H_n(x) \; H_m(x) \; \frac{s^n}{n!} \; \frac{t^m}{m!} \\ = & \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dx \; \exp \left[\; - \; x^2 \; \right] \; H_n(x) \; H_n(x) \; \frac{(\; s \; t \;)^n}{(n!)^2} \end{aligned} \tag{1093}$$

where we have used the orthogonality relation. However, one also has

$$\begin{aligned}
& \int_{-\infty}^{\infty} dx \; g(x,s) \; \exp \left[\; - \; x^2 \; \right] \; g(x,t) \\
= & \int_{-\infty}^{\infty} dx \; \exp \left[\; - \; x^2 \; \right] \; \exp \left[\; - \; t^2 \; + \; 2 \; x \; t \; \right] \; \exp \left[\; - \; s^2 \; + \; 2 \; x \; s \; \right] \\
= & \int_{-\infty}^{\infty} dx \; \exp \left[\; - \; x^2 \; + \; 2 \; x \; (\; s \; + \; t \;) \; \right] \; \exp \left[\; - \; t^2 \; - \; s^2 \; \right] \\
= & \sqrt{\pi} \; \exp \left[\; (\; s \; + \; t \;)^2 \; \right] \; \exp \left[\; - \; s^2 \; - \; t^2 \; \right] \\
= & \sqrt{\pi} \; \exp \left[\; 2 \; s \; t \; \right]
\end{aligned} \tag{1094}$$

On expanding in powers of (s t) one finds

$$\int_{-\infty}^{\infty} dx \; g(x,s) \; \exp \left[\; - \; x^2 \; \right] \; g(x,t) \; = \; \sqrt{\pi} \; \sum_{n=0}^{\infty} \frac{(\; 2 \; s \; t \;)^n}{n!} \tag{1095}$$

Hence on equating the coefficients of the powers of (s t), one has the equality

$$\int_{-\infty}^{\infty} dx \; \exp \left[\; - \; x^2 \; \right] \; H_n(x) \; H_n(x) \; = \; \sqrt{\pi} \; 2^n \; n! \tag{1096}$$

which gives the desired normalization.

Example:

The one dimensional quantum mechanical harmonic oscillator is a state with energy E is governed by the equation

$$- \; \frac{\hbar^2}{2 \; m} \; \frac{\partial^2 \psi}{\partial x^2} \; + \; \frac{1}{2} \; m \; \omega^2 \; x^2 \; \psi \; = \; E \; \psi \tag{1097}$$

The asymptotic large x behavior is found as

$$\lim_{x \; \rightarrow \; \infty} \; \psi(x) \; \rightarrow \; \exp \left[\; - \; \frac{m \; \omega}{2 \; \hbar} \; x^2 \; \right] \tag{1098}$$

and so we seek a solution of the form

$$\psi(x) \; = \; \exp \left[\; - \; \frac{m \; \omega}{2 \; \hbar} \; x^2 \; \right] \; \phi(x) \tag{1099}$$

From this, we we find that the first order derivative is given by

$$\frac{\partial \psi}{\partial x} \; = \; \exp \left[\; - \; \frac{m \; \omega}{2 \; \hbar} \; x^2 \; \right] \left(\; - \; \frac{m \; \omega}{\hbar} \; x \; + \; \frac{\partial}{\partial x} \; \right) \phi(x) \tag{1100}$$

and the second order derivative is

$$\frac{\partial^2 \psi}{\partial x^2} \; = \; \exp \left[\; - \; \frac{m \; \omega}{2 \; \hbar} \; x^2 \; \right] \left(\left(\frac{m \; \omega}{\hbar} \right)^2 x^2 \; - \; \frac{m \; \omega}{\hbar} \; (1 \; + \; 2 \; x \; \frac{\partial}{\partial x} \;) \; + \; \frac{\partial^2}{\partial x^2} \; \right) \phi(x) \tag{1101}$$

Inserting this last expression into the eigenvalue equation, we find that ϕ satisfies the differential equation

$$\frac{\partial^2 \phi}{\partial x^2} \; - \; 2 \; \frac{m \; \omega}{\hbar} \; x \; \frac{\partial \phi}{\partial x} \; = \; - \; \frac{m \; (\; 2 \; E \; - \; \hbar \; \omega \;)}{\hbar^2} \; \phi \tag{1102}$$

This differential equation can be put into Hermite's form by introducing a dimensionless variable

$$z \; = \; \sqrt{\frac{\hbar}{m \; \omega}} \; x \tag{1103}$$

Thus, we have

$$\frac{\partial^2 \phi}{\partial z^2} \; - \; 2 \; z \; \frac{\partial \phi}{\partial z} \; + \; \left(\; \frac{2 \; E}{\hbar \; \omega} \; - \; 1 \; \right) \phi \tag{1104}$$

which has the Hermite polynomial $H_n(z)$ as a solution when

$$2 \; n \; = \; \left(\; \frac{2 \; E}{\hbar \; \omega} \; - \; 1 \; \right) \tag{1105}$$

Thus, the allowed values of the energy are given by

$$E \; = \; \hbar \; \omega \; (\; n \; + \; \frac{1}{2} \;) \tag{1106}$$

Homework:

In quantum mechanics one encounters the Hermite polynomials in the context of one dimensional harmonic oscillators. If a system in the n-th state is perturbed by a potential $V(x)$, the probability of a transition from the n-th state to the m-th state is proportional to

$$\frac{1}{\pi \; 2^{n+m} \; n! \; m!} \; \left| \; \int_{-\infty}^{\infty} dx \; \exp \left[\; - \; x^2 \; \right] \; H_n(x) \; V(x) \; H_m(x) \; \right|^2 \tag{1107}$$

Evaluate the integrals

$$\int_{-\infty}^{\infty} dx \; \exp \left[\; - \; x^2 \; \right] \; x \; H_n(x) \; H_m(x) \tag{1108}$$

and

$$\int_{-\infty}^{\infty} dx \; \exp\left[\; - \; x^2 \; \right] \; x^2 \; H_n(x) \; H_m(x) \tag{1109}$$

11 Laguerre Polynomials

The generating function expansion for the Laguerre polynomials is given by

$$g(x,t) \; = \; \frac{\exp\left[\; - \; \frac{x \; t}{1 \; - \; t} \; \right]}{1 \; - \; t} \; = \; \sum_{n=0}^{\infty} \; L_n(x) \; t^n \tag{1110}$$

From which one obtains the series expansion as

$$L_n(x) \; = \; \sum_{s=0}^{n} \; (\; - \; 1 \;)^{n-s} \; \frac{n!}{(n-s)!^2 \; s!} \; x^{n-s} \tag{1111}$$

11.0.6 Recursion Relations

The recursion relations for the Laguerre polynomials can be obtained from the generating function expansion. By differentiating the generating function with respect to t one obtains the

$$\frac{(\; 1 \; - \; x \; - \; t \;)}{(\; 1 \; - \; t \;)^2} \; g(x,t) \; = \; \sum_{n=0}^{\infty} \; L_n(x) \; n \; t^{n-1} \tag{1112}$$

and hence on multiplying by $(\; 1 \; - \; t \;)^2$ to obtain the recurrence relation

$$(\; n \; + \; 1 \;) \; L_{n+1}(x) \; + \; n \; L_{n-1}(x) \; = \; (\; 2 \; n \; + \; 1 \; - \; x \;) \; L_n(x) \tag{1113}$$

Also, on differentiating with respect to x and then multiplying by $(\; 1 \; - \; t \;)$ one obtains

$$- \; t \; g(x,t) \; = \; (\; 1 \; - \; t \;) \; \sum_{n=0}^{\infty} \; \frac{\partial}{\partial x} \; L_n(x) \; t^n \tag{1114}$$

and hence the recursion relation is found as

$$- \; L_n(x) \; = \; \frac{\partial}{\partial x} \; L_{n+1}(x) \; - \; \frac{\partial}{\partial x} \; L_n(x) \tag{1115}$$

Differentiating the first recursion relation yields

$$(\; n \; + \; 1 \;) \; \frac{\partial}{\partial x} L_{n+1}(x) \; + \; n \; \frac{\partial}{\partial x} L_{n-1}(x) \; = \; (\; 2 \; n \; + \; 1 \; - \; x \;) \; \frac{\partial}{\partial x} \; L_n(x) \; - \; L_n(x) \tag{1116}$$

The previous relation can be used (twice, once with index n and the second time with index $n - 1$) to eliminate the differential of $L_{n+1}(x)$ and the differential of $L_{n-1}(x)$, giving the recursion relation

$$x \; \frac{\partial}{\partial x} L_n(x) \; = \; n \; L_n(x) \; - \; n \; L_{n-1}(x) \tag{1117}$$

11.0.7 Laguerre's Differential Equation

The Laguerre polynomials satisfy Laguerres differential equation. The differential equation for the Laguerre polynomials can be derived by combining the recursion relations. This is done by differentiating the prior relation

$$x \frac{\partial^2}{\partial x^2} L_n(x) \; + \; \frac{\partial}{\partial x} L_n(x) \; = \; n \frac{\partial}{\partial x} L_n(x) \; - \; n \frac{\partial}{\partial x} L_{n-1}(x) \tag{1118}$$

and subtracting the previous equation one has

$$x \frac{\partial^2}{\partial x^2} L_n(x) + (\, 1 - x \,) \frac{\partial}{\partial x} L_n(x) \; = \; n \frac{\partial}{\partial x} L_n(x) - n \frac{\partial}{\partial x} L_{n-1}(x) - n \, L_n(x) + n \, L_{n-1}(x) \tag{1119}$$

Finally, the right hand side can be identified as $- \; n \; L_n(x)$. Thus, we have Laguerre's differential equation

$$x \frac{\partial^2}{\partial x^2} L_n(x) \; + \; (\; 1 \; - \; x \;) \frac{\partial}{\partial x} L_n(x) \; + \; n \; L_n(x) \; = \; 0 \tag{1120}$$

This equation is not in Stürm-Liouville form, but can be put in the form by multiplying by $\exp[\, - \, x \,]$. Hence, we obtain

$$\frac{\partial}{\partial x} \left(\; x \; \exp[\, - \, x \,] \; \frac{\partial}{\partial x} L_n(x) \; \right) \; + \; n \; \exp[\, - \, x \,] \; L_n(x) \; = \; 0 \tag{1121}$$

The solution is defined on the interval $(0, \infty)$. Thus, the Laguerre functions are orthogonal with weighting factor $\exp[\, - \, x \,]$.

11.1 Associated Laguerre Polynomials

The associated Laguerre polynomials are defined by

$$L^p_n(x) \; = \; (\; - \; 1 \;)^p \; \frac{\partial^p}{\partial x^p} \; L_{n+p}(x) \tag{1122}$$

11.1.1 Generating Function Expansion

A generating function can be obtained by differentiating the generating function for the Laguerre polynomials p times. This yields the generating function expansion

$$\frac{\exp\left[\; - \; \frac{x \; t}{1 \; - \; t} \; \right]}{(\; 1 \; - \; t \;)^{p+1}} \; = \; \sum_{n=0}^{\infty} \; L^p_n(x) \; t^n \tag{1123}$$

A pair of recursion relations can be derived as

$$(\; n \; + \; 1 \;) \; L^p_{n+1}(x) \; = \; (\; 2 \, n \; + \; p \; + \; 1 \; - \; x \;) \; L^p_n(x) - \; (\; n \; + \; p \;) \; L^p_{n-1}(x) \tag{1124}$$

and

$$x \frac{\partial}{\partial x} L^p_n(x) \; = \; n \; L^p_n(x) \; - \; (\; n \; + \; p \;) \; L^p_{n-1}(x) \tag{1125}$$

From these, or by differentiating Laguerre's differential equation p times, one finds

$$x \frac{\partial^2}{\partial x^2} L^p_n(x) \; + \; (\; p \; + \; 1 \; - \; x \;) \frac{\partial}{\partial x} L^p_n(x) \; + \; n \; L^p_n(x) \; = \; 0 \tag{1126}$$

The weighting function is found to be

$$x^p \; \exp[\, - \, x \,] \tag{1127}$$

The orthogonality condition is found to be

$$\int_0^\infty dx \; x^p \; \exp[\, - \, x \,] \; L^p_n(x) \; L^p_m(x) \; = \; \delta_{m,n} \; \frac{(n+p)!}{n!} \tag{1128}$$

Example:

The associated Laguerre polynomials occur in the solution of the Schrödinger equation for the hydrogen atom. The Schrödinger equation for the electron wave function has the form

$$- \; \frac{\hbar^2}{2 \; m} \; \nabla^2 \; \psi \; - \; \frac{Z \; e^2}{r} \; \psi \; = \; E \; \psi \tag{1129}$$

which involves the spherically symmetric Coulomb potential of the nucleus of charge $Z \; e$ acting on the electrons. On separation of variables, and finding that due to the spherical symmetry, the angular dependence is given by the spherical harmonic $Y^m_l(\theta, \varphi)$, then the remaining radial function $R(r)$ is given by

$$- \; \frac{\hbar^2}{2 \; m} \; \frac{1}{r^2} \; \frac{\partial}{\partial r} \left(r^2 \; \frac{\partial R}{\partial r} \right) \; + \; \frac{\hbar^2}{2 \; m} \; \frac{l \; (\; l \; + \; 1 \;)}{r^2} \; R \; - \; \frac{Z \; e^2}{r} \; R \; = \; E \; R \tag{1130}$$

where the second term is the centrifugal potential. This equation can be put in a dimensionless form by defining a characteristic length scale r_0 by equating the centrifugal potential with the Coulomb attraction. (This just corresponds to the radius of the circular orbit in Classical Mechanics.) The radius is found as

$$r_0 \; = \; \frac{\hbar^2}{2 \; m \; Z \; e^2} \tag{1131}$$

Then, introducing a dimensionless radius ρ as the ratio of the radius to that of the circular orbit

$$\rho \; = \; \frac{r}{r_0} \tag{1132}$$

one sees that the on expressing the Laplacian in dimensionless form the energy term is given by the following constant

$$\frac{2\ m\ E\ r_0^2}{\hbar^2} \ = \ \frac{E\ \hbar^2}{2\ m\ Z^2\ e^4} \ = \ - \ \frac{1}{4\ \alpha^2} \tag{1133}$$

which must also be dimensionless. The second equality was found by substituting the expression for r_0. The dimensionless constant must be negative, since an electron that is bound to the hydrogen atom does not have enough energy to escape to infinity. The minimum energy required to escape to infinity is zero energy, since the potential falls to zero at infinity and the minimum of the kinetic energy is also zero. That is the minimum energy E is that in which the electron comes to rest at infinity. Thus, since E is less than this minimum it is negative. In terms of the variable, ρ and the constant α one has the differential equation

$$\frac{1}{\rho^2}\ \frac{\partial}{\partial\rho} \left(\rho^2\ \frac{\partial R(\rho\ r_0)}{\partial\rho} \right) + \left(\frac{1}{\rho} - \frac{l\ (\ l\ +\ 1\ )}{\rho^2} - \frac{1}{4\ \alpha^2} \right) R(\rho\ r_0) \ = \ 0 \tag{1134}$$

The form of the solution can be found by examining the equation near $\rho \ \rightarrow \ 0$. In this case, the centrifugal potential is much larger than the Coulomb potential so one can neglect the Coulomb potential. Also, for the same reason, the energy constant $\frac{1}{4\ \alpha^2}$ is also negligible compared with the centrifugal barrier. The equation reduces to

$$\frac{1}{\rho^2}\ \frac{\partial}{\partial\rho} \left(\rho^2\ \frac{\partial R(\rho\ r_0)}{\partial\rho} \right) \ - \ \frac{l\ (\ l\ +\ 1\ )}{\rho^2}\ R(\rho\ r_0) \ = \ 0 \tag{1135}$$

near the origin, and has a solution

$$R(r) \ \propto \ \rho^l \tag{1136}$$

since the other solution is proportional to $\rho^{-(l+1)}$ which diverges at the origin. It is not acceptable to have a solution that diverges too badly at the origin.

The form of the equation at $\rho \ \rightarrow \ \infty$ simplifies to

$$\frac{1}{\rho^2}\ \frac{\partial}{\partial\rho} \left(\rho^2\ \frac{\partial R(\rho\ r_0)}{\partial\rho} \right) \ - \ \frac{1}{4\ \alpha^2}\ R(\rho\ r_0) \ = \ 0 \tag{1137}$$

which can be written as

$$\frac{\partial^2 R(\rho\ r_0)}{\partial\rho^2} \ + \ \frac{2}{\rho}\ \frac{\partial R(\rho\ r_0)}{\partial\rho} \ - \ \frac{1}{4\ \alpha^2}\ R(\rho\ r_0) \ = \ 0 \tag{1138}$$

which for large ρ simply becomes

$$\frac{\partial^2 R(\rho\, r_0)}{\partial \rho^2} \; - \; \frac{1}{4\,\alpha^2}\, R(\rho\, r_0) \; = \; 0 \tag{1139}$$

which has the solution

$$R(\rho\, r_0) \; \propto \; \exp\left[\; - \; \frac{\rho}{2\,\alpha} \; \right] \tag{1140}$$

as the other solution which diverges exponentially as

$$R(\rho\, r_0) \; \propto \; \exp\left[\; + \; \frac{\rho}{2\,\alpha} \; \right] \tag{1141}$$

is physically unacceptable for an electron that is bound to the nucleus at a distance r_0. Thus, we have found that electrons are bound at a distance of $2\,\alpha\,r_0$ from the origin.

This motivates one looking for a solution with the right forms at the origin and at infinity. This form can be expressed as

$$R(\rho\, r_0) \; = \; \exp\left[\; - \; \frac{\rho}{2\,\alpha} \; \right] \rho^l \, L(\frac{\rho}{\alpha}) \tag{1142}$$

To substitute this form into the differential equation, one needs to evaluate the first and second order derivatives of the form. First note that

$$\frac{\partial R(\rho\, r_0)}{\partial \rho} \; = \; \exp\left[\; - \; \frac{\rho}{2\,\alpha} \; \right] \rho^l \; \left[\left(\; - \; \frac{1}{2\,\alpha} \; + \; \frac{l}{\rho} \; \right) L(\frac{\rho}{\alpha}) \; + \; \frac{1}{\alpha}\, L'(\frac{\rho}{\alpha}) \right] \tag{1143}$$

and then note that

$$\begin{aligned} \frac{\partial}{\partial \rho} \left(\rho^2 \, \frac{\partial R(\rho\, r_0)}{\partial \rho} \right) \; &= \; \exp\left[\; - \; \frac{\rho}{2\,\alpha} \; \right] \rho^{l+2} \times \\ \times \left[\left(\frac{1}{4\,\alpha^2} \; - \; \frac{(\, l \, + \, 1\,)}{\alpha\,\rho} \; + \; \frac{l\,(\, l \, + \, 1\,)}{\rho^2} \right) L(\frac{\rho}{\alpha}) \right. \\ \left. + \left(\; - \; \frac{1}{\alpha^2} \; + \; \frac{2\,l \, + \, 2}{\rho\,\alpha} \right) L'(\frac{\rho}{\alpha}) \; + \; \frac{1}{\alpha^2}\, L''(\frac{\rho}{\alpha}) \right] \end{aligned} \tag{1144}$$

Thus, one finds that L satisfies the equation

$$\frac{\rho}{\alpha^2}\, L'' \; + \; (\, 2\,l \; + \; 2 \; - \; \frac{\rho}{\alpha}\,)\, \frac{1}{\alpha}\, L' \; + \; \left(1 \; - \; \frac{(\, l \, + \, 1\,)}{\alpha} \right) L \; = \; 0 \tag{1145}$$

or

$$\frac{\rho}{\alpha}\, L'' \; + \; (\, 2\,l \; + \; 2 \; - \; \frac{\rho}{\alpha}\,)\, L' \; + \; \left(\alpha \; - \; (\, l \; + \; 1\,) \right) L \; = \; 0 \tag{1146}$$

Hence $L(x)$ is the associated Laguerre polynomial $L^{(2l+1)}_{\alpha \, - \, l \, - \, 1}(x)$, when α is an integer. If the function is to be normalizable, it is necessary for the series to terminate, and hence $\alpha \, - \, l \, - \, 1$ must be an integer. It is usual to set $n \, = \, \alpha$, and have the condition $n \, \geq \, l \, + \, 1$. The radial wave function is given by

$$R(r) \; \propto \; r^l \; \exp \left[\; - \; \frac{r}{2 \; n \; r_0} \; \right] \; L^{(2l+1)}_{(n-l-1)} \left(\frac{r}{n \; r_0} \right) \tag{1147}$$

Example:

The energy eigenvalue equation for a three dimensional harmonic oscillator is given by

$$- \; \frac{\hbar^2}{2 \; m} \; \nabla^2 \; \psi \; + \; \frac{1}{2} \; m \; \omega^2 \; r^2 \; \psi \; = \; E \; \psi \tag{1148}$$

On using separation of variables

$$\psi \; = \; R(r) \; Y^m_l(\theta, \varphi) \tag{1149}$$

one has

$$- \; \frac{\hbar^2}{2 \; m} \; \frac{1}{r^2} \; \frac{\partial}{\partial r} \; \left(\; r^2 \; \frac{\partial R}{\partial r} \; \right) \; R \; + \; \frac{\hbar^2 \; l \; (\; l \; + \; 1 \;)}{2 \; m \; r^2} \; R \; + \; \frac{m \; \omega^2 \; r^2}{2} \; R \; = \; E \; R \tag{1150}$$

On writing

$$R(r) \; = \; \rho^{\frac{l}{2}} \; \exp \left[\; - \; \frac{\rho}{2} \; \right] \; L(\rho) \tag{1151}$$

with a dimensionless variable

$$\rho \; = \; \frac{m \; \omega}{\hbar} \; r^2 \tag{1152}$$

one has

$$\frac{\partial R(r)}{\partial r} \; = \; 2 \; \sqrt{\frac{m \; \omega}{\hbar}} \; \rho^{\frac{l+1}{2}} \; \exp \left[\; - \; \frac{\rho}{2} \; \right] \; \left(\; \frac{l}{2 \; \rho} \; - \; \frac{1}{2} \; + \; \frac{\partial}{\partial \rho} \; \right) \; L \tag{1153}$$

and the second derivative is given by

$$\begin{aligned} \frac{\partial^2 R(r)}{\partial r^2} \; &= \; 4 \; \frac{m \; \omega}{\hbar} \; \rho^{\frac{l+2}{2}} \; \exp \left[\; - \; \frac{\rho}{2} \; \right] \; \left(\; \frac{l \; (\; l \; - \; 1 \;)}{4 \; \rho^2} \; - \; \frac{2 \; l \; + \; 1}{4 \; \rho} \; + \; \frac{1}{4} \right. \\ &+ \; \left. \left(\; \frac{2 \; l \; + \; 1}{2 \; \rho} \; - \; 1 \; \right) \; \frac{\partial}{\partial \rho} \; + \; \frac{\partial^2}{\partial \rho^2} \; \right) \; L \end{aligned} \tag{1154}$$

This leads to the equation

$$- \rho \, \frac{\partial^2 L}{\partial \rho^2} \; - \; \left(\frac{2 \, l \, + \, 3}{2} \; - \; \rho \right) \frac{\partial L}{\partial \rho} \; = \; \left(\frac{E}{2 \, \hbar \, \omega} \; - \; \frac{2 \, l \, + \, 3}{4} \right) L \qquad (1155)$$

which is the differential equation for the Associated Laguerre polynomials in which $p \; = \; \frac{2 \, l \, + \, 1}{2}$ and the quantum number n is given by

$$n \; = \; \left(\frac{E}{2 \, \hbar \, \omega} \; - \; \frac{2 \, l \, + \, 3}{4} \right) \qquad (1156)$$

Homework:

A quantum mechanical analysis of the Stark effect in parabolic coordinates leads to the differential equation

$$\frac{\partial}{\partial x} \left(x \, \frac{\partial u}{\partial x} \right) \; + \; \left(\frac{1}{2} \, E \, x \; + \; l \; - \; \frac{m^2}{4 \, x} \; - \; \frac{1}{4} \, F \, x^2 \right) u \; = \; 0 \qquad (1157)$$

where F is a measure of the strength of the electric field. Find the unperturbed wave function in terms of the Associated Laguerre polynomials.

12 Inhomogeneous Equations

12.1 Inhomogeneous Differential Equations

Inhomogeneous linear differential equations can be solved by Green's function methods. For example, if one has an equation of the type

$$\frac{\partial}{\partial x} \left(p(x) \, \frac{\partial \phi}{\partial x} \right) \; + \; (\; q(x) \; - \; \lambda \; w(x) \;) \; \phi(x) \; = \; f(x) \tag{1158}$$

where λ is a control parameter, and the solution is defined on an interval (a, b) and which satisfies boundary conditions at the ends of the interval, say of the type

$$\phi(a) \; = \; \phi(b) \; = \; 0 \tag{1159}$$

The solution of this equation can be found using Green's functions. The Green's function $G(x, x')$ is defined as the solution of the equation

$$\frac{\partial}{\partial x} \left(p(x) \, \frac{\partial G(x,x')}{\partial x} \right) \; + \; (\; q(x) \; - \; \lambda \; w(x) \;) \; G(x,x') \; = \; \delta(x-x') \tag{1160}$$

in which the inhomogeneous term is replaced by a delta function which is non-zero at the value of x given by $x \; = \; x'$. The Green's function must also satisfy the same boundary conditions as ϕ , which in this case is

$$G(a, x') \; = \; G(b, x') \; = \; 0 \tag{1161}$$

Since we can write the inhomogeneous term of our original equation in the form of an integral

$$f(x) \; = \; \int_a^b dx' \; \delta(x-x') \; f(x') \tag{1162}$$

then we can view the original inhomogeneous equation as a linear superposition of equations with δ function source terms, but in which the various terms are weighted with a factor of $f(x')$. That is, the solution can be expressed as

$$\phi(x) \; = \; \int_a^b dx' \; G(x,x') \; f(x') \tag{1163}$$

This expression satisfies the equation for $\phi(x)$, as can be seen by direct substitution. This means that once the Green's function has been found, the solution of the inhomogeneous equation, for any reasonable $f(x)$, can be found by integration.

12.1.1 Eigenfunction Expansion

One method of finding the Green's function is based on the completeness relation for the eigenvalues of the Stürm-Liouville equation in which the control parameter λ has been set to zero

$$\delta(x - x') \;=\; \sum_n \phi_n^*(x') \; w(x) \; \phi_n(x) \tag{1164}$$

Due to the completeness relation one can find an expansion of the Green's function in the form

$$G(x, x') \;=\; \sum_n G_n(x') \; \phi_n(x) \tag{1165}$$

where $G_n(x')$ is an unknown coefficient. As $\phi_n(x)$ satisfies the same boundary conditions as $G(x, x')$, this expansion is satisfies the boundary conditions. On substituting these two expansions in the equation one obtains

$$\sum_n (\; \lambda_n \; - \; \lambda \;) \; G_n(x') \; w(x) \; \phi_n(x) \;=\; \sum_n \phi_n^*(x') \; w(x) \; \phi_n(x) \tag{1166}$$

where we have used the Stürm-Liouville eigenvalue equation. On multiplying by $\phi_m^*(x)$ and integrating with respect to x and using the orthogonality of the eigenfunctions (where in the cases of degeneracies the eigenfunctions have been constructed via the Gram Schmidt process), one finds that

$$(\; \lambda_m \; - \; \lambda \;) \; G_m(x') \;=\; \phi_m^*(x') \tag{1167}$$

Thus, if the control parameter is chosen such that $\lambda_n \; \neq \; \lambda$ for all n, we have found that the Green's function is given in terms of a sum of the eigenfunctions

$$G(x, x') \;=\; \sum_n \frac{\phi_n^*(x') \; \phi_n(x)}{\lambda_n \; - \; \lambda} \tag{1168}$$

12.1.2 Piece-wise Continuous Solution

Alternatively, for one dimensional problems the Green's function which satisfies

$$\frac{\partial}{\partial x} \left(\; p(x) \; \frac{\partial G(x, x')}{\partial x} \; \right) \; + \; (\; q(x) \; - \; \lambda \; w(x) \;) \; G(x, x') \;=\; \delta(x - x') \tag{1169}$$

can be obtained from knowledge of the solutions of the homogeneous equation

$$\frac{\partial}{\partial x} \left(\; p(x) \; \frac{\partial \phi(x)}{\partial x} \; \right) \; + \; (\; q(x) \; - \; \lambda \; w(x) \;) \; \phi(x) \;=\; 0 \tag{1170}$$

utilizing the arbitrary constants of integration. In one dimension, the point x' separates the interval into two disjoint regions. The solution of the Green's function in the two regions $b\ x\ >\ x'$ and $x'\ >\ x\ >\ a$ coincide with the solution of the homogeneous equation with the appropriate boundary conditions. Then in the first region, $b\ >\ x\ >\ x'$, one can have

$$G(x,x') \ = \ C_1\ \phi_1(x) \tag{1171}$$

which satisfies the boundary condition at $x\ =\ b$. In the second region one can have $x'\ >\ x\ >\ a$

$$G(x,x') \ = \ C_2\ \phi_2(x) \tag{1172}$$

where $\phi_2(x)$ satisfies the boundary condition at $x\ =\ a$. The arbitrary constants C_1 and C_2 can be obtained from consideration of the other boundaries of the two intervals, that is the point $x\ =\ x'$. The Green's function must be continuous at $x\ =\ x'$, which requires that

$$C_1\ \phi_1(x') \ = \ C_2\ \phi_2(x') \tag{1173}$$

Furthermore, the Green's function must also satisfy the equation at $x\ =\ x'$. On integrating the differential equation for the Green's function from $x\ =\ x'\ -\ \epsilon$ and $x\ =\ x'\ +\ \epsilon$ and taking the limit $\epsilon\ \rightarrow\ 0$

$$p(x')\ \frac{\partial G(x,x')}{\partial x}\bigg|_{x=x'+\epsilon} \ - \ p(x')\ \frac{\partial G(x,x')}{\partial x}\bigg|_{x=x'-\epsilon} \ = \ 1 \tag{1174}$$

which leads to

$$C_1\ \frac{\partial\phi_1(x)}{\partial x}\bigg|_{x=x'} \ - \ C_2\ \frac{\partial\phi_2(x)}{\partial x}\bigg|_{x=x'} \ = \ \frac{1}{p(x')} \tag{1175}$$

The above pair of equations for the constants C_1 and C_2 has a solution if the Wronskian determinant is non-zero

$$W(\phi_1,\phi_2) \ = \ \begin{vmatrix} \phi_1(x') & \phi_2(x') \\ \frac{\partial\phi_1(x')}{\partial x} & \frac{\partial\phi_2(x')}{\partial x} \end{vmatrix} \tag{1176}$$

However, the Wronskian is given by

$$W(\phi_1,\phi_2) \ = \ \frac{C}{p(x')} \tag{1177}$$

where C is yet another constant. From linear algebra one has

$$\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} \ = \ \frac{\begin{pmatrix} \frac{\partial\phi_2}{\partial x}|_{x'} & -\ \phi_2(x') \\ \frac{\partial\phi_1}{\partial x}|_{x'} & -\ \phi_1(x') \end{pmatrix}}{W(\phi_1,\phi_2)} \begin{pmatrix} 0 \\ \frac{1}{p(x')} \end{pmatrix} \tag{1178}$$

So the constants C_1 and C_2 are found as

$$\begin{aligned} C_1 &= - \frac{\phi_2(x')}{C} \\ C_2 &= - \frac{\phi_1(x')}{C} \end{aligned} \tag{1179}$$

and so the Green's function is given by

$$G(x,x') = - \frac{1}{C} \phi_1(x) \phi_2(x') \tag{1180}$$

for $b > x > x'$ and

$$G(x,x') = - \frac{1}{C} \phi_1(x') \phi_2(x) \tag{1181}$$

for $x' > x > a$. Thus the Green's function is symmetric under the interchange of x and x'.

The solution of the inhomogeneous equation is found as

$$\begin{aligned} \phi(x) &= \int_a^b dx' \, G(x,x') \, f(x') \\ &= - \frac{1}{C} \int_a^x dx' \, \phi_1(x) \, \phi_2(x') \, f(x') - \frac{1}{C} \int_x^b dx' \, \phi_1(x') \, \phi_2(x) \, f(x') \\ &= - \frac{1}{C} \phi_1(x) \int_a^x dx' \, \phi_2(x') \, f(x') - \frac{1}{C} \phi_2(x) \int_x^b dx' \, \phi_1(x') \, f(x') \end{aligned} \tag{1182}$$

Example:

Show that the Green's function for the equation

$$\frac{\partial^2}{\partial x^2} \phi(x) = f(x) \tag{1183}$$

subject to the boundary conditions

$$\begin{aligned} \phi(0) &= 0 \\ \frac{\partial}{\partial x} \phi(x) \Big|_{x=1} &= 0 \end{aligned} \tag{1184}$$

is given by

$$\begin{aligned} G(x,t) &= -\,x \qquad \text{for } \; 0 \;\leq\; x \;<\; t \\ G(x,t) &= -\,t \qquad \text{for } \; t \;<\; x \;\leq\; 1 \end{aligned} \tag{1185}$$

This is solved by noting that for $x \neq x'$ the equation for the Green's function is given by the solution of

$$\frac{\partial^2 G(x,x')}{\partial x^2} \;=\; 0 \tag{1186}$$

This has a general solution

$$G(x,x') \;=\; a\,x \;+\; b \tag{1187}$$

The Green's function in the region $x' > x \geq 0$ must satisfy the boundary condition at $x = 0$. Thus, the Green's function has to satisfy the boundary condition

$$G_<(0,x') \;=\; a_<\,0 \;+\; b_< \;=\; 0 \tag{1188}$$

Hence, we have $b_< = 0$ so the Green's function in this region is given by

$$G_<(x,x') \;=\; a_<\,x \tag{1189}$$

In the second region, $1 \geq x > x'$, we have the boundary condition

$$\frac{\partial G_>(x,x')}{\partial x}\bigg|_1 \;=\; 0 \tag{1190}$$

which leads to

$$\frac{\partial G_>(x,x')}{\partial x}\bigg|_1 \;=\; a_> \;=\; 0 \tag{1191}$$

$$G_>(x,x') = \; b_> \tag{1192}$$

Continuity of the Green's function at $x = x'$ yields

$$a_<\,x' \;=\; b_> \tag{1193}$$

Furthermore, on integrating the differential equation between the limits $(x' - \epsilon, x' + \epsilon)$ we have

$$\begin{aligned} \int_{x'-\epsilon}^{x'+\epsilon} dx \left(\frac{\partial^2 G(x,x')}{\partial x^2} \right) &= \int_{x'-\epsilon}^{x'+\epsilon} \delta(\,x \;-\; x'\,) \\ \frac{\partial G(x,x')}{\partial x}\bigg|_{x'-\epsilon}^{x'+\epsilon} &= 1 \end{aligned} \tag{1194}$$

This leads to the second condition

$$0 \; - \; a_< \; = \; 1 \tag{1195}$$

Hence, we have

$$\begin{aligned} G_<(x,x') &= - \, x \\ G_>(x,x') &= - \, x' \end{aligned} \tag{1196}$$

Example:

Find the solution of the equation

$$\frac{\partial^2}{\partial x^2} \, \phi(x) \; + \; \phi(x) \; = \; f(x) \tag{1197}$$

subject to the boundary conditions

$$\begin{aligned} \phi(0) &= 0 \\ \frac{\partial}{\partial x} \, \phi(x) \Big|_{x=1} &= 0 \end{aligned} \tag{1198}$$

The Green's function can be obtained from knowledge of the solutions of the homogeneous equation. The general solution of the homogeneous equation is given by

$$G(x,x') \; = \; a \, \sin x \; + \; b \, \cos x \tag{1199}$$

In the first region ($<$) where $x' \; > \; x \; > \; 0$ the Green's function has to satisfy the boundary condition

$$G_<(0,x') \; = \; a_< \, \sin 0 \; + \; b_< \, \cos 0 \; = \; 0 \tag{1200}$$

Hence,

$$G_<(x,x') \; = \; a_< \, \sin x \tag{1201}$$

In the second region ($>$) where $1 \; > \; x \; > \; x'$ we have

$$\frac{\partial G_>(x,x')}{\partial x} \Big|_{x=1} \; = \; a_> \, \cos 1 \; - \; b_> \, \sin 1 \; = \; 0 \tag{1202}$$

Continuity, leads to the condition

$$\begin{aligned} G_<(x,x') &= G_>(x,x') \\ a_< \, \sin x' &= a_> \, \sin x' \; + \; b_> \, \cos x' \end{aligned} \tag{1203}$$

and since $G(x, x')$ satisfies the differential equation at $x = x'$ one finds on integrating the differential equation

$$\begin{aligned} \frac{\partial G_>(x,x')}{\partial x}\bigg|_{x'} \; - \; \frac{\partial G_<(x,x')}{\partial x}\bigg|_{x'} &= 1 \\ a_< \; \cos x' \; - \; a_> \; \cos x' \; + \; b_> \; \sin x' &= 1 \end{aligned} \tag{1204}$$

Eliminating $a_>$, using the relation $a_> = b_> \; \tan 1$, one obtains the pair of equations

$$\begin{aligned} a_< \; \sin x' \; \cos 1 &= b_> \; \cos(x' - 1) \\ a_< \; \cos x' \; \cos 1 \; + \; b_> \; \sin(x' - 1) &= \cos 1 \end{aligned} \tag{1205}$$

On solving these one finds the coefficients as

$$\begin{aligned} a_< &= \frac{\cos(x' - 1)}{\cos 1} \\ b_> &= \sin x' \\ a_> &= \frac{\sin x' \; \sin 1}{\cos 1} \end{aligned} \tag{1206}$$

Hence we have the Green's function as

$$\begin{aligned} G_<(x, x') &= \frac{\sin x \; \cos(x' - 1)}{\cos 1} \\ G_>(x, x') &= \frac{\sin x' \; \cos(x - 1)}{\cos 1} \end{aligned} \tag{1207}$$

The solution of the inhomogeneous differential equation is then given by

$$\phi(x) = \int_x^1 dx' \; G_<(x, x') \; f(x') \; + \; \int_0^x dx' \; G_>(x, x') \; f(x') \tag{1208}$$

Example:

Find the Green's function $G(x, x')$ that satisfies the equation

$$\frac{\partial}{\partial x}\left(x \; \frac{\partial G(x, x')}{\partial x} \right) = \delta(\; x \; - \; x' \;) \tag{1209}$$

subject to the boundary conditions $| \; G(0, x') \; | \; < \; \infty$ and $G(1, x') \; = \; 0$.

The homogeneous equation has the solution

$$G(x,x') = a \ln x + b \tag{1210}$$

The solution has to satisfy the boundary conditions

$$G_<(0,x') = a_< \ln 0 + b_< \neq \pm\infty \tag{1211}$$

and

$$G_>(1,x') = a_> \ln 1 + b_> = 0 \tag{1212}$$

The continuity condition leads to

$$G_>(x',x') = G_<(x',x') \tag{1213}$$

or

$$a_> \ln x' = b_< \tag{1214}$$

On integrating over a region of infinitesimal width ϵ around x', yields

$$\begin{aligned}\int_{x'-\epsilon}^{x'+\epsilon} dx \, \frac{\partial}{\partial x} \left(x \, \frac{\partial G(x,x')}{\partial x} \right) &= \int_{x'-\epsilon}^{x'+\epsilon} dx \; \delta(\, x - x' \,) \\ x' \left(\frac{\partial G_>(x,x')}{\partial x} \bigg|_{x'} - \frac{\partial G_<(x,x')}{\partial x} \bigg|_{x'} \right) &= 1 \end{aligned} \tag{1215}$$

Thus, $a_> = 1$ and from the continuity condition one has $b_< = \ln x'$. Hence, we find

$$\begin{aligned} G_<(x,x') &= \ln x' \\ G_>(x,x') &= \ln x \end{aligned} \tag{1216}$$

Example:

Find the series solution for the Green's function which satisfies the equation

$$\frac{\partial^2 G(x,x')}{\partial x^2} = \delta(\, x - x' \,) \tag{1217}$$

with boundary conditions

$$G(0,x') = G(1,x') = 0 \tag{1218}$$

The eigenvalue equation

$$\frac{\partial^2 \phi(x)}{\partial x^2} = \lambda \, \phi(x) \tag{1219}$$

satisfying the same boundary conditions has eigenfunctions $\phi_n(x)$ given by

$$\phi_n(x) \; = \; \sqrt{2} \; \sin n \pi x \tag{1220}$$

and eigenvalue $\lambda \; = \; - \; \pi^2 \; n^2$. On writing the Green's function as a series expansion in terms of a complete set of functions

$$G(x, x') \; = \; \sum_{n=1}^{\infty} \; G_n(x') \; \phi_n(x) \tag{1221}$$

then the expansion coefficients can be found by substitution into the differential equation

$$- \; \sum_{n=1}^{\infty} \; \pi^2 \; n^2 \; G_n(x') \; \phi_n(x) \; = \; \delta(\; x \; - \; x' \;) \tag{1222}$$

On multiplying by $\phi_m(x)$ and integrating over x we obtain

$$G_m(x') \; = \; - \; \frac{\phi_m(x')}{\pi^2 \; m^2} \tag{1223}$$

Thus, we have

$$G(x, x') \; = \; - \; \sum_{n=1}^{\infty} \; 2 \; \frac{\sin n \pi x \; \sin n \pi x'}{\pi^2 \; n^2} \tag{1224}$$

This can be compared with the expression

$$\begin{aligned} G_<(x, x') \; &= \; x \; (\; x' \; - \; 1 \;) \\ G_>(x, x') \; &= \; (\; x \; - \; 1 \;) \; x' \end{aligned} \tag{1225}$$

Example:

Consider a bowed stretched string. The bowing force is assumed to be transverse to the string, and has a force per unit length, at position x given by $f(x, t)$. Then, the displacement of the string, $u(x, t)$ is governed by the partial differential equation

$$\frac{\partial^2 u}{\partial x^2} \; - \; \frac{1}{c^2} \; \frac{\partial^2 u}{\partial t^2} \; = \; f(x, t) \tag{1226}$$

We assume a sinusoidal bowing force

$$f(x, t) \; = \; f(x) \; \text{Real} \; \exp \left[\; - \; i \; \omega \; t \; \right] \tag{1227}$$

The forced response is given by

$$u(x,t) \; = \; u(x) \text{ Real } \exp \left[\; - \; i \; \omega \; t \; \right] \tag{1228}$$

where $u(x)$ is determined by

$$\frac{\partial^2 u}{\partial x^2} \; + \; \frac{\omega^2}{c^2} \; u(x) \; = \; f(x) \tag{1229}$$

The string is fixed at the two ends, so

$$u(0) \; = \; u(l) \; = \; 0 \tag{1230}$$

The Green's function $G(x,x')$ satisfies the equation

$$\frac{\partial^2 G(x,x')}{\partial x^2} \; + \; \frac{\omega^2}{c^2} \; G(x,x') \; = \; \delta(x-x') \tag{1231}$$

along with the boundary conditions

$$G(0,x') \; = \; G(l,x') \; = \; 0 \tag{1232}$$

The solution can be found as

$$G(x,x') \; = \; \left\{ \begin{array}{cc} A \; \sin k \; x & x \; < \; x' \\ \\ B \; \sin k \; (\; x \; - \; l \;) & x \; > \; x' \end{array} \right\} \tag{1233}$$

where $k \; = \; \frac{\omega}{c}$. On integrating the differential equation over an infinitesimal region around the delta function yields

$$\frac{\partial}{\partial x} \; G(x,x') \; \Bigg|_{x'-\epsilon}^{x'+\epsilon} \; = \; 1 \tag{1234}$$

Thus,

$$k \; B \; \cos k \; (\; x' \; - \; l \;) \; - k \; A \; \cos k \; x' \; = \; 0 \tag{1235}$$

Continuity of the Green's function at $x \; = \; x'$ yields

$$G(x'+\epsilon,x') \; = \; G(x'-\epsilon,x') \tag{1236}$$

or

$$B \; \sin k \; (\; x' \; - \; l \;) \; = \; A \; \sin k \; x' \tag{1237}$$

This, leads to the determination of A and B as

$$\begin{aligned} A \;\; &= \;\; \frac{\sin k \; (\; x' \; - \; l \;)}{k \; \sin k \; l} \\ B \;\; &= \;\; \frac{\sin k \; x'}{k \; \sin k \; l} \end{aligned} \tag{1238}$$

Hence, the Green's function is given by

$$G(x,x') \; = \; \frac{\sin k \; x_< \; \sin k \; (\; x_> \; - \; l \;)}{k \; \sin k \; l} \tag{1239}$$

which is symmetric in x and x'. The solution of the forced equation is given by

$$\begin{aligned} u(x) \; &= \; \int_0^l dx' \; G(x,x') \; f(x') \\ &= \; \frac{\sin k \; (\; x \; - \; l \;)}{k \; \sin k \; l} \; \int_0^x dx' \; \sin k \; x' \; f(x') \\ &+ \; \frac{\sin k \; x}{k \; \sin k \; l} \; \int_x^l dx' \; \sin k \; (\; x' \; - \; l \;) \; f(x') \end{aligned} \tag{1240}$$

12.2 Inhomogeneous Partial Differential Equations

The Greens' function method can also be used for inhomogeneous partial differential equations. Examples of inhomogeneous partial differential equations which often occur in physics are given by

$$\begin{aligned} \nabla^2 \; \phi(\underline{r}) \; &= \; - \; 4 \; \pi \; \rho(\underline{r}) \\ \nabla^2 \; \phi(\underline{r},t) \; - \; \frac{1}{c^2} \; \frac{\partial^2 \phi(\underline{r},t)}{\partial t^2} \; &= \; - \; 4 \; \pi \; \rho(\underline{r},t) \\ \nabla^2 \; \phi(\underline{r},t) \; - \; \frac{1}{\kappa} \; \frac{\partial \phi(\underline{r},t)}{\partial t} \; &= \; - \; 4 \; \pi \; \rho(\underline{r},t) \end{aligned} \tag{1241}$$

subject to appropriate boundary conditions. These three equations can be solved, for arbitrary source terms ρ, from knowledge of the respective Green's functions which satisfy the differential equations

$$\begin{aligned} \nabla^2 \; G(\underline{r},\underline{r}') \; &= \; \delta^3(\underline{r}-\underline{r}') \\ \nabla^2 \; G(\underline{r},t;\underline{r}',t') \; - \; \frac{1}{c^2} \; \frac{\partial^2 G(\underline{r},t;\underline{r}',t')}{\partial t^2} \; &= \; \delta^3(\underline{r}-\underline{r}') \; \delta(t-t') \\ \nabla^2 \; G(\underline{r},t;\underline{r}',t') \; - \; \frac{1}{\kappa} \; \frac{\partial G(\underline{r},t;\underline{r}',t')}{\partial t} \; &= \; \delta^3(\underline{r}-\underline{r}') \; \delta(t-t') \end{aligned} \tag{1242}$$

with the same boundary conditions. In these equations we have introduced a three dimensional delta function. These are defined via

$$\int d^3\underline{r} \; \delta^3(\underline{r}-\underline{r}') \; f(\underline{r}) \; = \; f(\underline{r}') \tag{1243}$$

The three dimensional delta function includes the weighting function appropriate for the coordinate systems. In Cartesian coordinates one has

$$\delta^3 (\underline{r} - \underline{r}') \; = \; \delta (x - x') \; \delta (y - y') \; \delta (z - z') \tag{1244}$$

while in spherical polar coordinates

$$\delta^3 (\underline{r} - \underline{r}') \; = \; \frac{\delta (r - r')}{r^2} \; \frac{\delta (\theta - \theta')}{\sin \theta} \; \delta (\varphi - \varphi') \tag{1245}$$

It can be seen that on integrating the delta function over all three dimensional, the denominator cancels with the weight factors giving a result of unity. On finding the time dependent Green's function one obtains the solution of the inhomogeneous equation as

$$\phi (\underline{r} , t) \; = \; - \, 4 \, \pi \, \int_{-\infty}^{\infty} \, dt' \, \int \, d^3 \underline{r}' \; G (\underline{r} , t ; \underline{r}' , t') \; \rho (\underline{r}' , t') \tag{1246}$$

which is valid for any arbitrary source, $\rho (\underline{r} , t)$.

12.2.1 The Symmetry of the Green's Function.

The Green's function is symmetric in its arguments $(\underline{r} , \underline{r}')$, such that

$$G (\underline{r} , t ; \underline{r}' , t') \; = \; G (\underline{r}' , t' ; \underline{r} , t) \tag{1247}$$

This can be proved by examining the Stürm-Liouville Green's function equation with a source at $(\underline{r}' , t')$

$$\begin{aligned} \underline{\nabla} \, . \, \left[\, p (\underline{r} , t) \; \underline{\nabla} \; G (\underline{r} , t ; \underline{r}' , t') \, \right] \; + \; \lambda \; q (\underline{r} , t) \; G (\underline{r} , t ; \underline{r}' , t') & \\ - \; \frac{1}{c^2} \; \frac{\partial^2 G (\underline{r} , t ; \underline{r}' , t')}{\partial t^2} & \; = \; \delta^3 (\underline{r} - \underline{r}') \; \delta (t - t') \end{aligned} \tag{1248}$$

and the similar equation with a source at $(\underline{r}" , t")$. Multiplying the equation for $G (\underline{r} , t ; \underline{r}' , t')$ by $G (\underline{r} , t ; \underline{r}" , t")$ and subtracting it from $G (\underline{r} , t ; \underline{r}' , t')$ times the equation for $G (\underline{r} , t ; \underline{r}" , t")$, one obtains

$$\begin{aligned} G (\underline{r} , t ; \underline{r}" , t") \; \underline{\nabla} \, . \, \left[\, p (\underline{r} , t) \; \underline{\nabla} \; G (\underline{r} , t ; \underline{r}' , t') \, \right] \; - \; G (\underline{r} , t ; \underline{r}' , t') \; \underline{\nabla} \, . \, \left[\, p (\underline{r} , t) \; \underline{\nabla} \; G (\underline{r} , t ; \underline{r}" , t") \, \right] & \\ - \; \frac{1}{c^2} \; G (\underline{r} , t ; \underline{r}" , t") \; \frac{\partial^2 G (\underline{r} , t ; \underline{r}' , t')}{\partial t^2} \; + \; \frac{1}{c^2} \; G (\underline{r} , t ; \underline{r}' , t') \; \frac{\partial^2 G (\underline{r} , t ; \underline{r}" , t")}{\partial t^2} & \\ = \; G (\underline{r} , t ; \underline{r}" , t") \; \delta^3 (\underline{r} - \underline{r}') \; \delta (t - t') \; - \; G (\underline{r} , t ; \underline{r}' , t') \; \delta^3 (\underline{r} - \underline{r}") \; \delta (t - t") & \end{aligned} \tag{1249}$$

On integrating over $\underline{r}$ and t, one obtains

$$\begin{aligned}
& \int_{-\infty}^{\infty} dt \int d^2\underline{S} \; G(\underline{r}, t; \underline{r}", t") \; . \; \left[\; p(\underline{r}, t) \; \underline{\nabla} \; G(\underline{r}, t; \underline{r}', t') \; \right] \\
- & \int_{-\infty}^{\infty} dt \int d^2\underline{S} \; G(\underline{r}, t; \underline{r}', t') \; . \; \left[\; p(\underline{r}, t) \; \underline{\nabla} \; G(\underline{r}, t; \underline{r}", t") \; \right] \\
- & \frac{1}{c^2} \int d^3\underline{r} \; G(\underline{r}, t; \underline{r}", t") \; \frac{\partial G(\underline{r}, t; \underline{r}', t')}{\partial t} \Bigg|_{t=-\infty}^{t=\infty} \\
+ & \frac{1}{c^2} \int d^3\underline{r} \; G(\underline{r}, t; \underline{r}', t') \; \frac{\partial G(\underline{r}, t; \underline{r}", t")}{\partial t} \Bigg|_{t=-\infty}^{t=\infty} \\
= & \; G(\underline{r}', t'; \underline{r}", t") \; - \; G(\underline{r}", t"; \underline{r}', t')
\end{aligned} \tag{1250}$$

On imposing appropriate boundary conditions, the surfaces terms in space time vanish and one finds that the Green's function is symmetric in its variables

$$G(\underline{r}', t'; \underline{r}", t") \; = \; G(\underline{r}", t"; \underline{r}', t') \tag{1251}$$

We shall now illustrate the solution of the equation for the Green's function of Poisson's equation and the Wave Equation, in several different geometries.

Poisson's Equation

Example:

The Green's function for Poisson's equation inside a sphere is given by the solution of

$$\nabla^2 \; G(\underline{r}, \underline{r}') \; = \; \delta^3(\underline{r} - \underline{r}') \tag{1252}$$

In spherical coordinates the delta function can be written as

$$\begin{aligned}
\delta^3(\underline{r} - \underline{r}') \quad & = \quad \frac{\delta(r - r')}{r^2} \; \frac{\delta(\theta - \theta')}{\sin\theta} \; \delta(\varphi - \varphi') \\
& = \quad \frac{\delta(r - r')}{r^2} \; \sum_{l=0}^{\infty} \; \sum_{m=-l}^{m=l} \; Y^{*m}_{l}(\theta', \varphi') \; Y^{m}_{l}(\theta, \varphi)
\end{aligned} \tag{1253}$$

where we have used the completeness condition for the spherical harmonics. The Green's function can also be expanded in powers of the spherical harmonics

$$G(\underline{r}, \underline{r}') \; = \; \sum_{l=0}^{\infty} \; \sum_{m=-l}^{m=l} \; G_{l,m}(r, \underline{r}') \; Y^{*m}_{l}(\theta, \varphi) \tag{1254}$$

On substituting the expansion for the Green's function into the differential equation one obtains

$$\sum_{l,m} \left(\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} G_{l,m} \right) - \frac{l \, (\, l \, + \, 1 \,)}{r^2} G_{l,m} \right) Y_l^m(\theta, \varphi)$$
$$= \frac{\delta(r - r')}{r^2} \sum_{l,m} Y^{*m}_{\ l}(\theta, \varphi) \, Y_l^m(\theta, \varphi) \tag{1255}$$

On multiplying by the spherical harmonics, and integrating over the solid angle, the orthogonality of the spherical harmonics yields

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} G_{l,m} \right) - \frac{l \, (\, l \, + \, 1 \,)}{r^2} G_{l.m} = \frac{\delta(r - r')}{r^2} Y^{*m}_{\ l}(\theta', \varphi') \tag{1256}$$

Since the left hand side has no explicit dependence on the angle (θ', φ'), one can separate out the angular dependence

$$G_{l,m}(r, \underline{r}') = g_l(r, r') \, Y^{*m}_{\ l}(\theta', \varphi') \tag{1257}$$

and find

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} g_{l,m} \right) - \frac{l \, (\, l \, + \, 1 \,)}{r^2} g_{l.m} = \frac{\delta(r - r')}{r^2} \tag{1258}$$

This is the equation for a one dimensional Green's function. For $r \neq r'$, the inhomogeneous term vanishes so one has solutions of the form

$$g_l(r, r') = \begin{cases} A \, r^l \, + \, B \, \frac{1}{r^{(l+1)}} & r \, < \, r' \\ C \, r^l + \, D \, \frac{1}{r^{(l+1)}} & r \, > \, r' \end{cases} \tag{1259}$$

The boundary conditions that $G(\underline{r}, \underline{r}')$ is finite at $r = 0$ and vanishes at $r = a$ implies that

$$\begin{aligned} B &= 0 \\ C \, a^l \, + \, D \, \frac{1}{a^{l+1}} &= 0 \end{aligned} \tag{1260}$$

Thus, the purely radial part of the Green's function is given by

$$g_l(r, r') = \begin{matrix} A \, r^l & r \, < \, r' \\ C \left(r^l - \frac{a^{2l+1}}{r^{(l+1)}} \right) & r \, > \, r' \end{matrix} \tag{1261}$$

The two remaining coefficients A and C are determined by continuity at $r = r'$ and by the discontinuity in the slope. That is

$$g_l(r' + \epsilon, r') = g_l(r' - \epsilon, r') \tag{1262}$$

and by integrating the differential equation over the singularity one obtains

$$\frac{\partial}{\partial r} \left[g_l(r, r') \right] \Bigg|_{r'-\epsilon}^{r'+\epsilon} = \frac{1}{r'^2} \tag{1263}$$

From these we, obtain the matching conditions

$$\begin{aligned} C \left[r'^l - \frac{a^{2l+1}}{r'^{l+1}} \right] - A \, r'^l &= 0 \\ C \left[l \; r'^{l-1} + (\, l + 1 \,) \, \frac{a^{2l+1}}{r'^{l+2}} \right] - A \, l \, r'^{l-1} &= \frac{1}{r'^2} \end{aligned} \tag{1264}$$

These two equations can be solved for A and C, yielding

$$\begin{aligned} C &= \frac{r'^l}{(2l+1) \; a^{2l+1}} \\ A &= \frac{r'^l}{(2l+1) \; a^{2l+1}} \left[1 - \left(\frac{a}{r'} \right)^{2l+1} \right] \end{aligned} \tag{1265}$$

Hence, the radial part of the Green's function is

$$g_l(r, r') = \frac{r^l \; r'^l}{(2l+1) \; a^{2l+1}} \left\{ \begin{array}{ll} \left[1 - \left(\frac{a}{r'} \right)^{2l+1} \right] & r < r' \\ \left[1 - \left(\frac{a}{r} \right)^{2l+1} \right] & r > r' \end{array} \right\} \tag{1266}$$

In terms of this function, one can write the Green's function as

$$\begin{aligned} G(\underline{r}, \underline{r}') &= \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} g_l(r, r') \; Y^{*m}_{\;l}(\theta', \varphi') \; Y_l^m(\theta, \varphi) \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \frac{(\, 2 \, l \, + \, 1 \,)}{4 \, \pi} \; g_l(r, r') \; P_l(\cos \gamma) \end{aligned} \tag{1267}$$

where we have used the spherical harmonic addition theorem and γ is the angle between $\underline{r}$ and $\underline{r}'$.

In the limit that the boundaries are removed to infinity, $a \rightarrow \infty$, the Green's function simplifies to

$$\begin{aligned} g_l(r, r') & = - \frac{r^l \, r'^l}{(2l+1)} \left\{ \begin{array}{ll} \left(\frac{1}{r'} \right)^{2l+1} & r \, < \, r' \\ \left(\frac{1}{r} \right)^{2l+1} & r \, > \, r' \end{array} \right\} \\ & = - \frac{1}{(2l+1) \, r_>} \left(\frac{r_<}{r_<} \right)^l \end{aligned} \tag{1268}$$

Thus, the Green's function in infinite three-dimensional space is given by the familiar result

$$\begin{aligned} G(\underline{r}, \underline{r}') & = - \frac{1}{4 \, \pi \, r_>} \sum_{l=0}^{\infty} \left(\frac{r_<}{r_<} \right)^l P_l(\cos\gamma) \\ & = - \frac{1}{4 \, \pi \, \sqrt{r^2 \, - \, 2 \, r \, r' \, \cos\gamma \, + \, r'^2}} \\ & = - \frac{1}{4 \, \pi \, | \, \underline{r} \, - \, \underline{r}' \, |} \end{aligned} \tag{1269}$$

which is the Green's function for Laplace's equation.

Example:

The solution of Poisson's equation in two dimensions, for the potential $\phi(r)$ confined by a conducting ring of radius a can be obtained from the Green's function. The Green's function satisfies the partial differential equation

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \, \frac{\partial G(\underline{r}, \underline{r}')}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 G(\underline{r}, \underline{r}')}{\partial \theta^2} = \frac{\delta(\, r \, - \, r' \,)}{r} \, \delta(\, \theta \, - \, \theta' \,) \tag{1270}$$

On using the completeness relation

$$\delta(\, \theta \, - \, \theta' \,) = \frac{1}{2 \, \pi} \sum_{m=-\infty}^{\infty} \exp \left[\, i \, m \, (\, \theta \, - \, \theta' \,) \, \right] \tag{1271}$$

and the series expansion

$$G(\underline{r}, \underline{r}') = \sum_{m=-\infty}^{\infty} G_m(r, \underline{r}') \, \frac{1}{\sqrt{2 \, \pi}} \, \exp \left[\, i \, m \, \theta \, \right] \tag{1272}$$

one finds that the coefficient G_m must satisfy the ordinary differential equation

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial G_m(r, \underline{r}')}{\partial r} \right) - \frac{m^2}{r^2} G_m(r, \underline{r}') = \frac{\delta(r - r')}{r} \frac{1}{\sqrt{2 \pi}} \exp \left[- i \, m \, \theta' \right] \tag{1273}$$

Introducing the definition

$$G_m(r, \underline{r}') = g_m(r, r') \frac{1}{\sqrt{2 \pi}} \exp \left[- i \, m \, \theta' \right] \tag{1274}$$

which isolates the angular dependence of $G_m(r, \underline{r}')$, one finds that $g_m(r, r')$ satisfies the ordinary differential equation

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial g_m(r, r')}{\partial r} \right) - \frac{m^2}{r^2} g_m(r, r') = \frac{\delta(r - r')}{r} \tag{1275}$$

For $m = 0$ and $r \neq r'$ the differential equation has the general solution

$$g_0(r, r') = A_0 + B_0 \ln r \tag{1276}$$

while for $m \neq 0$ and $r \neq r'$ the equation has the general solution

$$g_m(r, r') = A_m \, r^m + B_m \, r^{-m} \tag{1277}$$

The boundary conditions at $r = 0$ leads to the vanishing of the coefficients of r^{-m}. Hence, the solution close to the origin must be of the form

$$g_m(r < r') = A_m \, r^m \tag{1278}$$

The boundary condition at $r = a$ leads to a relation between the coefficients of r^m and r^{-m}. The solution close to the edge of the ring has the form

$$g_m(r > r') = C_m \left[\left(\frac{r}{a} \right)^m - \left(\frac{a}{r} \right)^m \right] \tag{1279}$$

for $m \neq 0$. The solution for the Green's function for $m = 0$ is given by

$$g_0(r < r') = A_0 \tag{1280}$$

close to the origin and

$$g_0(r > r') = C_0 \ln \frac{r}{a} \tag{1281}$$

close to the ring. The boundary conditions at $r = r'$ are

$$\begin{aligned} g_m(r' + \epsilon, r') &= g_m(r' - \epsilon, r') \\ \frac{\partial g_m(r, r')}{\partial r} \bigg|_{r'-\epsilon}^{r'+\epsilon} &= \frac{1}{r'} \end{aligned} \tag{1282}$$

The boundary conditions at the intersection of the two intervals determine the remaining two coefficients via

$$A_m \, r'^m \;=\; C_m \left[\left(\frac{r'}{a} \right)^m - \left(\frac{a}{r'} \right)^m \right] \tag{1283}$$

and

$$m \, C_m \left[\left(\frac{r'}{a} \right)^m + \left(\frac{a}{r'} \right)^m \right] - m \, A_m \, r'^m \;=\; 1 \tag{1284}$$

These two equations can be solved resulting in

$$C_m \;=\; \frac{1}{2\,m} \left(\frac{r'}{a} \right)^m \tag{1285}$$

and

$$A_m \;=\; \frac{a^{-m}}{2\,m} \left[\left(\frac{r'}{a} \right)^m - \left(\frac{a}{r'} \right)^m \right] \tag{1286}$$

Hence, the solution is given by

$$\begin{aligned} g_m(r < r') &= \frac{1}{2\,m} \left(\frac{r}{a} \right)^m \left[\left(\frac{r'}{a} \right)^m - \left(\frac{a}{r'} \right)^m \right] \\ g_m(r > r') &= \frac{1}{2\,m} \left(\frac{r'}{a} \right)^m \left[\left(\frac{r}{a} \right)^m - \left(\frac{a}{r} \right)^m \right] \end{aligned} \tag{1287}$$

and

$$\begin{aligned} g_0(r < r') &= \ln \frac{r'}{a} \\ g_0(r > r') &= \ln \frac{r}{a} \end{aligned} \tag{1288}$$

The Green's function is given by

$$\begin{aligned} G(\underline{r}, \underline{r}') &= \frac{1}{2\,\pi} \sum_{m=-\infty}^{\infty} g_m(r, r') \, \exp \left[\, i \, m \, (\, \theta \, - \, \theta' \,) \, \right] \\ &= \frac{1}{2\,\pi} \left[\, g_0(r, r') \; + 2 \sum_{m=1}^{\infty} g_m(r, r') \, \cos \, m \, (\, \theta \, - \, \theta' \,) \, \right] \end{aligned} \tag{1289}$$

In the limit that the boundaries are removed to infinity $a \rightarrow \infty$ one has

$$g_m(r,r') = - \frac{1}{2\,m} \left(\frac{r_<}{r_>} \right)^m \tag{1290}$$

so

$$\begin{aligned} G(\underline{r},\underline{r}') &= \frac{1}{2\,\pi} \left[\ln \frac{r_>}{a} - \sum_{m=1}^{\infty} \frac{1}{m} \left(\frac{r_<}{r_>} \right)^m \cos\, m\,(\,\theta - \theta'\,) \right] \\ &= \frac{1}{4\,\pi} \ln \left[\frac{r^2 + r'^2 - 2\,r\,r' \cos\,(\,\theta - \theta'\,)}{a^2} \right] \\ &= \frac{1}{2\,\pi} \ln \frac{|\,\underline{r} - \underline{r}'\,|}{a} \end{aligned} \tag{1291}$$

which is the Green's function for the Laplacian operator in an infinite two dimensional space.

The Wave Equation.

Example:

Consider the forced drum head, described by the inhomogeneous partial differential equation

$$\left(\nabla^2 \phi - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} \right) = - \frac{1}{c^2\,\sigma} f(\underline{r},t) \tag{1292}$$

where f is the force per unit area normal to the drumhead and σ is the mass density. The boundary condition on the displacements is $\phi(\underline{r},t) = 0$. We shall assume that the driving force has a temporal Fourier decomposition

$$f(\underline{r},t) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\,\pi}} f(\underline{r},\omega) \exp\left[- i\,\omega\,t \right] \tag{1293}$$

Due to the linear nature of the equation one can find the solution $\phi(\underline{r},t)$ from the temporal Fourier transform $\phi(\underline{r},\omega)$ defined via

$$\phi(\underline{r},t) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\,\pi}} \phi(\underline{r},\omega) \exp\left[- i\,\omega\,t \right] \tag{1294}$$

On Fourier transforming the differential equation with respect to t one has

$$\begin{aligned} &\int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\,\pi}} \left(\nabla^2 \phi - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} \right) \exp\left[+ i\,\omega\,t \right] \\ &= - \frac{1}{c^2\,\sigma} \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\,\pi}} f(\underline{r},t) \exp\left[+ i\,\omega\,t \right] \end{aligned} \tag{1295}$$

On integrating the second derivative with respect to time by parts, twice, and assuming that $\lim_{t \to \pm\infty} \ \phi(\underline{r}, t) \ = \ 0$, one obtains

$$\left(\nabla^2 \ \phi(\underline{r}, \omega) \ + \ \frac{\omega^2}{c^2} \ \phi(\underline{r}, \omega) \right) \ = \ - \ \frac{1}{c^2 \ \sigma} \ f(\underline{r}, \omega) \tag{1296}$$

To solve this equation we introduce the frequency dependent Green's function, $G(\underline{r}, \underline{r}'; \omega)$, which satisfies

$$\left(\nabla^2 \ G(\underline{r}, \underline{r}'; \omega) \ + \ \frac{\omega^2}{c^2} \ G(\underline{r}, \underline{r}'; \omega) \right) \ = \ \frac{1}{\sqrt{2 \ \pi}} \ \delta^2(\underline{r} - \underline{r}') \tag{1297}$$

which is the Fourier transform of the equation for the real time Green's function. Note that this holds only because the homogeneous equation is only a function of $t \ - \ t'$ and does not depend on t and t' independently. This is expected to be true for most physical phenomenon due to the homogeneity of space time. The Green's function satisfies the boundary condition $G(\underline{r}, \underline{r}; \omega) \ = \ 0$, at the edge of the drum head.

The solution for $\phi(\underline{r}; \omega)$ is found in terms of the Green's function. From the partial differential equations one has

$$\begin{aligned} \int d^2\underline{r} \ \left(\phi(\underline{r}, \omega) \ \nabla^2 \ G(\underline{r}, \underline{r}'; \omega) \ - \ G(\underline{r}, \underline{r}'; \omega) \ \nabla^2 \ \phi(\underline{r}, \omega) \right) \\ = \ \frac{\phi(\underline{r}', \omega)}{\sqrt{2 \ \pi}} \ + \ \frac{1}{c^2 \ \sigma} \ \int \ d^2\underline{r} \ G(\underline{r}, \underline{r}'; \omega) \ f(\underline{r}, \omega) \end{aligned} \tag{1298}$$

Also, using the two dimensional version of Green's theorem, this is equal to

$$= \ \int \ dl \ \left(\phi(\underline{r}, \omega) \ \frac{\partial G(\underline{r}, \underline{r}'; \omega)}{\partial n} \ - \ G(\underline{r}, \underline{r}'; \omega) \ \frac{\partial \phi(\underline{r}; \omega)}{\partial n} \right) \tag{1299}$$

where the integral is over the perimeter of the two dimensional area and the derivative with respect to n ia taken along the normal to the perimeter. For a circular area of radius a, one has $dl \ = \ a \ d\theta$ and $\frac{\partial}{\partial n} \ = \ \frac{\partial}{\partial r}$. Since both terms vanish on the perimeter of the drumhead, $\phi(\underline{r}, \omega) \ = \ 0$ and $G(\underline{r}, \underline{r}'; \omega) \ = \ 0$, one has

$$\frac{\phi(\underline{r}', \omega)}{\sqrt{2 \ \pi}} \ = \ - \ \frac{1}{c^2 \ \sigma} \ \int \ d^2\underline{r} \ G(\underline{r}, \underline{r}'; \omega) \ f(\underline{r}, \omega) \tag{1300}$$

or using the symmetry of the Green's function

$$\frac{\phi(\underline{r}', \omega)}{\sqrt{2 \ \pi}} \ = \ - \ \frac{1}{c^2 \ \sigma} \ \int \ d^2\underline{r} \ G(\underline{r}', \underline{r}; \omega) \ f(\underline{r}, \omega) \tag{1301}$$

Thus, the solution of the forced equation can be obtained from the Green's function and the forcing function. In particular one has

$$\begin{aligned} \phi(\underline{r}, t) &= \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\,\pi}} \, \phi(\underline{r}, \omega) \, \exp \left[\, - \, i \, \omega \, t \, \right] \\ &= - \, \frac{1}{c^2 \, \sigma} \int_{-\infty}^{\infty} d\omega \int d^2\underline{r}' \, G(\underline{r}, \underline{r}'; \omega) \, f(\underline{r}', \omega) \, \exp \left[\, - \, i \, \omega \, t \, \right] \end{aligned} \tag{1302}$$

The Green's function can be obtained by expanding it in terms of a Fourier series in θ,

$$G(\underline{r}, \underline{r}'; \omega) = \sum_{m=-\infty}^{\infty} G_m(r, \underline{r}'; \omega) \, \frac{1}{\sqrt{2\,\pi}} \, \exp \left[\, i \, m \, \theta \, \right] \tag{1303}$$

The two dimensional Green's function can be expressed as

$$\begin{aligned} \delta^2(\underline{r} - \underline{r}') &= \frac{\delta(r - r')}{r} \, \delta(\theta - \theta') \\ &= \frac{\delta(r - r')}{r} \, \frac{1}{2\,\pi} \sum_{m=-\infty}^{\infty} \exp \left[\, i \, m \, (\, \theta \, - \, \theta' \,) \, \right] \end{aligned} \tag{1304}$$

where we have used the completeness relation for the Fourier series to expand the delta function of the angle.

On substituting these into the equation for the Green's function, multiplying by the complex conjugate basis function

$$\frac{1}{\sqrt{2\,\pi}} \, \exp \left[\, - \, i \, m \, \theta \, \right] \tag{1305}$$

and integrating over θ, one obtains

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \, \frac{\partial G_m(r, \underline{r}')}{\partial r} \right) + \left(\frac{\omega^2}{c^2} \, - \, \frac{m^2}{r^2} \right) G_m(r, \underline{r}') = \frac{1}{2\,\pi} \, \exp \left[\, - \, i \, m \, \theta' \, \right] \, \frac{\delta(r - r')}{r} \tag{1306}$$

On factoring out the θ' dependence via

$$G_m(r, \underline{r}') = g_m(r, r') \, \frac{1}{\sqrt{2\,\pi}} \, \exp \left[\, - \, i \, m \, \theta' \, \right] \tag{1307}$$

one finds that $g_m(r,r')$ satisfies the equation

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\,\frac{\partial g_m(r,r')}{\partial r}\right) + \left(\frac{\omega^2}{c^2} - \frac{m^2}{r^2}\right) g_m(r,r') = \frac{1}{\sqrt{2\pi}}\,\frac{\delta(r-r')}{r} \tag{1308}$$

The inhomogeneous term is zero for both regions $r > r'$ and $r' > r$, so that the solution is

$$\begin{aligned} g_m(r,r') &= A\,J_m(\frac{\omega}{c}\,r) \qquad r < r' \\ g_m(r,r') &= F\,J_m(\frac{\omega}{c}\,r) + G\,N_m(\frac{\omega}{c}\,r) \qquad r > r' \end{aligned} \tag{1309}$$

since the Green's function must be regular at $r = 0$. The boundary condition at $r = a$ is

$$g_m(a,r') = 0 \tag{1310}$$

Hence, we have

$$\begin{aligned} g_m(r,r') &= A\,J_m(\frac{\omega}{c}\,r) \qquad r < r' \\ g_m(r,r') &= B\left(N_m(\frac{\omega}{c}\,a)\,J_m(\frac{\omega}{c}\,r) - J_m(\frac{\omega}{c}\,a)\,N_m(\frac{\omega}{c}\,r)\right) \qquad r > r' \end{aligned} \tag{1311}$$

The matching conditions at $r = r'$ are given by

$$\begin{aligned} g_m(r'+\epsilon,r') &= g_m(r'-\epsilon,r') \\ \frac{\partial g_m(r,r')}{\partial r}\Bigg|_{r'-\epsilon}^{r'+\epsilon} &= \frac{1}{\sqrt{2\pi}}\,\frac{1}{r'} \end{aligned} \tag{1312}$$

Hence, the coefficients A and B satisfy the linear equations

$$\begin{aligned} A\,J_m(\frac{\omega}{c}\,r') &= B\left(N_m(\frac{\omega}{c}\,a)\,J_m(\frac{\omega}{c}\,r') - J_m(\frac{\omega}{c}\,a)\,N_m(\frac{\omega}{c}\,r')\right) \\ \frac{1}{\sqrt{2\pi}}\,\frac{1}{r'} &= \frac{\omega}{c}\left[B\left(N_m(\frac{\omega}{c}\,a)\,J'_m(\frac{\omega}{c}\,r') - J_m(\frac{\omega}{c}\,a)\,N'_m(\frac{\omega}{c}\,r')\right) - A\,J'_m(\frac{\omega}{c}\,r')\right] \end{aligned} \tag{1313}$$

The solution of these equations can be simplified by noting that the Wronskian of the solutions of the Bessel functions is given by

$$J_m(z)\,N'_m(z) - J'_m(z)\,N_m(z) = \frac{2}{\pi\,z} \tag{1314}$$

The solution can be written as

$$A = - \frac{1}{\sqrt{2\,\pi}} \frac{\pi}{2} \frac{\left(N_m(\frac{\omega}{c}\, a)\, J_m(\frac{\omega}{c}\, r') \; - \; J_m(\frac{\omega}{c}\, a)\, N_m(\frac{\omega}{c}\, r') \right)}{J_m(\frac{\omega}{c}\, a)}$$

$$B = - \frac{1}{\sqrt{2\,\pi}} \frac{\pi}{2} \frac{J_m(\frac{\omega}{c}\, r')}{J_m(\frac{\omega}{c}\, a)} \tag{1315}$$

The radial Green's function can be written as

$$g_m(r,r') = - \frac{1}{\sqrt{2\,\pi}} \frac{\pi}{2} \frac{J_m(\frac{\omega}{c}\, r)}{J_m(\frac{\omega}{c}\, a)} \left(N_m(\frac{\omega}{c}\, a)\, J_m(\frac{\omega}{c}\, r') \; - \; J_m(\frac{\omega}{c}\, a)\, N_m(\frac{\omega}{c}\, r') \right) \qquad r' > r$$

$$g_m(r,r') = - \frac{1}{\sqrt{2\,\pi}} \frac{\pi}{2} \frac{J_m(\frac{\omega}{c}\, r')}{J_m(\frac{\omega}{c}\, a)} \left(N_m(\frac{\omega}{c}\, a)\, J_m(\frac{\omega}{c}\, r) \; - \; J_m(\frac{\omega}{c}\, a)\, N_m(\frac{\omega}{c}\, r) \right) \qquad r' < r \tag{1316}$$

which is symmetric under the interchange $m \rightleftharpoons - m$. Then, the frequency dependent Green's function can be written as

$$\begin{aligned} G(\underline{r},\underline{r}';\omega) &= \sum_{m=-\infty}^{\infty} g_m(r,r')\, \frac{1}{2\,\pi}\, \exp\left[\, i\, m\, (\, \theta \, - \, \theta'\,)\, \right] \\ &= \frac{1}{2\,\pi} \left(g_0(r,r') \; + \; 2 \sum_{m=1}^{\infty} g_m(r,r')\, \cos m\, (\, \theta \, - \, \theta'\,) \right) \end{aligned} \tag{1317}$$

The time dependent Green's function is given by

$$G(\underline{r},\underline{r}';t-t') = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\,\pi}}\, G(\underline{r},\underline{r}';\omega)\, \exp\left[\, - \, i\, \omega\, (\, t \, - \, t'\,)\, \right] \tag{1318}$$

12.2.2 Eigenfunction Expansion

The Green's function can also be obtained by expanding the Green's function in terms of eigenfunctions of an appropriate operator and using the completeness relation for the delta function. The expansion coefficients can then be determined directly, using the orthogonality relation.

Poisson's Equation.

We shall consider examples of the eigenfunction expansion solution for the Green's functions for Poisson's equation, in various geometries.

Example:

The Green's function for Poisson's equation in an infinite three dimensional space can be obtained by an eigenfunction expansion method. The Green's function satisfies the equation

$$\nabla^2 \; G(\underline{r}, \underline{r}') \; = \; \delta^3(\underline{r} - \underline{r}') \tag{1319}$$

The eigenfunction of the Laplacian satisfy

$$\nabla^2 \; \phi_{\underline{k}}(\underline{r}) \; = \; \lambda_{\underline{k}} \; \phi_{\underline{k}}(\underline{r}) \tag{1320}$$

and has eigenfunctions

$$\phi_{\underline{k}}(\underline{r}) \; = \; \frac{1}{(\, 2 \, \pi \,)^{\frac{3}{2}}} \; \exp \left[\; i \; \underline{k} \; . \; \underline{r} \; \right] \tag{1321}$$

and have eigenvalues

$$\lambda_{\underline{k}} \; = \; - \; k^2 \tag{1322}$$

The Green's function can be expanded as

$$G(\underline{r}, \underline{r}') \; = \; \int \; d^3\underline{k} \; G_{\underline{k}}(\underline{r}') \; \phi_{\underline{k}}(\underline{r}) \tag{1323}$$

and the delta function can be expanded using the completeness relation for the eigenfunctions

$$\delta^3(\underline{r} - \underline{r}') \; = \; \int \; d^3\underline{k} \; \phi^*_{\underline{k}}(\underline{r}') \; \phi_{\underline{k}}(\underline{r}) \tag{1324}$$

Inserting both of these expansions in the equation for the Green's function we find the expansion coefficients of the Green's function satisfy the equation

$$- \int \; d^3\underline{k} \; k^2 \; G_{\underline{k}}(\underline{r}') \; \phi_{\underline{k}}(\underline{r}) \; = \; \int \; d^3\underline{k} \; \phi^*_{\underline{k}}(\underline{r}') \; \phi_{\underline{k}}(\underline{r}) \tag{1325}$$

Multiplying by $\phi^*_{\underline{k}'}(\underline{r})$ and integrating over $\underline{r}$ one has the orthogonality relation

$$\int \; d^3\underline{r} \; \phi^*_{\underline{k}'}(\underline{r}) \; \phi_{\underline{k}}(\underline{r}) \; = \; \delta^3(\underline{k} - \underline{k}') \tag{1326}$$

one projects out the coefficient $G_{\underline{k}'}(\underline{r})$ so

$$- \; k'^2 \; G_{\underline{k}'}(\underline{r}) \; = \; \phi^*_{\underline{k}'}(\underline{r}') \tag{1327}$$

Hence, the Green's function is given by

$$\begin{aligned} G(\underline{r}, \underline{r}') &= - \int d^3\underline{k} \; \frac{\phi^*_{\underline{k}}(\underline{r}') \; \phi_{\underline{k}}(\underline{r})}{k^2} \\ &= - \int \frac{d^3\underline{k}}{(\, 2 \, \pi \,)^3} \; \frac{\exp \left[\, i \, \underline{k} \, . \, (\, \underline{r} \, - \, \underline{r}' \,) \, \right]}{k^2} \end{aligned} \tag{1328}$$

It is seen that the Green's function only depends on the difference of the positions, $\underline{r} - \underline{r}'$, and not on $\underline{r}$ and $\underline{r}'$ separately. This is because we have assumed that space is homogeneous. To simplify further calculations we shall re-center our coordinates on the source point at $\underline{r}'$. In this case, the Green's function only depends on $\underline{r}$.

In spherical polar coordinates, one has

$$\begin{aligned} G(\underline{r}) &= - \int \frac{d^3\underline{k}}{(\, 2 \, \pi \,)^3} \; \frac{\exp \left[\, i \, \underline{k} \, . \, \underline{r} \, \right]}{k^2} \\ &= - \int_0^{2\pi} d\varphi \int_0^{\pi} d \, \theta \, \sin\theta \int_0^{\infty} \frac{dk \; k^2}{(\, 2 \, \pi \,)^3} \; \frac{\exp \left[\, i \, k \, r \, \cos\theta \, \right]}{k^2} \end{aligned} \tag{1329}$$

where the polar axis has been chosen along the direction of $\underline{r}$. The integral over φ and $\cos\theta$ can be performed as

$$\begin{aligned} G(\underline{r}) &= - \int_0^{2\pi} d\varphi \int_{-1}^{1} d \, \cos\theta \int_0^{\infty} \frac{dk}{(\, 2 \, \pi \,)^3} \; \exp \left[\, i \, k \, r \, \cos\theta \, \right] \\ &= - \int_0^{\infty} \frac{dk}{(\, 2 \, \pi \,)^2} \; \frac{\exp \left[\, i \, k \, r \, \right] \; - \; \exp \left[\, - \, i \, k \, r \, \right]}{i \, k \, r} \end{aligned} \tag{1330}$$

On writing $k \; = \; - \, k$ in the second term, one can extend the integration to $(-\infty, \infty)$, yielding

$$G(\underline{r}) \; = \; - \int_{-\infty}^{\infty} \frac{dk}{(\, 2 \, \pi \,)^2} \; \frac{\exp \left[\, i \, k \, r \, \right]}{i \, k \, r} \tag{1331}$$

where the integral over the singularity at $k = 0$ is interpreted as being just the principal part. That is, the integral is evaluated over two regions $(-\infty, -\varepsilon)$ and (ε, ∞), which end symmetrically around the singularity at $k = 0$. The integral is evaluated by taking the limit $\varepsilon \rightarrow 0$. The integration can be evaluated by Cauchy's theorem to yield $\pi \, i$ times the residue. Hence, we obtain

$$G(\underline{r}) \quad = \quad - \, \frac{1}{(\, 4 \, \pi \, r \,)} \tag{1332}$$

or re-instating the source position at $\underline{r}'$

$$G(\underline{r}, \underline{r}') \quad = \quad - \, \frac{1}{4 \, \pi \, | \, \underline{r} \; - \; \underline{r}' \, |} \tag{1333}$$

as expected from Coulomb's law.

Example:

The Green's function for the Laplacian in an infinite d-dimensional space satisfies

$$\nabla^2 \, G(\underline{r}, \underline{r}') \; = \; \delta^d(\underline{r} - \underline{r}') \tag{1334}$$

where in ultra-spherical polar coordinates one has the delta function

$$\delta^d(\underline{r} - \underline{r}') \; = \; \frac{\delta(r - r')}{r^{d-1}} \, \frac{\delta(\theta_{d-1} - \theta'_{d-1})}{\sin^{d-2} \theta_{d-1}} \, \frac{\delta(\theta_{d-2} - \theta'_{d-2})}{\sin^{d-3} \theta_{d-2}} \, \ldots \, \frac{\delta(\theta_2 - \theta'_2)}{\sin \theta_2} \, \delta(\varphi - \varphi') \tag{1335}$$

One can solve for the Green's function using the eigenfunction expansion method. The Green's function is expanded as

$$G(\underline{r}, \underline{r}') \; = \; \int \frac{d^d \underline{k}}{(\, 2 \, \pi \,)^{\frac{d}{2}}} \; G_{\underline{k}}(\underline{r}') \; \exp \left[\, i \, \underline{k} \, . \, \underline{r} \, \right] \tag{1336}$$

The delta function can also be expanded using the completeness relation

$$\delta^d(\underline{r} - \underline{r}') \; = \; \int \frac{d^d \underline{k}}{(\, 2 \, \pi \,)^d} \; \exp \left[\, i \, \underline{k} \, . \, (\, \underline{r} \; - \; \underline{r}' \,) \, \right] \tag{1337}$$

These are substituted into the equations of motion, which then gives an equation involving all the Green's function expansion coefficients. The orthogonality relation of the eigenfunctions

$$\int \frac{d^d \underline{r}}{(\, 2 \, \pi \,)^d} \; \exp \left[\, i \, \underline{r} \, . \, (\, \underline{k} \; - \; \underline{k}' \,) \, \right] \; = \; \delta^d(\underline{k} - \underline{k}') \tag{1338}$$

can be used to obtain the expansion coefficients as

$$G_{\underline{k}'}(\underline{r}') = \frac{\exp\left[- i \, \underline{k}' \, . \, \underline{r}' \right]}{(\, 2 \, \pi \,)^{\frac{d}{2}}} \tag{1339}$$

Hence, we find that due to the isotropy and translational invariance of space the Green's function is only a function of the spatial separation $\underline{r} - \underline{r}'$ and does not depend on $\underline{r}$ and $\underline{r}'$ separately

$$G(\underline{r} - \underline{r}') = - \int \frac{d^d \underline{k}}{(\, 2 \, \pi \,)^d} \, \frac{\exp\left[\, i \, \underline{k} \, . \, (\, \underline{r} \, - \, \underline{r}' \,) \, \right]}{k^2} \tag{1340}$$

or

$$G(\underline{r}) = - \int \frac{d^d \underline{k}}{(\, 2 \, \pi \,)^d} \, \frac{\exp\left[\, i \, \underline{k} \, . \, \underline{r} \, \right]}{k^2} \tag{1341}$$

The integration will be evaluated in spherical polar coordinates, in which the polar axis is chosen along the direction of $\underline{r}$. The integration over the d-dimensional volume $d^d \underline{k}$ can be expressed in spherical polar coordinates as

$$d^d \underline{k} = dk \, k^{d-1} \, d\theta_{d-1} \, \sin^{d-2} \theta_{d-1} \, d\theta_{d-2} \, \sin^{d-3} \theta_{d-2} \, \ldots \, d\theta_2 \, \sin \theta_2 \, d\varphi \tag{1342}$$

Thus, we have

$$\begin{aligned} G(\underline{r}) = & - \int_0^\infty \frac{dk \, k^{d-1}}{(\, 2 \, \pi \,)^d} \int_0^\pi d\theta_{d-1} \, \sin^{d-2} \theta_{d-1} \, \frac{\exp\left[\, i \, k \, r \, \cos \theta_{d-1} \, \right]}{k^2} \\ & \times \int_0^\pi d\theta_{d-2} \, \sin^{d-3} \theta_{d-2} \, \ldots \int_0^\pi d\theta_2 \, \sin \theta_2 \int_0^{2\pi} d\varphi \end{aligned} \tag{1343}$$

The angular integrations which only involve the weight factors can be performed using the formula

$$\int_0^\pi d\theta \, \sin^m \theta = \sqrt{\pi} \, \frac{\Gamma(\frac{m+1}{2})}{\Gamma(\frac{m+2}{2})} \tag{1344}$$

where the Γ function is the generalized factorial function defined by

$$\Gamma(z) = \int_0^\infty dx \, \exp\left[\, - \, x \, \right] \, x^{z-1} \tag{1345}$$

One can show that, by integrating by parts with respect to x, the Γ function satisfies the same recursion relation as the factorial function

$$\Gamma(z) = (\, z \, - \, 1 \,) \, \Gamma(z-1) \tag{1346}$$

and as

$$\Gamma(1) \; = \; \int_0^\infty \; dx \; \exp \left[\; - \; x \; \right] \; = \; 1 \tag{1347}$$

Thus, for integer n the Γ function reduces to n factorial

$$\Gamma(n+1) \; = \; n! \tag{1348}$$

Hence, the Green's function is expressed as

$$\begin{aligned} G(\underline{r}) \; = \; - \int_0^\infty \frac{dk \; k^{d-3}}{(\; 2 \; \pi \;)^d} \; \int_0^\pi \; d\theta_{d-1} \; \sin^{d-2} \theta_{d-1} \; \exp \left[\; i \; k \; r \; \cos \theta_{d-1} \; \right] \\ \times \; \sqrt{\pi} \; \frac{\Gamma(\frac{d-2}{2})}{\Gamma(\frac{d-1}{2})} \ldots \; \sqrt{\pi} \; \frac{\Gamma(\frac{2}{2})}{\Gamma(\frac{3}{2})} \; 2 \; \pi \end{aligned} \tag{1349}$$

The integration over the angle θ_{d-1} can be performed using

$$\int_0^\pi \; d\theta_{d-1} \; \sin^{d-2} \theta_{d-1} \; \exp \left[\; i \, k \, r \; \cos \theta_{d-1} \; \right] \; = \; \sqrt{\pi} \, \Gamma(\frac{d-1}{2}) \left(\frac{2}{k \; r} \right)^{\frac{d-2}{2}} \; J_{\frac{d-2}{2}}(kr) \tag{1350}$$

Thus, we find

$$\begin{aligned} G(\underline{r}) \; &= \; - \int_0^\infty \frac{dk \; k^{d-3}}{(\; 2 \; \pi \;)^{\frac{d}{2}}} \left(\frac{1}{k \; r} \right)^{\frac{d-2}{2}} \; J_{\frac{d-2}{2}}(kr) \\ &= \; - \left(\; \frac{1}{r} \; \right)^{\frac{d-2}{2}} \int_0^\infty \; \frac{dk}{(\; 2 \; \pi \;)^{\frac{d}{2}}} \; k^{\frac{d-4}{2}} \; J_{\frac{d-2}{2}}(kr) \end{aligned} \tag{1351}$$

Finally, the integral over k can be evaluated with the aid of the formula

$$\int_0^\infty \; dk \; k^\mu \; J_\nu(kr) \; = \; \frac{2^\mu}{r^{\mu+1}} \; \frac{\Gamma(\frac{\mu+\nu+1}{2})}{\Gamma(\frac{\mu-\nu+1}{2})} \tag{1352}$$

which yields the Green's function for the d-dimensional Laplacian as

$$G(\underline{r}) \; = \; - \; \frac{\Gamma(\frac{d-2}{2})}{4 \; \pi^{\frac{d}{2}}} \left(\frac{1}{r^{d-2}} \right) \tag{1353}$$

The d-dimensional Green's function for the Laplacian operator reduces to the three dimensional case previously considered, as can be seen by putting $d \; = \; 3$ and noting that $\Gamma(\frac{1}{2}) \; = \; \sqrt{\pi}$.

The Wave Equation

The Green's function for the wave equation can be obtained by expansion in terms of eigenfunctions.

Example:

The Green's function for the wave equation, inside a two dimensional area, satisfies the inhomogeneous equation

$$\left(\nabla^2 \; - \; \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) G(\underline{r}, \underline{r}'; t - t') \; = \; \delta^2(\underline{r} - \underline{r}') \; \delta(t - t') \tag{1354}$$

which on Fourier transforming with respect to t according to

$$G(\underline{r}, \underline{r}'; \omega) \; = \; \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2 \pi}} \; G(\underline{r}, \underline{r}'; t - t') \; \exp \left[\; + \; i \; \omega \; (\; t \; - \; t' \;) \; \right] \tag{1355}$$

yields

$$\left(\; \nabla^2 \; + \; \frac{\omega^2}{c^2} \; \right) G(\underline{r}, \underline{r}'; \omega) \; = \; \frac{1}{\sqrt{2 \pi}} \; \delta^2(\underline{r} - \underline{r}') \tag{1356}$$

The eigenfunctions of the operator satisfy the eigenvalue equation

$$\left(\; \nabla^2 \; + \; \frac{\omega^2}{c^2} \; \right) \phi_{k,m}(\underline{r}) \; = \; \lambda_{k,m} \; \phi_{k,m}(\underline{r}) \tag{1357}$$

where k, m label the eigenfunctions. The explicit form of the eigenvalue equation is given by

$$\left(\; \frac{1}{r} \frac{\partial}{\partial r} \left(\; r \; \frac{\partial \phi_{k,m}}{\partial r} \; \right) \; + \; \frac{1}{r^2} \; \frac{\partial^2 \phi_{k,m}}{\partial \theta^2} \; + \; \frac{\omega^2}{c^2} \; \phi_{k,m} \; \right) \; = \; \lambda_{k,m} \; \phi_{k,m} \tag{1358}$$

The eigenfunctions that satisfy the boundary conditions at the origin and vanish on a circle of radius a are given by

$$\phi_{k,m}(r, \theta) \; = \; N_m \; J_m(kr) \; \frac{1}{\sqrt{2 \pi}} \; \exp \left[\; i \; m \; \theta \; \right] \tag{1359}$$

where the normalization N_m is given by

$$N_m \; = \; \left[\; \frac{a}{\sqrt{2}} \; J'_m(ka) \; \right]^{-1} \tag{1360}$$

and the number k is given by the zeroes of the Bessel function

$$J_m(ka) \; = \; 0 \tag{1361}$$

The eigenvalues are given by

$$\lambda_{k,m} \; = \; \frac{\omega^2}{c^2} \; - \; k^2 \tag{1362}$$

The frequency dependent Green's function is given by

$$\begin{aligned} G(\underline{r}, \underline{r}'; \omega) \; &= \; \frac{1}{\sqrt{2 \, \pi}} \, \sum_{m=-\infty}^{\infty} \, \sum_{k} \, \frac{N_m^2}{2 \, \pi} \, \frac{J_m(kr) \; J_m(kr')}{\frac{\omega^2}{c^2} \; - \; k^2} \; \exp \left[\; i \; m \; (\; \theta \; - \; \theta' \;) \; \right] \\ G(\underline{r}, \underline{r}'; \omega) \; &= \; \frac{1}{\sqrt{2 \, \pi}} \, \sum_{k} \, \frac{N_0^2}{2 \, \pi} \, \frac{J_0(kr) \; J_0(kr')}{\frac{\omega^2}{c^2} \; - \; k^2} \\ &+ \; \frac{1}{\sqrt{2 \, \pi}} \, \sum_{m=1}^{\infty} \, \sum_{k} \, \frac{N_m^2}{\pi} \, \frac{J_m(kr) \; J_m(kr')}{\frac{\omega^2}{c^2} \; - \; k^2} \; \cos \; m \; (\; \theta \; - \; \theta' \;) \end{aligned} \tag{1363}$$

where we have used the symmetry of the product $J_m(x) \; J_m(y)$ under the interchange of m and $- \, m$.

Example:

The Green's function for the wave equation in an infinite three dimensional space can be found from the temporal Fourier transform

$$\left(\; \nabla^2 \; + \; \frac{\omega^2}{c^2} \; \right) \; G(\underline{r}, \underline{r}'\omega) \; = \; \frac{1}{\sqrt{2 \, \pi}} \; \delta^3(\underline{r} - \underline{r}') \tag{1364}$$

We expand the Green's function in terms of the plane wave eigenfunctions which satisfy

$$\left(\; \nabla^2 \; + \; \frac{\omega^2}{c^2} \; \right) \phi_{\underline{k}}(\underline{r}) \; = \; \left(\; - \, k^2 \; + \; \frac{\omega^2}{c^2} \; \right) \; \phi_{\underline{k}}(\underline{r}) \tag{1365}$$

in which the eigenfunction is found as

$$\phi_{\underline{k}}(\underline{r}) \; = \; \frac{1}{(\; 2 \; \pi \;)^{\frac{3}{2}}} \; \exp \left[\; + \; i \; \underline{k} \; . \; \underline{r} \; \right] \tag{1366}$$

One obtains the expression

$$G(\underline{r}, \underline{r}'; \omega) \; = \; \frac{1}{\sqrt{2 \, \pi}} \, \int \, \frac{d^3 \underline{k}}{(\; 2 \; \pi \;)^3} \; \frac{\exp \left[\; i \; \underline{k} \; . \; (\; \underline{r} \; - \; \underline{r}' \;) \; \right]}{\frac{\omega^2}{c^2} \; - \; k^2} \tag{1367}$$

and hence

$$G(\underline{r},t:\underline{r}',t') \;=\; \int_{-\infty}^{\infty} \frac{d\omega}{2\,\pi} \int \frac{d^3\underline{k}}{(\,2\,\pi\,)^3} \frac{\exp\left[\,i\,\underline{k}\,.\,(\,\underline{r}\,-\,\underline{r}'\,)\,-\,i\,\omega\,(\,t\,-\,t'\,)\,\right]}{\frac{\omega^2}{c^2}\,-\,k^2} \tag{1368}$$

The angular part of the integration over $\underline{k}$ can be performed by using $\underline{r}-\underline{r}'$ as the polar axis. In this case one finds

$$\begin{aligned} G(\underline{r},t:\underline{r}',t') \;&=\; \int_{0}^{\infty} \frac{dk\;k^2}{(\,2\,\pi\,)^2} \frac{\exp\left[\,+\,i\,k\,|\,\underline{r}\,-\,\underline{r}'\,|\,\right]\,-\,\exp\left[\,-\,i\,k\,|\,\underline{r}\,-\,\underline{r}'\,|\,\right]}{i\,k\,|\,\underline{r}\,-\,\underline{r}'\,|} \\ &\times\; \int_{-\infty}^{\infty} \frac{d\omega}{2\,\pi} \frac{\exp\left[\,-\,i\,\omega\,(\,t\,-\,t'\,)\,\right]}{\frac{\omega^2}{c^2}\,-\,k^2} \\ &=\; \int_{-\infty}^{\infty} \frac{dk\;k}{(\,2\,\pi\,)^2} \frac{\exp\left[\,+\,i\,k\,|\,\underline{r}\,-\,\underline{r}'\,|\,\right]}{|\,\underline{r}\,-\,\underline{r}'\,|} \\ &\times\; \int_{-\infty}^{\infty} \frac{d\omega}{2\,\pi\,i} \frac{\exp\left[\,-\,i\,\omega\,(\,t\,-\,t'\,)\,\right]}{\frac{\omega^2}{c^2}\,-\,k^2} \end{aligned} \tag{1369}$$

The integration over ω can be performed using Cauchy's theorem of contour integration. The contour has to be closed in the lower half complex ω plane for positive t, and in the upper half complex plane for negative t. There are poles at $\omega\;=\;\pm\,c\,k$ in the lower half plane. This leads to

$$\begin{aligned} G(\underline{r},t:\underline{r}',t') \;&=\; -\,i\,\frac{c\,\Theta(t-t')}{|\,\underline{r}\,-\,\underline{r}'\,|} \int_{-\infty}^{\infty} \frac{dk}{(\,2\,\pi\,)^2} \exp\left[\,i\,k\,|\,\underline{r}\,-\,\underline{r}'\,|\,\right] \sin\,c\,k\,(\,t\,-\,t'\,) \\ &=\; -\,\frac{c}{4\,\pi\,|\,\underline{r}\,-\,\underline{r}'\,|}\,\delta\Big(\,|\,\underline{r}\,-\,\underline{r}'\,|\,-\,c\,(\,t\,-\,t'\,)\,\Big) \end{aligned} \tag{1370}$$

Example:

The Green's function for the wave equation in an infinite d-dimensional space can also be obtained using this method. First, the Green's function equation is Fourier transformed with respect to time. The frequency dependent Green's function is then defined as the solution of the inhomogeneous partial differential equation

$$\left(\nabla^2 \ + \ \frac{\omega^2}{c^2} \right) G(\underline{r},\underline{r}';\omega) \ = \ \frac{1}{\sqrt{2 \ \pi}} \ \delta^d(\ \underline{r} \ - \ \underline{r}' \ ) \tag{1371}$$

This can be solved by using the completeness relation of the plane wave eigenfunctions of the Laplace operator. On expanding the Green's function in terms of plane waves and also using the representation of the d-dimensional delta function

$$\delta^d(\ \underline{r} \ - \ \underline{r}' \ ) \ = \ \int \frac{d^d\underline{k}}{(\ 2 \ \pi \ )^d} \ \exp \left[\ i \ \underline{k} \ . \ (\ \underline{r} \ - \ \underline{r}' \ ) \ \right] \tag{1372}$$

one finds that the frequency dependent Green's function can be written as

$$G(\underline{r},\underline{r}',\omega) \ = \ \frac{1}{(\ 2 \ \pi \ )^{(d+\frac{1}{2})}} \int d^d\underline{k} \ \frac{\exp \left[\ i \ \underline{k} \ . \ (\ \underline{r} \ - \ \underline{r}' \ ) \ \right]}{\frac{\omega^2}{c^2} \ - \ k^2} \tag{1373}$$

The time dependent Green's function is given by the inverse Fourier Transform of the frequency dependent Green's function

$$G(\underline{r},\underline{r}',t{-}t') \ = \ \frac{1}{(\ 2 \ \pi \ )^{(d+1)}} \int_{-\infty}^{\infty} d\omega \int d^d\underline{k} \ \frac{\exp \left[\ i \ \underline{k} \ . \ (\ \underline{r} \ - \ \underline{r}' \ ) \ - \ i \ \omega \ (\ t \ - \ t' \ ) \ \right]}{\frac{\omega^2}{c^2} \ - \ k^2} \tag{1374}$$

Note that because space time is homogeneous (we have no boundaries) the Green's function is invariant under translations through time and space.

The integral over the d-dimensional volume $d^d\underline{k}$ in ultra-spherical polar coordinates is given by

$$\int_0^{\infty} dk \ k^{d-1} \int_0^{\pi} d\theta_{d-1} \ \sin^{d-2}\theta_{d-1} \int_0^{\pi} d\theta_{d-2} \ \sin^{d-3}\theta_{d-2} \ \ldots \int_0^{\pi} d\theta_2 \ \sin\theta_2 \int_0^{2\pi} d\varphi \tag{1375}$$

The integral over the solid angle involves an integral over the principal polar angle of the form

$$\int d\theta \ \sin^{(d-2)}\theta \ \exp \left[\ i \ x \ \cos\theta \ \right] \ = \ \sqrt{\pi} \ \Gamma(\frac{d-1}{2}) \left(\frac{2}{x} \right)^{\frac{d-2}{2}} J_{\frac{d-2}{2}}(x) \tag{1376}$$

where $\Gamma(x)$ is the factorial function

$$\Gamma(x+1) \ = \ x \ \Gamma(x) \tag{1377}$$

and for integer n, with $\Gamma(1) \ = \ 1$, yields

$$\Gamma(n+1) \ = \ n! \tag{1378}$$

The subsequent angular integrations are performed using the formula

$$\int_0^{\pi} d\theta \ \sin^m \theta \ = \ \sqrt{\pi} \ \frac{\Gamma(\frac{m+1}{2})}{\Gamma(\frac{m+2}{2})} \tag{1379}$$

Thus, the angular integrations produce the factor

$$\begin{aligned} & \sqrt{\pi} \ \Gamma(\frac{d-1}{2}) \left(\frac{2}{x} \right)^{\frac{d-2}{2}} J_{\frac{d-2}{2}}(x) \ \sqrt{\pi} \ \frac{\Gamma(\frac{d-2}{2})}{\Gamma(\frac{d-1}{2})} \ \sqrt{\pi} \ \frac{\Gamma(\frac{d-3}{2})}{\Gamma(\frac{d-2}{2})} \ \ldots \ \sqrt{\pi} \ \frac{\Gamma(\frac{2}{2})}{\Gamma(\frac{3}{2})} \ 2 \ \pi \\ = & \ 2 \ \pi^{\frac{d}{2}} \left(\frac{2}{x} \right)^{\frac{d-2}{2}} J_{\frac{d-2}{2}}(x) \\ = & \ (\ 2 \ \pi \ )^{\frac{d}{2}} \ x^{-\frac{d-2}{2}} \ J_{\frac{d-2}{2}}(x) \end{aligned} \tag{1380}$$

as the Γ function is defined such that $\Gamma(1) \ = \ 1$.

Also the integral over ω can be performed, using contour integration. Since we only want the causal part of the Green's function for physical reasons, the poles on the real ω axis at $\omega \ = \ \pm \ c \ k$ are displaced into the lower half complex plane, giving

$$\int_{-\infty}^{\infty} d\omega \ \frac{\exp \left[\ - \ i \ \omega \ t \ \right]}{\frac{\omega^2}{c^2} \ - \ k^2} \ = \ \frac{2 \ \pi \ c}{k} \ \Theta(t) \ \sin \ c \ k \ t \tag{1381}$$

where $\Theta(t)$ is the Heaviside step function defined by

$$\Theta(t) \ = \ \begin{cases} 1 & t \ > \ t' \\ 0 & t \ < \ t' \end{cases} \tag{1382}$$

This leads to the expression

$$G(\underline{r}-\underline{r}';t-t') \ = \ - \ \frac{c \ \Theta(t-t')}{(\ 2 \ \pi \ )^{\frac{d}{2}} \ | \ \underline{r} \ - \ \underline{r}' \ |^{\frac{d-2}{2}}} \int_0^{\infty} dk \, k^{\frac{d-2}{2}} \ J_{\frac{d-2}{2}}(k| \ \underline{r} - \underline{r}' \ |) \ \sin \ c \, k \ (\ t - t' \ ) \tag{1383}$$

For convenience of notation we re-center the origin of our coordinate system on the source at $(\underline{r}', t')$, so the Green's function only explicitly depends on the field point coordinates. The integral over k can be evaluated with the aid of the formula

$$\int_0^{\infty} dx \ x^{\nu} \ J_{\nu}(\alpha x) \ \exp \left[\ - \ \beta \ x \ \right] \ = \ \frac{(\ 2 \ \alpha \ )^{\nu} \ \Gamma(\nu + \frac{1}{2})}{\sqrt{\pi} \ (\ \alpha^2 \ + \ \beta^2 \ )^{\nu + \frac{1}{2}}} \tag{1384}$$

where $\Gamma(n+1) \; = \; n!$ is the factorial function. However, to ensure that the integrals over k converge we add a convergence factor of

$$\lim_{\varepsilon \to 0} \; \exp \left[\; - \; k \; \varepsilon \; \right] \tag{1385}$$

to the integrals. Thus, one finds the integral

$$\begin{aligned} & \lim_{\varepsilon \to 0} \int_0^\infty \; dk \; k^\nu \; J_\nu(kr) \; \sin kr \; \exp \left[\; - \; k \; \varepsilon \; \right] \; = \\ = \; & \lim_{\varepsilon \to 0} \; (\; 2 \; r \;)^\nu \; \frac{\Gamma(\frac{2\nu+1}{2})}{2 \; i \; \sqrt{\pi}} \left[\frac{1}{[\; r^2 \; + \; (\; - \; i \; c \; t \; + \; \varepsilon \;)^2 \;]^{\frac{2\nu+1}{2}}} \; - \; \frac{1}{[\; r^2 \; + \; (\; i \; c \; t \; + \; \varepsilon \;)^2 \;]^{\frac{2\nu+1}{2}}} \right] \end{aligned} \tag{1386}$$

Then on defining

$$s \; = \; r^2 \; + \; (\; - \; i \; c \; t \; + \; \varepsilon \;)^2 \tag{1387}$$

and using the identity

$$s^{-n} \; = \; (\; - \; 1 \;)^n \; \frac{1}{(n-1)!} \; \frac{\partial^{n-1}}{\partial s^{n-1}} \; s^{-1} \tag{1388}$$

one has

$$\left[\; r^2 \; + \; (\; - \; i \; c \; t \; + \; \varepsilon \;)^2 \; \right]^{-n} \; = \; \frac{1}{(n-1)!} \left(\; - \; \frac{1}{2 \; r} \; \frac{\partial}{\partial r} \; \right)^{n-1} \left[\; r^2 \; + \; (\; - \; i \; c \; t \; + \; \varepsilon \;)^2 \; \right]^{-1} \tag{1389}$$

After some elementary manipulations one obtains the time dependent Green's function

$$G(r;t) \; = \; - \; \frac{c \; \Theta(t)}{4 \; \pi} \left(\; - \; \frac{1}{2 \; \pi \; r} \; \frac{\partial}{\partial r} \; \right)^{\frac{d-3}{2}} \left[\; \frac{\delta(\; r \; - \; c \; t \;)}{r} \; \right] \tag{1390}$$

The term involving a second delta function has been dropped as it does not contribute, due to the presence of the Heaviside function. The Green's function is retarded, in the sense that the solution at point $(\underline{r}, t)$ only experiences the effect of the source at the point $(\underline{r}', t')$ only if t is later than t'. Thus, the retarded Green's function expresses causality. However, it also shows that the an effect at point $(\underline{r}, t)$ only occurs if the signal from the point source at $(\underline{r}', t')$ exactly reaches the point $(\underline{r}, t)$, and that in between the signal travels with speed c.

13 Complex Analysis

Consider a function of a complex variable $z = x + i\, y$. Then the function $f(z)$ of the complex variable also has a real and imaginary part, so

$$f(z) = u(x,y) + i\, v(x,y) \tag{1391}$$

where u and v are real functions of x and y. The derivative of a complex function is defined by the limit

$$\frac{df(z)}{dz} = \lim_{\Delta z \to 0} \frac{f(z + \Delta z) - f(z)}{\Delta z} \tag{1392}$$

provided that the limit exists and is independent of the path in which the limit is taken. For example, if one considers

$$\Delta z = \Delta x + i\, \Delta y \tag{1393}$$

then one can take two independent limits, either $\Delta x \to 0$ or $\Delta y \to 0$. In general

$$\frac{\Delta f}{\Delta z} = \frac{\Delta u + i\, \Delta v}{\Delta x + i\, \Delta y} \tag{1394}$$

On taking the limit $\Delta x \to 0$ one obtains

$$\lim_{\Delta x \to 0} \frac{\Delta f}{\Delta x} = \left(\frac{\partial u}{\partial x} \right) + i \left(\frac{\partial v}{\partial x} \right) \tag{1395}$$

while on the path $\Delta z = i\, \Delta y$ the derivative takes the value

$$\lim_{\Delta y \to 0} \frac{\Delta f}{i\, \Delta y} = -\, i \left(\frac{\partial u}{\partial y} \right) + \left(\frac{\partial v}{\partial y} \right) \tag{1396}$$

If the derivative is to be well defined, these expressions must be equal, so one must have

$$\left(\frac{\partial u}{\partial x} \right) = \left(\frac{\partial v}{\partial y} \right) \tag{1397}$$

and

$$\left(\frac{\partial u}{\partial y} \right) = - \left(\frac{\partial v}{\partial x} \right) \tag{1398}$$

These are the Cauchy-Riemann conditions. They are necessary conditions, for if a unique derivative is to exist the Cauchy Riemann conditions must hold. Note that a function that satisfies the Cauchy Riemann conditions automatically is a solution of Laplace's equation.

Conversely, if the Cauchy Riemann conditions are satisfied then $f(z)$ is continuous, and the derivative exists. This can be formulated as a theorem.

Theorem.

Let $u(x,y)$ and $v(x,y)$ be the real and imaginary parts of a function of a complex variable $f(z)$, which obey the Cauchy Riemann conditions and also posses continuous partial derivatives (with respect to x and y) at all points in some region of the complex plane, then $f(z)$ is differentiable in this region.

Proof.

Since u and v have continuous first partial derivatives there exist four numbers, $\epsilon_1, \epsilon_2, \delta_1, \delta_2$ that can be made arbitrarily small as Δx and Δy tend to zero, such that

$$u(x+\Delta x, y+\Delta y) - u(x,y) = \left(\frac{\partial u}{\partial x}\right)\Delta x + \left(\frac{\partial u}{\partial y}\right)\Delta y + \epsilon_1\,\Delta x + \delta_1\,\Delta y \quad (1399)$$

and

$$v(x+\Delta x, y+\Delta y) - v(x,y) = \left(\frac{\partial v}{\partial x}\right)\Delta x + \left(\frac{\partial v}{\partial y}\right)\Delta y + \epsilon_2\,\Delta x + \delta_2\,\Delta y \quad (1400)$$

Multiplying the second of these equations by i and adding them one has

$$\begin{aligned} f(z+\Delta z) \;-\; f(z) \;&=\; \left(\frac{\partial u}{\partial x}\right)\Delta x \;+\; \left(\frac{\partial u}{\partial y}\right)\Delta y \;+\; i\,\left(\frac{\partial v}{\partial x}\right)\Delta x \;+\; i\,\left(\frac{\partial v}{\partial y}\right)\Delta y \\ &+\; \epsilon_1\,\Delta x \;+\; \delta_1\,\Delta y \;+\; i\,\epsilon_2\,\Delta x \;+\; i\,\delta_2\,\Delta y \end{aligned} \quad (1401)$$

Using the Cauchy Riemann conditions one has

$$\begin{aligned} f(z+\Delta z) \;-\; f(z) \;&=\; \left(\frac{\partial u}{\partial x}\right)\Delta x \;-\; \left(\frac{\partial v}{\partial x}\right)\Delta y \;+\; i\,\left(\frac{\partial v}{\partial x}\right)\Delta x \;+\; i\,\left(\frac{\partial u}{\partial x}\right)\Delta y \\ &+\; \epsilon_1\,\Delta x \;+\; \delta_1\,\Delta y \;+\; i\,\epsilon_2\,\Delta x \;+\; i\,\delta_2\,\Delta y \\ &=\; \left[\left(\frac{\partial u}{\partial x}\right) \;+\; i\,\left(\frac{\partial v}{\partial x}\right)\right]\left[\Delta x \;+\; i\,\Delta y\right] \\ &+\; \epsilon_1\,\Delta x \;+\; \delta_1\,\Delta y \;+\; i\,\epsilon_2\,\Delta x \;+\; i\,\delta_2\,\Delta y \end{aligned} \quad (1402)$$

Thus, on dividing by Δz, and taking the limit one has

$$\frac{df(z)}{dz} \;=\; \left(\frac{\partial u}{\partial x}\right) \;+\; i\,\left(\frac{\partial v}{\partial x}\right) \quad (1403)$$

Example:

The function $f(z) \; = \; z^2$ satisfies the Cauchy Riemann conditions, at all points in the complex plane as

$$u(x,y) \; = \; x^2 \; - \; y^2 \tag{1404}$$

and

$$v(x,y) \; = \; 2 \; i \; x \; y \tag{1405}$$

Hence,

$$\left(\frac{\partial u}{\partial x} \right) \; = \; 2 \; x \; = \; \left(\frac{\partial v}{\partial y} \right) \tag{1406}$$

and

$$\left(\frac{\partial u}{\partial y} \right) \; = \; - \; 2 \; y \; = \; - \; \left(\frac{\partial v}{\partial x} \right) \tag{1407}$$

However, the function $f(z) \; = \; (z^*)^2$ does not satisfy the Cauchy Riemann conditions, but is still continuous.

On applying the Cauchy Riemann conditions to a function which is assumed to be expandable as a Taylor series in some region around (x_0, y_0) one can show that

$$u(x,y) \; + \; i \; v(x,y) \; - \; u(x_0,y_0) \; - \; i \; v(x_0,y_0) \; =$$

$$= \; \sum_{n=1}^{\infty} \frac{1}{n!} \left[\; x \; + \; i \; y \; - \; x_0 \; - \; i \; y_0 \; \right]^n \frac{\partial^n}{\partial x_0^n} \left(\; u(x_0,y_0) \; + \; i \; v(x_0,y_0) \; \right) \tag{1408}$$

That is, the function only depends on $z \; = \; x \; + \; i \; y$ and not on the complex conjugate $z^* \; = x \; - \; i \; y$. It should be noted that not all functions can be Taylor expanded about an arbitrary point, for example the functions

$$f(z) \; = \; \frac{1}{z} \tag{1409}$$

and

$$f(z) \; = \; \exp \left[\; - \; \frac{1}{z} \; \right] \tag{1410}$$

can not be Taylor expanded around the point $z \; = \; 0$. The partial derivatives do not exist, and the Cauchy-Riemann conditions do not hold at $z \; = \; 0$. The radius of convergence of the Taylor expansion about the origin is zero.

Analytic Functions

A function $f(z)$ is analytic at the point z_0 if it satisfies the Cauchy Riemann conditions at z_0. If $f(z)$ is analytic at all points in the entire complex z plane it is defined to be an entire function.

13.1 Contour Integration

The integration of a complex function, is defined as an integration over a curve in the complex plane. The curve is known as a contour, and may be parameterized by

$$\begin{aligned} x &= x(s) \\ y &= y(s) \end{aligned} \tag{1411}$$

The integral of $f(z)$ over a specific contour C can be evaluated as

$$\begin{aligned} \int_C dz \; f(z) &= \int_{s_0}^{s_1} ds \left(\frac{dx(s)}{ds} + i \, \frac{dy(s)}{ds} \right) f(z(s)) \\ &= \int_{s_0}^{s_1} ds \left(\frac{dx(s)}{ds} \, u(x(s), y(s)) - \frac{dy(s)}{ds} \, v(x(s), y(s)) \right) \\ &+ i \int_{s_0}^{s_1} ds \left(\frac{dx(s)}{ds} \, v(x(s), y(s)) + \frac{dy(s)}{ds} \, u(x(s), y(s)) \right) \end{aligned} \tag{1412}$$

which reduces the contour integration to the sum of two Riemann integrations.

Example:

Consider the integration of the function $f(z) = z^2$ over an open contour from $z = 0$ to $z \; 1 + i$ along two different paths, the contour C_1 which is a parabola

$$\begin{aligned} x(s) &= s \\ y(s) &= s^2 \end{aligned} \tag{1413}$$

and a second contour C_2 which consists of a straight line segment

$$\begin{aligned} x(s) &= s \\ y(s) &= s \end{aligned} \tag{1414}$$

The integral over contour C_1 is evaluated as

$$\begin{aligned}
\int_{C_1} dz\ f(z) &= \int_0^1 ds \left(\frac{dz(s)}{ds} \right) \left((x^2 - y^2) + i\ 2\ x\ y \right) \\
&= \int_0^1 ds \left(\frac{dx(s)}{ds} + i\ \frac{dy(s)}{ds} \right) \left((x^2 - y^2) + i\ 2\ x\ y \right) \\
&= \int_0^1 ds \left(1 + i\ 2\ s \right) \left((s^2 - s^4) + i\ 2\ s^3 \right) \\
&= \int_0^1 ds \left((s^2 - 5\ s^4) + i\ (4\ s^3 - 2\ s^5) \right) \\
&= \left((\frac{1}{3}\ s^3 - s^5) + i\ (s^4 - \frac{2}{6}\ s^6) \right) \Bigg|_{s=0}^{s=1} \\
&= \left(- \frac{2}{3} + i\ \frac{2}{3} \right)
\end{aligned} \tag{1415}$$

The integral over the contour C_2 is evaluated as

$$\begin{aligned}
\int_{C_2} dz\ f(z) &= \int_0^1 ds \left(\frac{dz(s)}{ds} \right) \left((x^2 - y^2) + i\ 2\ x\ y \right) \\
&= \int_0^1 ds \left(\frac{dx(s)}{ds} + i\ \frac{dy(s)}{ds} \right) \left((x^2 - y^2) + i\ 2\ x\ y \right) \\
&= \int_0^1 ds \left(1 + i \right) \left((s^2 - s^2) + i\ 2\ s^2 \right) \\
&= \int_0^1 ds \left(- 2\ s^2 + i\ 2\ s^2 \right) \\
&= \left(- \frac{2}{3}\ s^3 + i\ \frac{2}{3}\ s^3 \right) \Bigg|_{s=0}^{s=1} \\
&= \left(- \frac{2}{3} + i\ \frac{2}{3} \right)
\end{aligned} \tag{1416}$$

Thus, the integration over an entire function appears to be independent of the contour on which it is evaluated.

Example:

Important examples of contour integration are given by the integration of a mono-nomial z^n over a closed circle of radius r centered on the origin of the complex z plane. The integral can be evaluated as

$$\frac{1}{2 \pi i} \int_C dz \, z^n \; = \; \frac{r^n}{2 \pi} \int_0^{2\pi} d\theta \, \exp \left[\, i \, (\, n \, + \, 1 \,) \, \theta \, \right] \tag{1417}$$

where we have used the polar form for the complex number

$$z \; = \; r \, \exp \left[\, i \, \theta \, \right] \tag{1418}$$

and on the contour one has

$$dz \; = \; r \, \exp \left[\, i \, \theta \, \right] \, i \, d\theta \tag{1419}$$

The integral is easily evaluated for integer values of n as

$$\begin{aligned} \frac{1}{2 \pi i} \int_C dz \, z^n \; &= \; \frac{r^n}{2 \pi} \int_0^{2\pi} d\theta \, \exp \left[\, i \, (\, n \, + \, 1 \,) \, \theta \, \right] \\ &= \; \frac{r^{n+1}}{2 \pi} \int_0^{2\pi} d\theta \, \exp \left[\, i \, (\, n \, + \, 1 \,) \, \theta \, \right] \\ &= \; \frac{r^{n+1}}{2 \pi i \, (\, n \, + \, 1 \,)} \, \exp \left[\, i \, (\, n \, + \, 1 \,) \, \theta \, \right] \Bigg|_0^{2\pi} \\ &= \; 0 \end{aligned} \tag{1420}$$

for integer n, $n \; \neq \; - \, 1$. This occurs since the exponential is $2 \, \pi$ periodic, and the result is independent of the radius r of the contour.

A second important example is found by examining the case where $n \; = \; - \, 1$. In this case, the closed contour integral is evaluated as

$$\begin{aligned} \frac{1}{2 \pi i} \int_C dz \, z^{-1} \; &= \; \frac{1}{2 \pi} \int_0^{2\pi} d\theta \\ &= \; \frac{1}{2 \pi} \, \theta \Bigg|_0^{2\pi} \\ &= \; 1 \end{aligned} \tag{1421}$$

It is noteworthy, that the function z^{-1} does not satisfy the Cauchy Riemann conditions at the origin, and the contour wraps around the origin once. The function and the derivatives are not defined at the origin.

Both of these examples yield results which are independent of r, the radius of the closed circular contour.

A contour integral of function, that satisfies the Cauchy Riemann conditions at every point of a region of the complex plane which contains the function, is independent of the path of integration. There is an analogy between integration of analytic functions and conservative forces in Mechanics; the analytic function plays the role of a conservative force and the integral plays the role of the potential. Alternatively, there is an analogy between integration of an analytic function and functions of state in thermodynamics.

The contour integral of an analytic function $f(z)$ can be calculated as the difference of a function $F(z)$ evaluated the end points,

$$\int_C dz \; f(z) \; = \; F(z_1) \; - \; F(z_0) \tag{1422}$$

where the function $F(z)$ satisfies

$$\frac{dF(z)}{dz} \; = \; f(z) \tag{1423}$$

The function $F(z)$ is the primitive of the function $f(z)$. This is the content of Cauchy's Integral Theorem.

13.2 Cauchy's Integral Theorem

If a function $f(z)$ is analytic and its partial derivatives are continuous everywhere inside a (simply connected) region, then the contour integration over any closed path entirely contained within the region is zero

$$\oint_C dz \; f(z) \; = \; 0 \tag{1424}$$

A simply connected region means a region in which there are no holes.

Stokes's Proof.

Consider the integration over the closed loop

$$\oint_C dz \; f(z) \; = \; \oint_C (\left(\; u \; + \; i \; v \; \right) \left(\; dx \; + \; i \; dy \; \right)$$

$$= \oint_C \left(u\, dx \; - \; v\, dy \right) \; + \; i \oint_C \left(v\, dx \; + \; u\, dy \right) \tag{1425}$$

The integration consists of two line integrals. Each line integral can be thought of as a integration of a scalar product of a vector with the vector displacement around the loop in the (x, y) plane. That is, the integration can be considered as an integration representing the work performed by a force.

The real part of integration involves the scalar product of a vector

$$\underline{A} \; = \; \hat{e}_1 \, u \; - \; \hat{e}_2 \, v \tag{1426}$$

and a displacement. The displacement is represented by

$$d\underline{r} \; = \; \hat{e}_1 \, dx \; + \hat{e}_2 \, dy \tag{1427}$$

and the integration is given by

$$\oint_C d\underline{r} \; . \; \underline{A} \tag{1428}$$

The contour integration can be evaluated by Stokes's theorem

$$\oint_C d\underline{r} \; . \; \underline{A} \; = \; \int d^2\underline{S} \; . \; (\; \underline{\nabla} \; \wedge \; \underline{A} \;) \tag{1429}$$

in terms of an integral inside the area of the (x, y) enclosed by the loop or

$$\oint_C \left(u\, dx \; - \; v\, dy \right) \; = \; - \int dx \int dy \left(\frac{\partial v}{\partial x} \; + \; \frac{\partial u}{\partial y} \right) \tag{1430}$$

The imaginary part can be evaluated in the same way, but this time the vector $\underline{B}$ in the loop integral

$$\oint_C d\underline{r} \; . \; \underline{B} \tag{1431}$$

is identified as

$$\underline{B} \; = \; \hat{e}_1 \, v \; + \; \hat{e}_2 \, u \tag{1432}$$

leading to

$$\oint_C \left(v\, dx \; + \; u\, dy \right) \; = \; \int dx \int dy \left(\frac{\partial u}{\partial x} \; - \; \frac{\partial v}{\partial y} \right) \tag{1433}$$

where the last integral is evaluated over the area enclosed by the loop.

Since the functions u and v satisfy the Cauchy conditions inside the region enclosed by the loop, both integrands vanish. Hence, we have Cauchy's integral theorem

$$\oint_C dz \ f(z) \ = \ 0 \tag{1434}$$

if $f(z)$ is analytic at all points enclosed by the loop.

Since the contour integration around a loop contained entirely in a simply connected region where the function is analytic, one finds that the integration along two segments C_1 and C_2 of our arbitrary closed loop cancel

$$\oint_C dz \ f(z) \ = \ \int_{A \ C_1}^{B} dz \ f(z) \ + \ \int_{B \ C_2}^{A} dz \ f(z) \ = \ 0 \tag{1435}$$

Then, on reversing the direction of the integration on one segment, the integrals in the same direction are equal

$$\int_{A \ C_1}^{B} dz \ f(z) \ = \ \int_{A \ C_2}^{B} dz \ f(z) \tag{1436}$$

Since the integral of the analytic function between A and B is independent of the path, the integral can only depend upon the end points. Hence, we have

$$\int_{A}^{B} dz \ f(z) \ = \ F(z_B) \ - \ F(z_A) \tag{1437}$$

which is independent of the path of integration (as long as it is entirely contained inside the simply connected region where $f(z)$ is analytic).

Multiply Connected Regions.

A contour that lies within a simply connected region can be continuously shrunk to a point, without leaving the region. In a multiply connected region there exists contours that can not be shrunk to a point without leaving the region. Cauchy's integral theorem is not valid for a contour that can not be shrunk to a point without the contour leaving the region of analyticity.

A multiply connected region can be reduced to a simply connected region by introducing one or more lines connecting the disjoint regions in which the function is non-analytic, and demanding that the contours can not cross the lines. That is the lines are considered to cut the plane, so that the region is simply connected. Due to the cut lines, Cauchy's theorem can be applied.

Example:

Consider the integral

$$\oint_C dz \, \frac{1}{z \, (\, z \, + \, 1 \,)} \tag{1438}$$

around a contour C circling the origin counterclockwise with $| \, z \, | \, > \, 1$.

The Cauchy Riemann conditions are not satisfied at two point $z \, = \,$ and $z \, = \, - \, 1$ where the derivative is not defined. The function is analytic at all points in the surrounding area. The region is multiply connected. Two cut lines can be chosen linking the singularities to infinity, making the region simply connected. We shall choose the line running along the positive imaginary axis from the origin and the parallel line running from $z \, = \, - \, 1$ to infinity.

Cauchy's theorem can be applied to the contour C and its completion running along oppositely directed segments on each side of the line cuts extending to the singularities, and two small circles C_1 and C_2 of radius r circling the singularities in a clockwise direction.

Then, from Cauchy's theorem one has

$$\oint_C dz \, \frac{1}{z \, (\, z \, + \, 1 \,)} \, + \, \oint_{C_1} dz \, \frac{1}{z \, (\, z \, + \, 1 \,)} \, + \, \oint_{C_2} dz \, \frac{1}{z \, (\, z \, + \, 1 \,)} \, = \, 0 \tag{1439}$$

since the contour is in a singly connected region in which the function is analytic. The contributions from the anti-parallel line segments cancel in pairs, as the function is single valued on these lines.

The integral around C_1 enclosing $z \, = \, - \, 1$ in a clockwise direction is evaluated on the contour

$$z \, = \, - \, 1 \, + \, r \, \exp[\, i \, \theta \,] \tag{1440}$$

and θ runs from 0 to $- \, 2 \, \pi$. The integral around C_1 is given by the limit $r \, \rightarrow \, 0$

$$\begin{aligned} \oint_{C_1} dz \, \frac{1}{z \, (\, z \, + \, 1 \,)} \, &= \, \lim_{r \rightarrow 0} \, i \, \int_0^{-2\pi} d\theta \, r \, \exp[\, i \, \theta \,] \, \frac{1}{(\, - \, 1 \, + \, r \, \exp[\, i \, \theta \,] \,) \, r \, \exp[\, i \, \theta \,]} \\ &= \, \lim_{r \rightarrow 0} \, i \, \int_0^{-2\pi} d\theta \, \frac{1}{(\, - \, 1 + \, r \, \exp[\, i \, \theta \,] \,)} \\ &= \, i \, 2 \, \pi \end{aligned} \tag{1441}$$

The integral around the contour C_2 running clockwise around the origin is evaluated along the curve

$$z \, = \, r \, \exp[\, i \, \theta \,] \tag{1442}$$

and θ runs from 0 to $- \, 2 \, \pi$. The integral is evaluated as

$$\begin{aligned} \oint_{C_2} dz \, \frac{1}{z \, (\, z \, + \, 1 \,)} &= \lim_{r \to 0} \, i \, \int_0^{-2\pi} d\theta \, r \, \exp[\, i \, \theta \,] \, \frac{1}{r \, \exp[\, i \, \theta \,] \, (\, 1 \, + \, r \, \exp[\, i \, \theta \,] \,)} \\ &= \lim_{r \to 0} \, i \, \int_0^{-2\pi} d\theta \, \frac{1}{(\, 1 + \, r \, \exp[\, i \, \theta \,] \,)} \\ &= - \, i \, 2 \, \pi \end{aligned} \tag{1443}$$

Thus, we have the final result

$$\oint_C dz \, \frac{1}{z \, (\, z \, + \, 1 \,)} \, + \, 2 \, \pi \, i \, - \, 2 \, \pi \, i \, = \, 0 \tag{1444}$$

or

$$\oint_C dz \, \frac{1}{z \, (\, z \, + \, 1 \,)} \, = \, 0 \tag{1445}$$

This can be verified by explicitly evaluating the integral over a circular contour $z \, = \, R \, \exp[\, i \, \theta]$ of very large radius, $R \, \to \, \infty$. In this case one has

$$\begin{aligned} \oint_C dz \, \frac{1}{z \, (\, z \, + \, 1 \,)} &\sim \frac{i}{R} \int_0^{2\pi} d\theta \, \exp[\, - \, i \, \theta \,] \, + \, O(R^{-2}) \\ &= 0 \end{aligned} \tag{1446}$$

Example:

Consider the integral

$$\oint_C dz \, \frac{2 \, z \, + \, 1}{z \, (\, z \, + \, 1 \,)} \tag{1447}$$

around a contour C circling the origin counterclockwise with $| \, z \, | \, > \, 1$.

The Cauchy Riemann conditions are not satisfied at two point $z \, =$ and $z \, = \, - \, 1$ where the derivative is not defined. The function is analytic at all points in the surrounding area. The region is multiply connected. Two cuts can be chosen linking the singularities to infinity, cutting the region so that it is simply connected. We shall choose the cut running along the positive imaginary axis from the origin to $i \, \infty$ and a parallel cut running from $z \, = \, - \, 1$ to $i \, \infty$.

Cauchy's theorem can be applied to the contour C and its completion running along oppositely directed segments on each side of the cuts, and two small circles C_1 and C_2 of radius r circling the singularities in a clockwise direction.

Then, from Cauchy's theorem one has

$$\oint_C dz \, \frac{2 \, z \, + \, 1}{z \, (\, z \, + \, 1 \,)} + \oint_{C_1} dz \, \frac{2 \, z \, + \, 1}{z \, (\, z \, + \, 1 \,)} + \oint_{C_2} dz \, \frac{2 \, z \, + \, 1}{z \, (\, z \, + \, 1 \,)} \; = \; 0 \quad (1448)$$

since the contour is in a singly connected region in which the function is analytic. The contributions from the anti-parallel line segments cancel in pairs, as the function is single valued on these lines.

The integral around C_1 enclosing $z \; = \; - \, 1$ in a clockwise direction is evaluated on the contour

$$z \; = \; - \, 1 \; + \; r \; \exp[\, i \, \theta \,] \qquad (1449)$$

and θ runs from 0 to $- \, 2 \, \pi$. The integral around C_1 is given by the limit $r \; \rightarrow \; 0$

$$\begin{aligned} \oint_{C_1} dz \, \frac{2 \, z \, + \, 1}{(\, z \, + \, 1 \,)} \; &= \; \lim_{r \rightarrow 0} \; i \int_0^{-2\pi} d\theta \; r \; \exp[\, \theta \,] \, \frac{- \, 1 \, + \, 2 \, r \, \exp[\, i \, \theta \,]}{(\, - \, 1 \, + \, r \, \exp[\, i \, \theta \,] \,) \, r \, \exp[\, i \, \theta \,]} \\ &= \; \lim_{r \rightarrow 0} \; i \int_0^{-2\pi} d\theta \, \frac{- \, 1 \, + \, 2 \, r \, \exp[\, i \, \theta \,]}{(\, - \, 1 + \, r \, \exp[\, i \, \theta \,] \,)} \\ &= \; - \, i \, 2 \, \pi \end{aligned} \qquad (1450)$$

The integral around the contour C_2 running clockwise around the origin is evaluated along the curve

$$z \; = \; r \; \exp[\, i \, \theta \,] \qquad (1451)$$

and θ runs from 0 to $- \, 2 \, \pi$. The integral is evaluated as

$$\begin{aligned} \oint_{C_2} dz \, \frac{2 \, z \, + \, 1}{z \, (\, z \, + \, 1 \,)} \; &= \; \lim_{r \rightarrow 0} \; i \int_0^{-2\pi} d\theta \; r \; \exp[\, \theta \,] \, \frac{1 \, + \, 2 \, r \, \exp[\, i \, \theta \,]}{r \, \exp[\, i \, \theta \,] \, (\, 1 \, + \, r \, \exp[\, i \, \theta \,] \,)} \\ &= \; \lim_{r \rightarrow 0} \; i \int_0^{-2\pi} d\theta \, \frac{1 \, + \, 2 \, r \, \exp[\, i \, \theta \,]}{(\, 1 + \, r \, \exp[\, i \, \theta \,] \,)} \\ &= \; - \, i \, 2 \, \pi \end{aligned} \qquad (1452)$$

Thus, we have the final result

$$\oint_C dz \, \frac{2 \, z \, + \, 1}{z \, (\, z \, + \, 1 \,)} \; - \; 2 \, \pi \, i \; - \; 2 \, \pi \, i \; = \; 0 \qquad (1453)$$

or

$$\oint_C dz \, \frac{2 \, z \, + \, 1}{z \, (\, z \, + \, 1 \,)} \; = \; 4 \, \pi \, i \tag{1454}$$

13.3 Cauchy's Integral Formula

We shall assume that $f(z)$ is a function that is analytic in a simply connected region containing a contour C. Cauchy's integral formula states that

$$\frac{1}{2 \, \pi \, i} \oint_C dz \, \frac{f(z)}{z \, - \, z_0} \; = \; f(z_0) \tag{1455}$$

if z_0 is a point inside the contour C.

Although the function $f(z)$ is analytic in the region, the function

$$\frac{f(z)}{z \, - \, z_0} \tag{1456}$$

is not analytic everywhere inside the region. The function diverges at $z \; = \; z_0$ if $f(z_0) \; \neq \; 0$ and the function and derivative is not defined at z_0. Cauchy's theorem can not be applied until the region is converted into a simply connected region. This is performed by introducing a line from z_0 to ∞, which runs through the region of analyticity.

A contour can be constructed that runs around a contour C that almost encloses the point z_0, but continuous along both sides of the line towards z_0 and traverses around a small circle C" of radius r in the opposite sense of rotation. Thus, the contour excludes the point z_0.

The contour integration lies within the simply connected region of analyticity and, thus, Cauchy's theorem can be applied. The integral is evaluated as four segments

$$\begin{aligned} 0 \; = \; & \oint_C dz \, \frac{f(z)}{z \, - \, z_0} \; + \; \int_{z_0}^{z+\epsilon} dz \, \frac{f(z)}{z \, - \, z_0} \\ + \; & \oint_{C"} dz \, \frac{f(z)}{z \, - \, z_0} \; + \; \int_{z-\epsilon}^{z_0} dz \, \frac{f(z)}{z \, - \, z_0} \end{aligned} \tag{1457}$$

Since $f(z)$ is single valued, the integral along both sides of the line cancel. Hence we have

$$0 \; = \; \oint_C dz \, \frac{f(z)}{z \, - \, z_0} \; + \; \oint_{C"} dz \, \frac{f(z)}{z \, - \, z_0} \tag{1458}$$

On reversing the direction of the contour C" around z_0 such that $C" \; = \; - \, C'$, then

$$\oint_C dz \, \frac{f(z)}{z \, - \, z_0} \; = \; \oint_{C'} dz \, \frac{f(z)}{z \, - \, z_0} \tag{1459}$$

where both contours are traversed in the same sense of rotation. The contour C' is evaluated over a path of radius ϵ around z_0, i.e.

$$z \; = \; z_0 \; + \; r \; \exp[\; i \; \theta \;] \tag{1460}$$

We shall assume that the contour C and hence C' both run in a counter clockwise direction, so that θ runs from 0 to 2 π. Hence, in the limit $r \; \rightarrow \; 0$ one has

$$\begin{aligned} \oint_C dz \, \frac{f(z)}{z \, - \, z_0} \; &= \; \int_0^{2\pi} i \, d\theta \; r \; \exp[\; i \; \theta \;] \; \frac{f(\; z_0 \; + \; r \; \exp[\; i \; \theta \;] \;)}{r \; \exp[\; i\theta \;]} \\ &= \; i \int_0^{2\pi} d\theta \; f(z_0) \\ &= \; 2 \; \pi \; i \; f(z_0) \end{aligned} \tag{1461}$$

since $f(z)$ is analytic and continuous at z_0. Thus, Cauchy's integral theorem has been proved.

Cauchy's theorem can be expressed as

$$\frac{1}{2 \; \pi \; i} \oint_C dz \, \frac{f(z)}{z \, - \, z_0} \; = \; \begin{cases} f(z_0) & z_0 \;\; \text{interior} \\ 0 & z_0 \;\; \text{exterior} \end{cases} \tag{1462}$$

corresponding to z_0 either inside or outside the contour C.

Example:

Evaluate the integral

$$\frac{1}{2 \; \pi \; i} \oint_C dz \, \frac{f(z)}{z \, - \, 1} \; = \; \frac{1}{2 \; \pi \; i} \oint_C dz \, \frac{z \; + \; 3}{z \; - \; 1} \tag{1463}$$

over two contours which run counterclockwise, the contour C' enclosing the point $z \; = \; 1$ and another C" which does not enclose $z \; = \; 1$.

From Cauchy's integral formula one obtains the result

$$\frac{1}{2 \; \pi \; i} \oint_C dz \, \frac{f(z)}{z \, - \, 1} \; = \; \begin{cases} 4 & C' \\ 0 & C" \end{cases} \tag{1464}$$

which can be verified by explicit integration.

Thus, Cauchy's integral formula avoids any need to explicitly construct and evaluate the integral.

13.4 Derivatives

Cauchy's integral formula may be used to express the derivative of a function $f(z)$ at a point z_0 in a region which is analytic. The point z_0 is assumed to be enclosed by a loop C contained inside the region of analyticity.

The derivative is defined as

$$\lim_{\Delta z \to 0} \frac{f(z_0 + \Delta z) - f(z_0)}{\Delta z} \tag{1465}$$

on using Cauchy's integral formula at $z_0 + \Delta z$

$$\frac{1}{2 \pi i} \oint_C dz \, \frac{f(z)}{z - z_0 - \Delta z} = f(z_0 + \Delta z) \tag{1466}$$

and z_0

$$\frac{1}{2 \pi i} \oint_C dz \, \frac{f(z)}{z - z_0} = f(z_0) \tag{1467}$$

So one has

$$\begin{aligned} \lim_{\Delta z \to 0} \frac{f(z_0 + \Delta z) - f(z_0)}{\Delta z} &= \lim_{\Delta z \to 0} \frac{1}{2 \pi i \, \Delta z} \oint_C dz \left[\frac{f(z)}{z - z_0 - \Delta z} - \frac{f(z)}{z - z_0} \right] \\ &= \lim_{\Delta z \to 0} \frac{1}{2 \pi i} \oint_C dz \left[\frac{f(z)}{(z - z_0 - \Delta z) (z - z_0)} \right] \\ &= \frac{1}{2 \pi i} \oint_C dz \left[\frac{f(z)}{(z - z_0)^2} \right] \end{aligned} \tag{1468}$$

Thus, we have the derivative given by the contour integral

$$\frac{df(z_0)}{dz_0} = \frac{1}{2 \pi i} \oint_C dz \left[\frac{f(z)}{(z - z_0)^2} \right] \tag{1469}$$

where C encloses z_0, and $f(z)$ is analytic at all points of the region enclosed by C.

The higher order derivatives can also be evaluated in the same way. This procedure leads to

$$\frac{d^n f(z_0)}{dz_0^n} = \frac{n!}{2 \pi i} \oint_C dz \left[\frac{f(z)}{(z - z_0)^{n+1}} \right] \tag{1470}$$

which is basically the n-th order derivative of the Cauchy integral formula with respect to z_0.

Thus, Cauchy's integral formula proves that if $f(z)$ is analytic then all the derivatives are also analytic.

Example:

Explicitly evaluate the integral

$$\frac{1}{2 \pi i} \oint_C dz \, \frac{z^n}{(z - z_0)^2} \tag{1471}$$

where the integral runs over a clockwise contour enclosing z_0 and compare the result with Cauchy's integral formula for the derivative.

The integral can be evaluated on the circular contour

$$z = z_0 + r \exp[i \theta] \tag{1472}$$

traversed in the counter clockwise direction. The integral is evaluated through the binomial expansion of z^n about z_0

$$\begin{aligned} \frac{1}{2 \pi i} \oint_C dz \, \frac{z^n}{(z - z_0)^2} &= \frac{1}{2 \pi} \int_0^{2\pi} d\theta \, \frac{\left(z_0 + r \exp[i \theta] \right)^n}{r \exp[i \theta]} \\ &= \frac{1}{2 \pi} \int_0^{2\pi} d\theta \sum_{m=0}^{n} C(n,m) \, z_0^{n-m} \, r^{m-1} \exp[i (m - 1) \theta] \\ &= \sum_{m=0}^{n} C(n,m) \, z_0^{n-m} \, r^{m-1} \, \delta_{m,1} \\ &= C(n,1) \, z_0^{n-1} \\ &= n \, z_0^{n-1} \\ &= \frac{dz_0^n}{dz_0} \end{aligned} \tag{1473}$$

since only the term with $m = 1$ is non-zero. The result coincides with the derivative of z^n evaluated at z_0.

Example:

Evaluate the integral

$$\frac{1}{2 \pi i} \oint_C dz \, \frac{1}{z^2 (z + 1)} \tag{1474}$$

over a contour that contains the point $z = 0$ but excludes the point $z = - 1$.

This can be evaluated by using Cauchy's integral formula for derivatives as

$$\frac{1}{2\,\pi\,i}\oint_C dz\,\frac{1}{z^2\,(\,z\,+\,1\,)} \;=\; -\,\frac{1}{(\,z\,+\,1\,)^2}\bigg|_{z=0} \;=\; -\,1 \tag{1475}$$

Alternatively, on expressing the integrand in terms of partial fractions

$$\frac{1}{z^2\,(\,z\,+\,1\,)} \;=\; \frac{1}{z^2}\;-\;\frac{1}{z}\;+\;\frac{1}{z\,+\,1} \tag{1476}$$

and then performing a direct integration over a circle of radius ε around $z\;=\;0$ one obtains the result

$$\frac{1}{2\,\pi\,i}\oint_C dz\,\frac{1}{z^2\,(\,z\,+\,1\,)} \;=\; -\,1 \tag{1477}$$

which agrees with the previous result.

Cauchy's integral formula for derivatives automatically provides the result of the integral.

13.5 Morera's Theorem.

Morera's Theorem is the converse of Cauchy's theorem. That is, if a function is continuous in a simply connected region and

$$\oint_C dz\;f(z) \;=\; 0 \tag{1478}$$

for every closed contour C in the region, then $f(z)$ is analytic in the region.

This is proved by noting that since the integral on every closed contour is zero, an integral on an open contour (in the region) can only depend upon the end points

$$F(z_f)\;-\;F(z_i)\;=\;\int_{z_i}^{z_f} dz\;f(z) \tag{1479}$$

Furthermore, as

$$f(z_i)\;=\;\frac{f(z_i)}{z_f\;-\;z_i}\int_{z_i}^{z_f} dz \tag{1480}$$

one has the identity

$$\frac{F(z_f)\;-\;F(z_i)}{z_f\;-\;z_i}\;-\;f(z_i)\;=\;\int_{z_i}^{z_f} dz\left[\,\frac{f(z)\;-\;f(z_i)}{z_f\;-\;z_i}\,\right] \tag{1481}$$

In the limit $z_f \rightarrow z_i$ the righthand side goes to zero as $f(z)$ is continuous. Hence, the left hand side is equal to zero. Thus,

$$\lim_{z_f \rightarrow z_i} \frac{F(z_f) - F(z_i)}{z_f - z_i} - f(z_i) = 0 \tag{1482}$$

and

$$\lim_{z_f \rightarrow z_i} \frac{F(z_f) - F(z_i)}{z_f - z_i} = \frac{dF(z)}{dz}\bigg|_{z_i} = f(z_i) \tag{1483}$$

Since $F(z)$ is analytic, then Cauchy's integral formula for the derivatives shows that all the derivatives of $F(z)$ are analytic, in particular the first derivative $f(z)$ is also analytic.

Cauchy's Inequality

If one has a Taylor series expansion of $f(z)$

$$f(z) = \sum_n C_n \, z^n \tag{1484}$$

and the function is bounded such that

$$| \, f(z) \, | < M \tag{1485}$$

for all values of z within a radius r from the origin and where M is a positive constant, then Cauchy's inequality provides an upper bound on the coefficients

$$| \, C_n \, | \, r^n < M \tag{1486}$$

This can be proved using the Cauchy integral

$$C_n = \frac{1}{2 \pi i} \oint_{|z|=r} dz \, \frac{f(z)}{z^{n+1}} \tag{1487}$$

since only the term proportional to z^{-1} gives a finite contribution to the integral. Then

$$| \, C_n \, | = \frac{1}{2 \pi} \left| \oint_{|z|=r} dz \, \frac{f(z)}{z^{n+1}} \right| < M \, \frac{2 \pi r}{2 \pi r^{n+1}} \tag{1488}$$

which leads to the inequality

$$| \, C_n \, | \, r^n < M \tag{1489}$$

Liouville's Theorem

Liouville's theorem states that if $f(z)$ is analytic and bounded in the complex plane then $f(z)$ is a constant.

This is easily proved by using the Cauchy inequality.

$$| \ C_n \ | \ < \ \frac{M}{r^n} \tag{1490}$$

and let $r \rightarrow \ \infty$ be an arbitrarily large radius in the complex plane. Then for $n \ > \ 0$ one has

$$C_n \ = \ 0 \tag{1491}$$

Hence, the only non-zero coefficient is C_0 and the function is just a constant.

Conversely, if the function deviates from a constant the function must have a singularity somewhere in the complex plane. In the next section we shall consider properties of more general functions of a complex variable z

14 Complex Functions

We shall first examine the properties of a function that is analytic throughout a simply connected region.

14.1 Taylor Series

Consider a function that is analytic in a simply connected region containing two point z and z_0. Then Cauchy's integral formula at the point z yields

$$f(z) \; = \; \frac{1}{2 \, \pi \, i} \oint_C dz' \, \frac{f(z')}{z' \, - \, z} \tag{1492}$$

The contour C has to enclose z and we choose it such that it also encloses z_0. Then on writing

$$f(z) \; = \; \frac{1}{2 \, \pi \, i} \oint_C dz' \, \frac{f(z')}{(\, z' \, - \, z_0 \,) \, - \, (\, z \, - \, z_0 \,)} \tag{1493}$$

The denominator may be expanded in powers of $(\, z \, - \, z_0 \,)$ if the contour is such that for all points z' we have $| \, z \, - \, z_0 \, | \, < \, | \, z' \, - \, z_0 \, |$. In this case the series may be expected to converge. From this one finds the Taylor series expansion

$$\begin{aligned} f(z) \; &= \; \frac{1}{2 \, \pi \, i} \oint_C dz' \, \sum_{n=0}^{\infty} \frac{f(z')}{(\, z' \, - \, z_0 \,)^{n+1}} \, (\, z \, - \, z_0 \,)^n \\ &= \; \sum_{n=0}^{\infty} \frac{1}{n!} \, \frac{d^n f(z_0)}{dz_0^n} \, (\, z \, - \, z_0 \,)^n \end{aligned} \tag{1494}$$

where Cauchy's integral formula for the n-th order derivative has been used. If $f(z)$ is analytic at z_0 the Taylor expansion exists and is convergent for z sufficiently close to z_0.

Schwartz Reflection

The Schwartz reflection principle states that if a function $f(z)$ is analytic over a region that contains the real axis, and $f(z)$ is real when z is real, i.e, $z \, = \, x$, then

$$f(z^*) \; = \; f^*(z) \tag{1495}$$

That is, in this case the complex conjugate of the function of z is a function of the complex conjugate variable z^*.

The Schwartz reflection principle can be proved by using the Taylor expansion about some point x_0 on the real axis. Then

$$f(z) \; = \; \sum_{n=0} \frac{1}{n!} \; (\; z \; - \; x_0 \;)^n \; \frac{d^n f(x_0)}{dx_0^n} \tag{1496}$$

Since $f(x)$ is real on the real axis, then so are all the derivatives. Hence,

$$\begin{aligned} f^*(z) \; &= \; \sum_{n=0} \frac{1}{n!} \left((\; z \; - \; x_0 \;)^n \right)^* \frac{d^n f(x_0)}{dx_0^n} \\ &= \; \sum_{n=0} \frac{1}{n!} \; (\; z^* \; - \; x_0 \;)^n \; \frac{d^n f(x_0)}{dx_0^n} \\ &= \; f(z_0^*) \end{aligned} \tag{1497}$$

where the last line is obtained by identifying the Taylor expansion as $f(z)$ with the replacement $z \; = \; z^*$.

14.2 Analytic Continuation

If two functions $f_1(z)$ and $f_2(z)$ are analytic in a region R and agree in a smaller region R' that is contained in R, then the functions are equal everywhere in R. This allows the function $f_1(z)$ which is only known explicitly in some smaller region to be found in a much larger region.

A function $f(z)$ may be analytic in some region of space, around a point z_0. The region, by definition does not include the closest singularity, which may be at z_s. In the region around z_0 the function may be Taylor expanded, however it can not be expanded for values of $| \; z \; - \; z_0 \; |$ which are larger than $| \; z_s \; - \; z_0 \; |$ since the contour C involved in the proof of Taylors theorem must encloses a point z' which is nearer to z_0 than the singularity at z_s. That is there is a radius of convergence which is given by the distance from z_0 to the closest singularity z_s.

However, since $f(z)$ is analytic inside the radius of convergence we may choose to Taylor expand about another point, z_2 inside the radius of convergence of the expansion about z_0. The point z_2 can be chosen to be further from the singularity than z_0 is. Hence, the expansion about z_2 may have a larger radius of convergence.

Thus we have a region in which the both Taylor series converge, and yield the function. However, the second expansion defines the function at points which lie outside the original circle of convergence. Thus, the function $f(z)$ has been expressed as an analytic function in a region that contains points not included in the original circle. Thus, the analytic properties of the function has been continued into a different region of the complex plane.

This process is known as analytic continuation and may be repeated many times.

It should be noted that analytic continuation can take many different forms and is not restricted to series expansion.

Example:

Consider the function

$$f(z) \ = \ \frac{1}{z \ + \ 1} \tag{1498}$$

which can be expanded around $z_0 \ = \ 0$ as

$$f(z) \ = \ \sum_{n=0}^{\infty} (\ - \ 1 \ )^n \ z^n \tag{1499}$$

and the radius of convergence is determined by the distance to the nearest singularity, which is at $z_s \ = \ - \ 1$. The radius of convergence of the expansion about $z_0 \ = \ 0$ is unity. The Taylor expansion converges for all the points inside the unit circle.

This function can be analytically continued, by expanding about any other point inside the circle of radius 1 from the origin.

Let us first choose to expand about the new point $z_2 = \ + \ 1$. The function can be expanded about $z_2 \ = \ 1$ by writing

$$f(z) \ = \ \frac{1}{2 \ + \ (\ z \ - \ 1 \ )} \tag{1500}$$

The series is found as

$$f(z) \ = \ \sum_{n=0}^{\infty} (\ - \ 1 \ )^n \ (\ z \ - \ 1 \ )^n \ \frac{1}{2^{n+1}} \tag{1501}$$

and has a radius of convergence determined by the distance to the closest singularity which is at $z_s \ = \ -1$, so the radius of convergence is 2. Thus, the analytic properties of the function been extended to a circle of radius 2. The new circle of convergence includes the point $z \ = \ 3$. We can now iterate the process, an define the function over the whole positive real axis.

Alternatively, one may wish to examine the function on the negative real axis, or some other region. In this case, one might choose another point inside the original circle of convergence, say $z_2 = i$. The expansion about this point is expanded about $z_2 = 1$ via

$$f(z) = \frac{1}{1 + i + (z - i)} \tag{1502}$$

as

$$f(z) = \sum_{n=0}^{\infty} (- 1)^n (z - i)^n \frac{1}{(1 + i)^{n+1}} \tag{1503}$$

which has a radius of convergence determined by the distance to the closest singularity which is at $z_s = -1$. The series converges within the region

$$| z - i | < | 1 + i | = | z_s - i | = \sqrt{2} \tag{1504}$$

so the radius of convergence is $\sqrt{2}$. By choosing a suitable series of overlapping circles, one can analytically continue the function to the negative real axis, but the circles always have to exclude the point $z = - 1$.

It should be noted that a function $f(z)$ may have more than one singularity, in which case the circle of convergence for an expansion about some point is limited by the closest singularity.

Example:

A function that can not be analytic continued is given by the Taylor expansion about $z = 0$, of the function

$$\begin{aligned} f(z) &= 1 + \sum_{n=0}^{\infty} z^{2^n} \\ &= 1 + z^2 + z^4 + z^8 + z^{16} + \ldots \end{aligned} \tag{1505}$$

It can be seen that the function satisfies the relation

$$f(z) = z^2 + f(z^2) \tag{1506}$$

Furthermore, at the point $z = 1$ one has

$$f(1) = 1 + f(1) \tag{1507}$$

which makes $f(z)$ singular at $z = 1$. Furthermore, since

$$f(z) = z^2 + f(z^2) \tag{1508}$$

and the term $f(z^2)$ on the right hand side is singular when $z^2 = 1$, one finds that $f(z)$ is singular at all the roots of $z^2 = 1$. This process can be iterated to show that $f(z)$ is singular at all the roots of $z^{2^m} = 1$ for each integer value of m. There are 2^m such singularities for each integer value of m and the singularities are uniformly distributed on the unit circle. The singularities corresponding to $m \rightarrow \infty$ are separated by infinitesimally small distances. Hence, the radius of convergence for z values on the unit circle is infinitesimally small. Thus, it is impossible to analytically continue the function $f(z)$ outside the unit circle.

14.3 Laurent Series

Some functions are analytic in a finite area but is not analytic in some inner region. That is the area of analyticity may not be simply connected. For example, one may have

$$f(z) = \frac{R_0}{z - z_0} + 2 + z^2 + \ldots \tag{1509}$$

in which case one can not obtain a simple Taylor series expansion about the point z_0.

More generally, the function may be analytic inside a ring shaped area of inner radius r and outer radius R, where $R > r$. The the area is not simply connected. It is possible to introduce a line which cuts the plane making it into a simply connected region. A particular line can be chosen which runs from a point on the inner perimeter to a point on the outer perimeter. Since the area is now simply connected one can apply Cauchy's integral formula to any contour in the annular region which does not cross the cut we have chosen. In particular let us choose a contour that consists of two circular segments which are concentric, the center of the circles is denoted as the point z_0. The radius of the circles r_1 and r_2 are such that $R > r_1 > r_2 > r$. The contour is completed by anti-parallel paths running along opposite sides of the cut.

For any point z inside the singly connected region where $f(z)$ is analytic one has

$$f(z) = \frac{1}{2 \pi i} \oint_{C_1} dz' \frac{f(z')}{z' - z} + \frac{1}{2 \pi i} \oint_{C_2} dz' \frac{f(z')}{z' - z} \tag{1510}$$

where the first circular contour is traversed in the counter clockwise direction and the second contour is traversed in the counterclockwise direction. The contribution from the oppositely directed paths along a segment of the cut has cancelled, since our function is analytic and single valued in the entire annular region. That is the function $f(z)$ has the same value at points immediately adjacent to the cut.

The denominator in both of the integrands of the above expression can be written as

$$z' \; - \; z \; = \; (\; z' \; - \; z_0 \;) \; - \; (\; z \; - \; z_0 \;) \tag{1511}$$

and can be expanded. However, it is important to note that for C_1 one has

$$| \; z' \; - \; z_0 \; | \; = \; r_1 \; > \; | \; z \; - \; z_0 \; | \tag{1512}$$

while for the Contour C_2 one has

$$| \; z \; - \; z_0 \; | \; > \; | \; z' \; - \; z_0 \; | \; = \; r_2 \tag{1513}$$

This has the consequence the expansion on contour C_1 only converges if it consists of a power series in

$$\left(\frac{z \; - \; z_0}{z' \; - \; z_0} \right) \tag{1514}$$

whereas the expansion on contour C_2 is in powers of

$$\left(\frac{z' \; - \; z_0}{z \; - \; z_0} \right) \tag{1515}$$

Hence we have,

$$\begin{aligned} f(z) \; &= \; \frac{1}{2 \; \pi \; i} \; \sum_{n=0}^{\infty} \; \oint_{C_1} \; dz' \; f(z') \; \frac{(\; z \; - \; z_0 \;)^n}{(\; z' \; - \; z_0 \;)^{n+1}} \\ &- \; \frac{1}{2 \; \pi \; i} \; \sum_{n=0}^{\infty} \; \oint_{C_2} \; dz' \; f(z') \; \frac{(\; z' \; - \; z_0 \;)^n}{(\; z \; - \; z_0 \;)^{n+1}} \\ &= \; \sum_{n=}^{\infty} \; A_n \; (\; z \; - \; z_0 \;)^n \; + \; \sum_{n=0}^{\infty} \; \frac{B_n}{(\; z \; - \; z_0 \;)^{n+1}} \end{aligned} \tag{1516}$$

where

$$A_n \; = \; \frac{1}{2 \; \pi \; i} \oint_{C_1} \; dz' \; \frac{f(z')}{(\; z' - \; z_0 \;)^{n+1}} \tag{1517}$$

in which the contour C_1 runs clockwise. One can define

$$B_{n-1} \; = \; A_{-n} \tag{1518}$$

and have A_{-n} given by

$$A_{-n} \; = \; - \; \frac{1}{2 \; \pi \; i} \oint_{C_2} \; dz' \; f(z') \; (\; z' - \; z_0 \;)^{n-1} \tag{1519}$$

and the contour C_2 runs clockwise. Thus, we have the Laurent expansion of the function

$$f(z) = \sum_{n=-\infty}^{\infty} A_n \, (\, z \, - \, z_0 \,)^n \tag{1520}$$

Example:

The function

$$f(z) = \frac{1}{z \, (\, z \, - \, 1 \,)} \tag{1521}$$

has a Laurent series expansion about $z = 0$. The simplest method of obtaining the expansion consists of expressing the function in partial fractions and then expanding about $z = 0$

$$\begin{aligned} f(z) &= \frac{1}{z \, - \, 1} - \frac{1}{z} \\ &= - \frac{1}{z} - \sum_{n=0}^{\infty} z^n \end{aligned} \tag{1522}$$

Hence, the non zero coefficients are A_{-1} and A_n for $n \geq 0$ and are all unity.

$$A_{-1} = A_0 = A_1 = \ldots = 1 \tag{1523}$$

The Laurent series differs from the Taylor series due to the occurrence of negative powers of $(\, z \, - \, z_0 \,)$, which makes the series diverge at $z = z_0$.

Example:

The Fermi-Dirac distribution function of Statistical Mechanics has the form

$$f(z) = \frac{1}{\exp[z] \, - \, 1} \tag{1524}$$

find the Laurent expansion about $z = 0$.

14.4 Branch Points and Branch Cuts

In the above analysis, the functions $f(z)$ were single valued. That is they have a unique value at each point in the complex plane. This is ensured by the function only having positive or negative integral powers in the Laurent or Taylor expansions. Certain functions of a complex variable are multi-valued, in that more than one value of $f(z)$ is assigned to each point in the complex plane.

As a primitive example, consider the function

$$f(z) \;=\; z^{\frac{1}{m}} \tag{1525}$$

for integer m. What this equation actually means is that $f(z)$ is described by the solutions of

$$\left(\, f(z) \, \right)^m \;=\; z \tag{1526}$$

The solutions are found by expressing the complex number z in polar form

$$z \;=\; r_z \, \exp \left[\, i \, \theta_z \, \right] \tag{1527}$$

and the solution are found in the same form

$$f(z) \;=\; r_f \, \exp \left[\, i \, \theta_f \, \right] \tag{1528}$$

This leads to the relation between the positive magnitudes

$$r_f^m \;=\; r_z \tag{1529}$$

which has a unique solution

$$r_f \;=\; r_z^{\frac{1}{m}} \tag{1530}$$

However, the phases are not uniquely defined. They are only defined up to a multiple of $2 \, \pi$. Hence, on equating the phases one has

$$m \, \theta_f \;=\; \theta_z \;+\; 2 \, \pi \, n \tag{1531}$$

where n is an undetermined positive or negative integer. From this we see that the function is given by

$$f(z) \;=\; r_z^{\frac{1}{m}} \, \exp \left[\, i \, \frac{\theta_z}{m} \, \right] \, \exp \left[\, i \, \frac{2 \, \pi \, n}{m} \, \right] \tag{1532}$$

which involves the undetermined integer n. Hence, there exists more than one solution. One can see that there are m different solutions corresponding to $n \;=\; 0$ and every integer up to and including $n \;=\; m \;-\; 1$. These solutions form m equally spaced points on a circle of radius $r_z^{\frac{1}{m}}$ in the complex z plane. Thus, the function $z^{\frac{1}{m}}$ is multi-valued.

In general a function such as z^α, where α is either an arbitrary rational or irrational number, the function is expected to be multi-valued.

The function $z^{\frac{1}{m}}$ has m different values, but on changing z continuously each of the values change continuously. That is, the function has m branches which are continuous in z. Each branch can be considered to define a single valued function, as long as two branches do not give the same value at one point. However, we see that if z traverses a contour wrapping around the origin exactly once, then θ_z increases by exactly $2\,\pi$, and one branch merges with the next as the phase of $f(z)$ has increased by $\frac{2\,\pi}{m}$. In this case, the origin is a branch point of the function.

The function can be converted into a single valued function by introducing a branch cut and agreeing that the contour shall not cross the branch cut. However, it should be noted that the function does not have the same value on either side of the branch cut, as the phases are different by $\pm\,\frac{2\,\pi}{m}$.

Since a function is not single valued on any contour that wraps around $z\;=\;0$, the branch cut is chosen to start at the branch point $z\;=\;0$ and runs to infinity, where the function is not analytic. For convenience we might choose the cut to run along the positive real axis. In any case, once a branch cut has been chosen θ_z is restricted to be greater than 0 and less than $2\,\pi$ so there should be no confusion as to which value of the function belongs to which branch. With this convention, each of the branches define singly valued functions. Again, it should be stressed that the function does not have the same value on both sides of the branch cut as the phases are different.

If the contour where chosen to cross the branch cut, the function would be identified with the value on the next branch etc. In this case, one could define the complex plane to consist of several copies, (in which the phase of z is advanced by $2\,\pi$ between otherwise identical points in successive copies). The function in this enlarged complex plane is single valued.this manner of extending the complex plane to different phases, is akin to cutting identical sheets representing the complex plane, and joining the edge of the cut adjoining the lower half complex plane of one sheet to the edge of the cut adjoining the upper half complex plane of the next sheet. Thus, one has a spiral of continuously connected copies of the complex plane. The function $z^{\frac{1}{m}}$ is single valued on this spiral sheet, and also repeats after m sheets have been crossed. The m-th sheet is identified with the zeroth sheet, and this construct is the Riemann surface of $z^{\frac{1}{m}}$. The Riemann surface consists of m sheets.

If a contour is chosen to wind around the origin by $2\,\pi$ then, starting with the phase given by $n\;=\;0$, one has

$$\begin{aligned}
\oint_c dz\; z^{\frac{1}{m}} \;&=\; i\; r^{\frac{m+1}{m}} \int_0^{2\pi} d\theta\; \exp\left[\; i\; \frac{(\;m\;+\;1\;)}{m}\;\theta\;\right] \\
&=\; r^{\frac{m+1}{m}}\; \frac{m}{m\;+\;1} \left(\; \exp\left[\; i\; \frac{2\;\pi}{m}\;\right]\;-\;1\;\right)
\end{aligned}$$

$$= \quad z^{\frac{1}{m}} \, r \, \frac{m}{m \, + \, 1} \left(\exp \left[\, i \, \frac{2 \, \pi}{m} \, \right] \, - \, 1 \right) \tag{1533}$$

This integral is non zero if $m \neq 1$ and is zero when $m = 1$ for which the function is single valued. The multi-valued nature of functions can make Cauchy's theorem inapplicable.

Example:

Another important example is given by

$$f(z) \; = \; \ln z \tag{1534}$$

or in polar coordinates

$$f(z) \; = \; \ln \, r \; + \; i \, \theta \tag{1535}$$

Thus, $\ln z$ is infinitely multi-valued. Furthermore, it is the multi-valued nature of $\ln z$ that makes the integral

$$\oint \frac{dz}{z} \; = \; \ln z \, \Bigg| \; = \; 2 \, \pi \, i \tag{1536}$$

when integrating around a contour circling about the origin once.

Example:

The function

$$f(z) \; = \; (\, z^2 \, - \, 1 \,)^{\frac{1}{2}} \tag{1537}$$

can be factorized as

$$f(z) \; = \; (\, z \, - \, 1 \,)^{\frac{1}{2}} \, (\, z \, + \, 1 \,)^{\frac{1}{2}} \tag{1538}$$

The first factor has a branch point at $z = 1$ and the second factor has a branch point at $z = - 1$. The branch cut has to connect the two branch points. For convenience one can represent

$$z \, - \, 1 \; = \; r_1 \, \exp \left[\, i \, \varphi_1 \, \right] \tag{1539}$$

and

$$z \, + \, 1 \; = \; r_2 \, \exp \left[\, i \, \varphi_2 \, \right] \tag{1540}$$

Then the phase of $f(z)$ is given by

$$\frac{1}{2} \, (\, \varphi_1 \, + \, \varphi_2 \,) \tag{1541}$$

The introduction of the branch cut makes the function single valued. Consider a contour starting at $+ 1$ running down to $- 1$ in the upper half complex plane and returning to $+ 1$ below in the lower half complex plane just below the branch cut.

As the contour rotates around the branch point $+ 1$ the phase φ_1 changes from 0 to π while $\varphi_2 = 0$. As the contour rounds the branch point $- 1$, the phase φ_2 changes by 2π. Secondly, as the contour returns to the point $+ 1$ and circles around it back to the start φ_1 changes from π to 2π. In this loop the total phase changes by 2π, hence, the function is single valued.

14.5 Singularities

An point z_0 where a function is not analytic or single valued, but is analytical at all neighboring points is known as an isolated singularity. In this case one can draw a contour around the singularity on which the function only has no other singularity within it. The Laurent expansion yields a series which exhibits isolated singularities.

A function that is analytic in the entire complex plane except at isolated singularities is known as a meromorphic function. Examples of meromorphic functions are given by entire functions, (as they have no singularities in the finite complex plane), functions which are ratios of polynomials (as they only have isolated singularities) and functions like $\tan z$ and

$$f(z) = \frac{1}{\exp[z] - 1} \tag{1542}$$

This function has isolated singularities at

$$z = i \, 2 \, \pi \, n \tag{1543}$$

for integer n.

Poles

In the Laurent expansion one has

$$f(z) = \sum_{n=-\infty}^{\infty} a_n \, (\, z - z_0 \,)^n \tag{1544}$$

Let the highest negative order for which the coefficient is non zero be $- n$. That is $a_{-n} \neq 0$, and the higher order terms a_{-m} are zero for $- n > - m$. In this case one has a pole of order n. In this case, one has

$$f(z) \; = \; \frac{a_n}{(\; z \; - \; z_0 \;)^n} + \frac{a_{n-1}}{(\; z \; - \; z_0 \;)^{n-1}} + \ldots + a_0 + a_1 \, (\; z - z_0 \;) + \ldots \quad (1545)$$

A pole of order one is called a simple pole. It should be noted that the function is single valued on a contour going round a pole, as it does return to its original value after it has completed the contour, and $f(z)$ varies continuously on the contour.

Example:

The function

$$f(z) \; = \; \frac{\sin z}{z^6} \quad (1546)$$

has a pole of order 5 as

$$\sin z \; = \; \sum_{n=0}^{\infty} (\; - \; 1 \;)^n \, \frac{z^{2n+1}}{(\; 2 \; n \; + \; 1 \;)!} \quad (1547)$$

so

$$\frac{\sin z}{z^6} \; = \; \sum_{n=0}^{\infty} (\; - \; 1 \;)^n \, \frac{z^{2n-5}}{(\; 2 \; n \; + \; 1 \;)!} \quad (1548)$$

which leads to a pole of order 5.

Essential Singularities

If the Laurent expansion has terms of negative orders running up to $- \, \infty$ then the function has an essential singularity. The behavior of a function near an essential singularity is pathological.

Example:

The function

$$f(z) \; = \; \exp \left[\; \frac{1}{z} \; \right] \quad (1549)$$

has an essential singularity at $z \; = \; 0$. The function has the expansion

$$f(z) \; = \; \sum_{n=0} \frac{1}{n!} \left(\frac{1}{z} \right)^n \quad (1550)$$

which contains terms of arbitrarily high negative orders. The pathological behavior of this function is seen by examining how the function varies as z tends to zero. If z approaches zero from the positive axis then $f(z)$ tends to infinity, on the other hand if z tends to zero along the negative real axis, then $f(z)$ tends to zero. In fact by choosing an arbitrary path to the point $z = 0$ one can have $lim_{z \rightarrow 0} \, f(z) = b$ for any complex b. For example, on inverting the equation one can find solutions

$$z = \frac{1}{2 \, \pi \, i \, n \, + \ln \, b} \tag{1551}$$

where n are integers, as n approaches to infinity z approaches zero, while the function remains equal to b.

Branch Points

A point z_0 is a branch point of a function if, when z moves around the point z_0 on a contour of small but non-zero radius, the function does not return to its original value on completing the contour. It is assumed that $f(z)$ varies continuously on the contour.

Example:

The function

$$f(z) = \sqrt{z^2 - a^2} \tag{1552}$$

has branch points at $z = \pm \, a$. The function does not return to the same value if the contour warps around one pole once, say $z = a$, but does return to the same value if the contour encloses both branch points.

Singularities at Infinity

If one makes the transformation

$$z = \frac{1}{\xi} \tag{1553}$$

and

$$f(z) = g(\xi) \tag{1554}$$

then, if the function $g(\xi)$ has a singularity at $\xi = 0$ the function has a singularity at infinity.

Example:

The function

$$f(z) = \sin z \tag{1555}$$

has an essential singularity at infinity since

$$g(\xi) = \sin \frac{1}{\xi}$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^{2n+1}}{(2n+1)!} \frac{1}{\xi^{(2n+1)}} \tag{1556}$$

has terms of all negative orders.

15 Calculus of Residues

15.1 Residue Theorem

If a function $f(z)$ which has a Laurent expansion

$$f(z) \; = \; \sum_{n=-\infty}^{n=\infty} A_n \; (\; z \; - \; z_0 \;)^n \tag{1557}$$

then if $f(z)$ is integrated around a counterclockwise contour that only encloses the isolated singularity at z_0 one has

$$\frac{1}{2 \; \pi \; i} \oint_c dz \; f(z) \; = \; A_{-1} \tag{1558}$$

where A_{-1} is the coefficient of $(\; z \; - \; z_0 \;)^{-1}$ in the Laurent expansion is known as the residue of $f(z)$ at the pole z_0. We shall denote the residue at the polez_0 by $R(z_0)$.

The residue theorem states that the integral of a function around a contour C that only encloses a set of isolated singularities, then the integral

$$\frac{1}{2 \; \pi \; i} \oint_C dz \; f(z) \; = \; \sum_n \; R(z_n) \tag{1559}$$

is just the sum of the residues of the enclosed poles.

The Residue Theorem can be proved by using Cauchy's theorem on the counterclockwise contour C supplemented by segments C_n that run from C to the isolated poles and circle them in the opposite sense of rotation. The straight-line portion of the segments C_n cancel in pairs, leaving only the contributions circling the poles in the opposite sense of rotation. The circular integral around any singularity C_n can be evaluated on an infinitesimal circle around the pole, leading to the result $- \; R(z_n)$. The negative sign occurs, because we have evaluated the integral on a clockwise contour. Hence, Cauchy's theorem leads to

$$\frac{1}{2 \; \pi \; i} \oint_C dz \; f(z) \; - \; \sum_n \; R(z_n) \; = \; 0 \tag{1560}$$

Thus, the problem of evaluating the contour integral is reduced to an algebraic problem of summing the residues.

Example:

Evaluate the integral

$$\int_{-\infty}^{\infty} dx \; \frac{\Gamma}{x^2 \; + \; \Gamma^2} \tag{1561}$$

This can be evaluated by decomposing the integrand as partial fractions

$$f(x) \;=\; \frac{\Gamma}{x^2 \;+\; \Gamma^2} \;=\; \frac{1}{2\,i} \left[\frac{1}{x \;-\; i\,\Gamma} \;-\; \frac{1}{x \;+\; i\,\Gamma} \right] \tag{1562}$$

which shows the poles at $x \;=\; \pm\, i\,\Gamma$ with residues $\mp\,\frac{1}{2}\,i$.

The contour integral can be evaluated by closing the contour on a semi-circle at infinity in either the upper or lower half complex plane. The contribution from the semi-circular contour at infinity vanishes since if

$$z \;=\; R\,\exp\left[\,i\,\theta\,\right] \tag{1563}$$

then

$$\lim_{R\,\rightarrow\,\infty} \;|\,f(z)\,| \;\sim\; \frac{\Gamma}{R^2} \;\rightarrow\; 0 \tag{1564}$$

Hence, the contour at infinity is given by

$$R\,\int_0^\pi \,d\theta\;|\,f(z)\,| \;\sim\; \pi\,\frac{\Gamma}{R} \tag{1565}$$

which tends to zero as $R\;\rightarrow\;\infty$.

One completing the contour in the upper half complex plane one encloses the pole at $z \;=\; i\,\Gamma$ in a counter clockwise sense and obtains the final result

$$\int_{-\infty}^{\infty} dx\;\frac{\Gamma}{x^2 \;+\; \Gamma^2} \;=\; \frac{2\,\pi\,i}{2\,i}\;1 \;=\; \pi \tag{1566}$$

If the contour had been evaluated in the lower half plane, the contour would enclose the pole at $z \;=\; -\,i\,\Gamma$ in a clockwise sense, since the residue at this pole is negative, and the clockwise contour produces another negative sign, we obtain the same result.

15.2 Jordan's Lemma

Consider the integral on an open curve C_R consisting of the semi-circle of radius R in the upper half complex plane. The semi-circle is centered on the origin. Let the function $f(z)$ be a function that tends to zero as $\frac{M}{|\,z\,|}$ as $|\,z\,|\;\rightarrow\;\infty$, then

$$\lim_{R\,\rightarrow\,\infty}\;\frac{1}{2\,\pi\,i}\;\oint_{C_R} dz\;\exp\left[\,i\,k\,z\,\right]\;f(z)\;\rightarrow\;0 \tag{1567}$$

where k is a positive number.

Proof

On the contour one has

$$z \; = \; R \; \exp \left[\; i \; \theta \; \right] \tag{1568}$$

so the integral can be expressed as

$$\begin{aligned} & \left| \; \frac{1}{2 \; \pi \; i} \; \oint_{C_R} \; dz \; \exp \left[\; i \; k \; z \; \right] \; f(z) \right| \\ = & \; \frac{R}{2 \; \pi} \; \left| \; \int_0^\pi \; d\theta \; \exp \left[\; - \; k \; R \; \sin \theta \; + \; i \; k \; R \; \cos \theta \; \right] \; f(R \; \exp[\; i \; \theta \;]) \; \right| \\ < & \; \frac{R}{2 \; \pi} \; \int_0^\pi \; d\theta \; \exp \left[\; - \; k \; R \; \sin \theta \; \right] \; \left| \; f(R \; \exp[\; i \; \theta \;]) \; \right| \\ < & \; \frac{R}{2 \; \pi} \; \int_0^\pi \; d\theta \; \exp \left[\; - \; k \; R \; \frac{2}{\pi} \; \theta \; \right] \; \left| \; f(R \; \exp[\; i \; \theta \;]) \; \right| \\ < & \; \frac{M}{2 \; \pi \; k \; R} \; \left(\; 1 \; - \; \exp \left[\; - \; k \; R \; \right] \; \right) \end{aligned} \tag{1569}$$

which tends to zero as $R \; \rightarrow \; \infty$.

It should be noted that any attempt to evaluate the integration on a semi-circle in the lower complex plane may diverge if k is positive. Likewise, if k is a negative number the integration may diverge if evaluated on a semi-circle in the upper half complex plane of radius infinity, but will tend to zero on the semi-circle in the lower half complex plane.

15.3 Cauchy's Principal Value

The Principal Value of an integral of a function $f(x)$ which has only one simple pole at x_0 on the real axis, is defined as

$$\mathrm{Pr} \; \int_{-\infty}^{+\infty} \; dx \; f(x) \; = \; \lim_{\varepsilon \to 0} \; \int_{-\infty}^{x_0 - \varepsilon} \; dx \; f(x) \; + \; \int_{x_0 + \varepsilon}^{\infty} \; dx \; f(x) \tag{1570}$$

The integral is independent of ε since the contributions to the integral within ε of the pole are of the order of the residue and have opposite sign. Furthermore, as the intervals are symmetrically located about the pole the contributions cancel to order ε.

Integrals of this kind can often be evaluated using contour integration.

For example, if the function only has simple poles in the upper half complex plane and can be evaluated on the semi-circle C_R at infinity in the upper half complex plane. The principal value integral can be evaluated by integrating over a contour that runs from $- \infty$ to $(x_0 - \varepsilon)$ then follows a small semi-circle of radius ε around the pole at x_0, joins the real axis at $(x_0 + \varepsilon)$ then follows the real axis to $+ \infty$ and then completes the contour by following a semi-circle of infinite radius ($R \rightarrow \infty$) in the upper half complex plane.

Then the principal value integral and the integral over the small semi-circle of radius ε around x_0 is equal to $2 \pi i$ times the sum of the residues enclosed by the contour.

For example, if $f(z)$ is analytic in the upper half complex plane on the semi-circle at infinity in the upper half complex plane we have

$$\mathrm{Pr} \int_{-\infty}^{+\infty} dx \, \frac{f(x)}{x - x_0} + \oint_{C_R} dz \, \frac{f(z)}{z - x_0} = i \, \pi \, f(x_0) \tag{1571}$$

It does not matter if the semi-circle of radius ε is taken to be in the upper half complex plane or the lower half complex plane.

If the small semi-circle is chosen in the lower half complex plane the integral runs counter clockwise and runs half way around the pole, and contributes $\pi \, i \, f(x_0)$ to the left hand side, but the right hand side has the contribution of $2 \, \pi \, f(x_0)$ as the pole at x_0 is enclosed by the contour.

On the other hand if the contour is closed in the upper half complex plane, the semi-circle is in the clockwise direction and contributes $- \pi \, i \, f(x_0)$ to the left hand side and the right hand side is zero, as the pole at x_0 is not enclosed by the contour.

Example:

Consider the integral

$$I = \int_0^{\infty} dx \, \frac{\sin x}{x} \tag{1572}$$

this is evaluated as

$$\begin{aligned} I &= \frac{1}{2 \, i} \int_0^{\infty} dx \, \frac{\exp[+ i \, x] - \exp[- i \, x]}{x} \\ &= \frac{1}{2 \, i} \, \mathrm{Pr} \int_{-\infty}^{+\infty} dx \, \frac{\exp[\, i \, x \,]}{x} \end{aligned} \tag{1573}$$

However, on using Jordan's Lemma and the Cauchy Principal value formula one has

$$\Pr \int_{-\infty}^{+\infty} dx \, \frac{\exp[\, i \, x \,]}{x} \; = \; i \, \pi \; \exp[\, 0 \,] \; = \; i \, \pi \tag{1574}$$

Hence, we have shown that

$$I \; = \; \int_0^\infty dx \, \frac{\sin x}{x} \; = \; \frac{\pi}{2} \tag{1575}$$

An alternate method of evaluating a Cauchy Principal integral consists of deforming the contour. The contour is deformed to lie ε above the real axis. In this case, the integral becomes

$$\int_{-\infty}^{+\infty} dx \, \frac{f(x + i\varepsilon)}{x \; + \; i \, \varepsilon \; - \; x_0} \tag{1576}$$

on changing variable from x to z one has

$$\int_{-\infty}^{+\infty} dz \, \frac{f(z + i\varepsilon)}{z \; - \; x_0 \; + \; i \, \varepsilon} \; = \; \int_{-\infty}^{+\infty} dz \, \frac{f(z)}{z \; - \; x_0 \; + \; i \, \varepsilon} \tag{1577}$$

since $f(z)$ is continuous at all points on the contour.

This is equivalent to the principal value integral and the small semi-circle, or

$$\Pr \int_{-\infty}^{+\infty} dx \, \frac{f(z)}{z \; - \; x_0} \; - \; i \, \pi \, f(x_0) \tag{1578}$$

Hence, we have

$$\int_{-\infty}^{+\infty} dz \, \frac{f(z)}{z \; - \; x_0 \; + \; i \, \varepsilon} \; = \; \Pr \int_{-\infty}^{+\infty} dz \, \frac{f(z)}{z \; - \; x_0} \; - \; i \, \pi \, f(x_0) \tag{1579}$$

which yields the identity

$$\lim_{\varepsilon \to 0} \frac{1}{z \; - \; x_0 \; + \; i \, \varepsilon} = \; \Pr \frac{1}{z \; - \; x_0} \; - \; i \, \pi \, \delta(\, z \; - \; x_0 \,) \tag{1580}$$

The truth of this result can also be seen by writing

$$\frac{1}{z \; - \; x_0 \; + \; i \, \varepsilon} = \; \frac{z \; - \; x_0}{(\, z \; - \; x_0 \,)^2 \; + \; \varepsilon^2} \; - \; i \, \frac{\varepsilon}{(\, z \; - \; x_0 \,)^2 \; + \; \varepsilon^2} \tag{1581}$$

in which the first term on the right not only does not diverge at $z \; = \; x_0$ but is zero. This term cuts off at a distance ε from the pole, and thus corresponds to the Principal value. The second term on the right is a Lorentzian of width ε

centered at x_0. As the integrated weight is π, this represents the delta function term in the limit $\varepsilon \to 0$.

Example:

Evaluate the function

$$\Theta(k) = \frac{1}{2 \pi i} \int_{-\infty}^{+\infty} \frac{\exp \left[i k x \right]}{x - i \varepsilon} \tag{1582}$$

where $\varepsilon > 0$.

For $k > 0$ the integral can be evaluated by completing the contour in the upper half complex plane as the semi-circle at infinity vanishes, whereas for $k < 0$ the contour can be completed in the lower half complex plane. If $k > 0$ we close the contour in the upper half complex plane, and the integral encloses the pole at $z = i\varepsilon$. Hence, we have

$$\frac{1}{2 \pi i} \int_{-\infty}^{+\infty} \frac{\exp \left[i k x \right]}{x - i \varepsilon} + \frac{1}{2 \pi i} \oint_{C_R} \frac{\exp \left[i k z \right]}{z - i \varepsilon} = \exp \left[i k \varepsilon \right] \tag{1583}$$

or on using Jordan's Lemma

$$\frac{1}{2 \pi i} \int_{-\infty}^{+\infty} \frac{\exp \left[i k x \right]}{x - i \varepsilon} + 0 = 1 \tag{1584}$$

Hence, for $k > 0$ one has

$$\Theta(k) = 1 \tag{1585}$$

On the other hand, when $k < 0$, the integral must be closed in the lower half complex plane. The contour does not enclose the pole and Jordan's Lemma shows the contour at infinity yields a vanishing contribution. Hence for $k < 0$ one has

$$\Theta(k) = 0 \tag{1586}$$

Thus, $\Theta(k)$ is the Heaviside step function.

Example:

Evaluate the integral

$$\int_{-\infty}^{\infty} dx \, \frac{\exp \left[i t x \right]}{x^2 - k^2} \tag{1587}$$

First we write

$$\int_{-\infty}^{\infty} dx \, \frac{\exp \left[\, i \, t \, x \, \right]}{(\, x \, - \, k \,) \, (\, x \, + \, k \,)} \tag{1588}$$

The integrand has two poles, at $x \; = \; \pm \, k$. The integral can be evaluated as a principal value integral and the contribution on two small semicircles of radius ε about $x \; = \; \pm \, k$.

For $t \; > \; 0$ the integral can be evaluated by completing the contour in the upper half complex plane, in which case no poles are enclosed. The contour at infinity yields zero by Jordan's Lemma. Hence, one has

$$\mathrm{Pr} \int_{-\infty}^{\infty} dx \, \frac{\exp \left[\, i \, t \, x \, \right]}{x^2 \, - \, k^2} \; - \; \pi \, i \, \frac{\exp \left[\, - \, i \, t \, k \, \right]}{- \, 2 \, k} \; - \; \pi \, i \, \frac{\exp \left[\, + \, i \, t \, k \, \right]}{2 \, k} \; = \; 0 \tag{1589}$$

Hence, for $t \; > \; 0$, we have

$$\mathrm{Pr} \int_{-\infty}^{\infty} dx \, \frac{\exp \left[\, i \, t \, x \, \right]}{x^2 \, - \, k^2} \; = \; - \, \frac{\pi \, \sin t \, k}{k} \tag{1590}$$

For $t \; < \; 0$ the integral can be evaluated by completing the contour in the lower half complex plane, in which case no poles are enclosed. The contour at infinity yields zero by Jordan's Lemma. Hence, one has

$$\mathrm{Pr} \int_{-\infty}^{\infty} dx \, \frac{\exp \left[\, i \, t \, x \, \right]}{x^2 \, - \, k^2} \; + \; \pi \, i \, \frac{\exp \left[\, - \, i \, t \, k \, \right]}{- \, 2 \, k} \; + \; \pi \, i \, \frac{\exp \left[\, + \, i \, t \, k \, \right]}{2 \, k} \; = \; 0 \tag{1591}$$

Hence, for $t \; < \; 0$, we have

$$\mathrm{Pr} \int_{-\infty}^{\infty} dx \, \frac{\exp \left[\, i \, t \, x \, \right]}{x^2 \, - \, k^2} \; = \; + \, \frac{\pi \, \sin t \, k}{k} \tag{1592}$$

Thus, combining these results we have the single formula

$$\mathrm{Pr} \int_{-\infty}^{\infty} dx \, \frac{\exp \left[\, i \, t \, x \, \right]}{x^2 \; - \; k^2} \; = \; - \; \frac{\pi \; \sin | \, t \, | \; k}{k} \tag{1593}$$

15.4 Contour Integration

Example:

Evaluate the integral

$$I \; = \; \int_0^{2\pi} \, \frac{d\theta}{a \; + \; b \; \cos\theta} \tag{1594}$$

Using the substitution

$$z \; = \; \exp \left[\, i \, \theta \, \right] \tag{1595}$$

one can write the integral as a contour integral around the unit circle in the complex plane

$$\begin{aligned} I \quad &= \quad - \, i \oint_C \frac{dz}{z} \, \frac{1}{a \; + \; \frac{b}{2} \; (\; z \; + \; z^{-1} \;)} \\ &= \quad - \, i \oint_C \, dz \, \frac{2}{b \; z^2 \; + \; 2 \; a \; z \; + \; b} \\ &= \quad - \, \frac{2 \, i}{b} \oint_C \, dz \, \frac{1}{z^2 \; + \; 2 \; \frac{a}{b} \; z \; + \; 1} \end{aligned} \tag{1596}$$

The denominator has zeroes at

$$z \; = \; - \, \frac{a}{b} \; \pm \; \sqrt{ \left(\frac{a}{b} \right)^2 \; - \; 1 } \tag{1597}$$

For $a \; > \; b$ the solution

$$z \; = \; - \, \frac{a}{b} \; + \; \sqrt{ \left(\frac{a}{b} \right)^2 \; - \; 1 } \tag{1598}$$

lies inside the unit circle. As can be seen directly from the coefficients of the quadratic equation, the product of the solutions is equal to unity. Thus, the second solution has to lie outside the unit circle. In the case $a > b$, one has

$$\begin{aligned} I &= - \frac{2\,i}{b} \oint_C dz \, \frac{1}{(\, z + \frac{a}{b} + \sqrt{(\frac{a}{b})^2 - 1}\,)(\, z + \frac{a}{b} - \sqrt{(\frac{a}{b})^2 - 1}\,)} \\ &= - \frac{2\,i}{b} \, \frac{2\,\pi\,i}{2\sqrt{(\frac{a}{b})^2 - 1}} \\ &= \frac{2\,\pi}{\sqrt{a^2 - b^2}} \end{aligned} \tag{1599}$$

Example:

Evaluate the integral

$$I = \int_0^{2\pi} d\theta \; \cos^{2n}\theta \tag{1600}$$

by contour integration.

On the unit circle

$$z = \exp\left[\, i\,\theta \,\right] \tag{1601}$$

one has

$$\begin{aligned} I &= - i \oint_C \frac{dz}{z} \left(\frac{z + z^{-1}}{2} \right)^{2n} \\ &= 2\,\pi \, \frac{C(2n,n)}{2^{2n}} \\ &= \frac{\pi}{2^{2n-1}} \, \frac{(2n)!}{n!\;n!} \end{aligned} \tag{1602}$$

where we have used the binomial expansion and noted the integral only picks up the term which gives rise to the pole at $z = 0$. The binomial coefficient of the term z^0 in the expansion is $C(2n,n)$, which leads to the final result.

Example:

Evaluate the integral

$$\int_0^{2\pi} d\theta \, \frac{1}{a + b\,\sin\theta} \tag{1603}$$

with $a > b$.

We shall change variables from θ to z via

$$z = \exp \left[i \theta \right] \tag{1604}$$

so the integral can be written as a contour integral over the unit circle

$$\begin{aligned} I &= \oint \frac{dz}{i z} \frac{1}{a + b \frac{(z - z^{-1})}{2 i}} \\ &= \frac{2}{b} \oint dz \frac{1}{z^2 + 2 i \frac{a}{b} z - 1} \end{aligned} \tag{1605}$$

The denominator has poles at

$$z = - i \frac{a}{b} \pm i \sqrt{ \left(\frac{a}{b} \right)^2 - 1 } \tag{1606}$$

The pole at

$$z = - i \frac{a}{b} + i \sqrt{ \left(\frac{a}{b} \right)^2 - 1 } \tag{1607}$$

is inside the unit circle. The integral can be written as

$$\begin{aligned} I &= \frac{2}{b} \oint dz \frac{1}{\left(z + i \frac{a}{b} - i \sqrt{ \left(\frac{a}{b} \right)^2 - 1 } \right) \left(z + i \frac{a}{b} + i \sqrt{ \left(\frac{a}{b} \right)^2 - 1 } \right)} \\ &= \frac{1}{i \sqrt{a^2 - b^2}} \oint dz \left[\frac{1}{\left(z + i \frac{a}{b} - i \sqrt{ \left(\frac{a}{b} \right)^2 - 1 } \right)} - \frac{1}{\left(z + i \frac{a}{b} + i \sqrt{ \left(\frac{a}{b} \right)^2 - 1 } \right)} \right] \\ &= \frac{2 \pi}{\sqrt{b^2 - a^2}} \end{aligned} \tag{1608}$$

The last line of the integral is evaluated by noting that only the pole of the first term is inside the unit circle.

Example:

Evaluate the integral

$$I = \int_0^{2\pi} \frac{d\theta}{(a + b \cos\theta)^2} \tag{1609}$$

Using the substitution

$$z = \exp \left[i \theta \right] \tag{1610}$$

one can write the integral as a contour integral around the unit circle in the complex plane

$$\begin{aligned} I &= - i \oint_C \frac{dz}{z} \frac{1}{\left(a + \frac{b}{2} (z + z^{-1}) \right)^2} \\ &= - i \oint_C dz \frac{4 z}{\left(b z^2 + 2 a z + b \right)^2} \\ &= - \frac{4 i}{b^2} \oint_C dz \frac{z}{\left(z^2 + 2 \frac{a}{b} z + 1 \right)^2} \end{aligned} \tag{1611}$$

The denominator has double zeroes at

$$z = - \frac{a}{b} \pm \sqrt{\left(\frac{a}{b} \right)^2 - 1} \tag{1612}$$

For $a > b$ the pole at

$$z = z_\alpha = - \frac{a}{b} + \sqrt{\left(\frac{a}{b} \right)^2 - 1} \tag{1613}$$

lies inside the unit circle. The other pole is located at the inverse of the position of the above pole, and therefore lies outside the unit circle. In this case, one has

$$\begin{aligned} I &= - \frac{4 i}{b^2} \oint_C dz \frac{z}{(z + \frac{a}{b} + \sqrt{(\frac{a}{b})^2 - 1})^2 (z + \frac{a}{b} - \sqrt{(\frac{a}{b})^2 - 1})^2} \\ &= \frac{8 \pi}{b^2} \frac{d}{dz} \left(\frac{z}{(z + \frac{a}{b} + \sqrt{(\frac{a}{b})^2 - 1})^2} \right) \Bigg|_{z_\alpha} \\ &= \frac{8 \pi}{b^2} \left(\frac{\frac{a}{b} + \sqrt{(\frac{a}{b})^2 - 1} - z}{(z + \frac{a}{b} + \sqrt{(\frac{a}{b})^2 - 1})^3} \right) \Bigg|_{z_\alpha} \end{aligned}$$

$$= \quad \frac{2 \pi a}{(a^2 - b^2)^{\frac{3}{2}}} \tag{1614}$$

where Cauchy's integral formula for derivatives has been used to evaluate the contribution from the pole of order 2.

Example:

The function

$$\frac{2}{\pi} \frac{\sin^2 \omega T}{\omega^2 T} \tag{1615}$$

occurs in the derivation of the Fermi-Golden transition rate, in second order time dependent perturbation theory. In the limit $T \rightarrow \infty$ this becomes a Dirac delta function expressing energy conservation. Evaluate the integral

$$\int_{-\infty}^{\infty} d\omega \, \frac{\sin^2 \omega T}{\omega^2 T} \tag{1616}$$

The integral can be expressed as

$$\int_{-\infty}^{\infty} d\omega \, \frac{1 - \cos 2 \omega T}{2 \omega^2 T} = \int_{-\infty}^{\infty} d\omega \, \frac{1 - \exp[+ i \omega T]}{4 \omega^2 T} + \int_{-\infty}^{\infty} d\omega \, \frac{1 - \exp[- i \omega T]}{4 \omega^2 T} \tag{1617}$$

The two contributions can be expressed as contour integrals, the first can be closed by the semi-circle at infinity in the upper half complex plane, and a small semi-circle of radius r around the double pole

$$\begin{aligned} & \oint_C dz \, \frac{1 - \exp[+ i z T]}{4 z^2 T} \\ = & \int_{-\infty}^{\infty} d\omega \, \frac{1 - \exp[+ i \omega T]}{4 \omega^2 T} + i \int_{\pi}^{0} d\theta \, \exp[- i \theta] \, \frac{1}{4 r T} \bigg(- i r T \exp[+ i \theta] \bigg) \\ = & \; 0 \end{aligned} \tag{1618}$$

where we have Taylor expanded the function about $r = 0$, and the contour does not enclose the pole. Hence, we have

$$\int_{-\infty}^{\infty} d\omega \, \frac{1 - \exp[+ i \omega T]}{4 \omega^2 T} = i \, \frac{\pi}{4} \tag{1619}$$

Likewise, the other term can be evaluated by closing the contour in the lower half complex plane

$$\int_{-\infty}^{\infty} d\omega \, \frac{1 - \exp[- i \omega T]}{4 \omega^2 T} = i \, \frac{\pi}{4} \tag{1620}$$

On adding these two contributions one has the final result

$$\int_{-\infty}^{\infty} d\omega \, \frac{\sin^2 \omega \, T}{\omega^2 \, T} \; = \; \frac{\pi}{2} \tag{1621}$$

which shows that the function has weight unity. Furthermore, the weight is distributed in a frequency interval of width given by $\frac{1}{T}$, so for $T \; \rightarrow \; \infty$ one obtains the energy conserving delta function

$$\lim_{T \, \rightarrow \infty} \frac{2}{\pi} \left(\frac{\sin^2 \omega \, T}{\omega^2 \, T} \right) \; = \; \delta(\, \omega \,) \tag{1622}$$

Example:

Evaluate the integral

$$\int_{-\infty}^{\infty} dx \, \frac{\sin^3 x}{x^3} \tag{1623}$$

As the function is analytic at $x \; = \; 0$ the integration along the real axis can be deformed slightly near the origin in a semi-circle of radius ε in the lower half complex plane. This contour does not contribute to the integral in the limit $\varepsilon \; \rightarrow \; 0$. The integrand can be expressed as

$$\frac{\exp[\, + \, 3 \, i \, x \,] \; - \; 3 \; \exp[\, + \, i \, x \,] \; + \; 3 \; \exp[\, - \, i \, x \,] \; - \; \exp[\, - \, 3 \, i \, x \,]}{8 \; i^3 \; x^3} \tag{1624}$$

and the contribution to the small semi-circle from the terms with the positive phases cancel to order ε with those with the negative phases.

The contour can be closed in the upper half complex plane for the terms with the positive phases. The contour encloses the pole of order three at $x \; = \; 0$, while the contour for the term with the negative phases must be closed in the lower half complex plane. This contour excludes the pole at $x \; = \; 0$. The end result is that the integration is determined by the residue at $x \; = \; 0$ which is evaluated from Cauchy's formulae for derivatives as

$$\frac{6}{16 \; i} \tag{1625}$$

Hence, the integral is evaluated as

$$\int_{-\infty}^{\infty} dx \, \frac{\sin^3 x}{x^3} \; = \; \frac{3 \; \pi}{4} \tag{1626}$$

Example:

Evaluate the integral

$$I = \int_{-\infty}^{\infty} dx \, \frac{\exp[\, a \, x \,]}{\exp[\, x \,] \, + \, 1} \tag{1627}$$

where $0 < \, a \, < \, 1$.

The integral is convergent as when $x \, \to \, \infty$ the fact that $a \, < \, 1$ makes the integrand tends to zero. Also, when $x \, \to \, - \, \infty$ the integrand also tends to zero as $a \, > \, 0$.

The integration is evaluated on a contour which runs along the real axis between $(-R, R)$ then up to $R \, + \, 2 \, \pi \, i$ and then runs anti-parallel to the real axis from $R \, + \, 2 \, \pi \, i$ to $R \, - \, 2 \, \pi \, i$ and then back down to $- \, R$. This particular contour is chosen due to the fact that the integration on the upper line has

$$\frac{1}{\exp[\, x \, + \, i \, 2 \, \pi \,] \, - \, 1} \, = \, \frac{1}{\exp[\, x \,] \, - \, 1} \tag{1628}$$

The two vertical segments vanish as $R \, \to \, \infty$ as the integrand vanishes as $\exp[\, - \, a \, R \,]$ or $\exp[\, - \, (\, 1 \, - \, a \,) \, R \,]$. Thus, the contour integral is given by

$$\begin{aligned} \oint dz \, \frac{\exp[\, a \, z \,]}{\exp[\, z \,] \, + \, 1} \, &= \, \int_{-\infty}^{\infty} dx \, \frac{\exp[\, a \, x \,]}{\exp[\, x \,] \, + \, 1} \, - \, \int_{-\infty}^{\infty} dx \, \frac{\exp[\, a \, x \, + \, i \, 2 \, \pi \, a \,]}{\exp[\, x \,] \, + \, 1} \\ &= \, (\, 1 \, - \, \exp[\, i \, 2 \, \pi \, a \,] \,) \int_{-\infty}^{\infty} dx \, \frac{\exp[\, a \, x \,]}{\exp[\, x \,] \, + \, 1} \end{aligned} \tag{1629}$$

This contour encloses the pole at $z \, = \, \pi \, i$, which has a residue given by

$$\exp[\, (\, a \, - \, 1 \,) \, \pi \, i \,] \, = \, - \, \exp[\, i \, \pi \, a \,] \tag{1630}$$

Hence, we have

$$\left(1 \, - \, \exp[\, i \, 2 \, \pi \, a \,] \right) \int_{-\infty}^{\infty} dx \, \frac{\exp[\, a \, x \,]}{\exp[\, x \,] \, + \, 1} \, = \, - \, 2 \, \pi \, i \, \exp[\, i \, \pi \, a \,] \tag{1631}$$

or in final form, one has

$$\int_{-\infty}^{\infty} dx \, \frac{\exp[\, a \, x \,]}{\exp[\, x \,] \, + \, 1} \, = \, \frac{\pi}{\sin \, \pi \, a} \tag{1632}$$

Example:

The gamma function is defined by

$$\Gamma(x+1) \; = \; \int_0^\infty dt \; t^x \; \exp \left[\; - \; t \; \right] \tag{1633}$$

for $x \; > \; - \; 1$. Show that

$$\begin{aligned} \int_0^\infty dt \; t^x \; \sin \, t \quad &= \quad \Gamma(x+1) \; \cos \frac{\pi \; x}{2} \\ \int_0^\infty dt \; t^x \; \cos \, t \quad &= \quad - \; \Gamma(x+1) \; \sin \frac{\pi \; x}{2} \end{aligned} \tag{1634}$$

Consider the contour integral defined by

$$\oint_C dz \; z^t \; \exp \left[\; - \; z \; \right] \tag{1635}$$

where C starts at the origin and runs to infinity, then follows a segment of a circular path until the positive imaginary axis is reached. The contour is closed by the segment running down the positive imaginary axis back to the origin.

This integral is zero, as no singularities are enclosed

$$\oint_C dz \; z^t \; \exp \left[\; - \; z \; \right] \; = \; 0 \tag{1636}$$

In addition, due to the presence of the exponential factor

$$\exp \left[\; - \; R \; \cos \theta \; \right] \tag{1637}$$

in the integrand, integral over the quarter circle of radius $R \; \rightarrow \; \infty$ vanishes. Thus,

$$\int_0^\infty dx \; x^t \; \exp \left[\; - \; x \; \right] \; = \; i \; \int_0^\infty dy \; i^t \; y^t \; \exp \left[\; - \; i \; y \; \right] \tag{1638}$$

or on using the definition of the Gamma function

$$\Gamma(t+1) \; = \; i \; \exp \left[\; i \; \frac{\pi \; t}{2} \; \right] \; \int_0^\infty dy \; y^t \; \exp \left[\; - \; i \; y \; \right] \tag{1639}$$

On multiplying by a factor of

$$\exp \left[- \, i \, \frac{\pi \, t}{2} \, \right] \tag{1640}$$

one obtains

$$\exp \left[- \, i \, \frac{\pi \, t}{2} \, \right] \Gamma(t+1) \; = \; i \int_0^\infty \, dy \; y^t \; \exp \left[\; - \; i \; y \; \right] \tag{1641}$$

and on taking the real and imaginary parts one obtains the results

$$\begin{aligned} \int_0^\infty \, dt \; t^x \; \sin \; t \quad &= \quad \Gamma(x+1) \; \cos \frac{\pi \; x}{2} \\ \int_0^\infty \, dt \; t^x \; \cos \; t \quad &= \quad - \; \Gamma(x+1) \; \sin \frac{\pi \; x}{2} \end{aligned} \tag{1642}$$

as was to be shown.

Example:

Evaluate the integral

$$I \; = \; \int_0^\infty \, dx \frac{x^\alpha}{1 \; + \; x^2} \tag{1643}$$

for $\alpha \; < \; 1$.

The function has a branch point at $x \; = \; 0$. A branch cut can be drawn along the positive real axis. A contour can be drawn which performs a circle of radius R at infinity and a counter clockwise contour at radius r and two anti-parallel segments on opposite sides of the real axis.

The contribution from the circular contour at infinity vanishes as the integrand vanishes as $R^{\alpha-2}$. The contribution from the clockwise contour around the origin vanishes as $r^{\alpha+1}$ as $r \; \rightarrow \; 0$. The contribution from the two anti-parallel segments do not cancel as the function just below the real axis differs from the function just above the real axis by the phase $\exp[\; i \; 2 \; \pi \; \alpha \;]$. Hence, the integral around the contour reduces to

$$\oint_C \, dz \, \frac{z^\alpha}{z^2 \; + \; 1} \; = \; \left(\, 1 \; - \; \exp \left[\, i \; 2 \; \pi \; \alpha \, \right] \, \right) \int_0^\infty \, dx \, \frac{x^\alpha}{x^2 \; + \; 1} \tag{1644}$$

The contour encloses the two poles at $x = \pm i$ which have residues

$$R_{\pm} = \frac{\exp\left[i \frac{(2 \mp 1)}{2} \pi \alpha \right]}{\pm 2 i} \tag{1645}$$

Hence, one has

$$\left(1 - \exp\left[i 2 \pi \alpha \right] \right) \int_0^\infty dx \frac{x^\alpha}{x^2 + 1} = \pi \left(\exp\left[i \frac{\pi \alpha}{2} \right] - \exp\left[i \frac{3 \pi \alpha}{2} \right] \right) \tag{1646}$$

and on factoring out $\exp[i \pi \alpha]$ from both sides, one has the result

$$\begin{aligned} \int_0^\infty dx \frac{x^\alpha}{x^2 + 1} &= \pi \left(\frac{\sin \frac{\pi \alpha}{2}}{\sin \pi \alpha} \right) \\ &= \left(\frac{\pi}{2 \cos \frac{\pi \alpha}{2}} \right) \end{aligned} \tag{1647}$$

Example:

Prove that

$$\int_0^\infty dx \frac{x^\alpha}{(1 + x^2)^2} = \frac{\pi (1 - \alpha)}{4 \cos \frac{\pi \alpha}{2}} \tag{1648}$$

Example:

Evaluate the integral

$$\int_0^\infty dx \frac{\ln x}{x^2 + a^2} \tag{1649}$$

The integrand has a branch point at $x = 0$. A branch cut can be introduced along the positive real axis. The integral can be represented as the sum of a clockwise semi-circular contour around the branch point of radius r and a counter clockwise semi-circular contour at infinity of radius R, and an integral just over the entire real axis. The contour at infinity yields a result of the order R^{-1} which vanishes as $R \to \infty$. The contour around the semi-circle of radius r has the magnitude $r \ln r$ which vanishes as $r \to 0$. The remaining integral over the real axis result in the expression

$$\oint_C dx \frac{\ln z}{z^2 + a^2} = 2 \int_0^\infty d\rho \frac{\ln \rho}{\rho^2 + a^2} + i \pi \int_0^\infty d\rho \frac{1}{\rho^2 + a^2} \tag{1650}$$

where we have used the polar representation of the complex number $z = \rho \exp[\, i \, \theta \,]$.

The contour encloses the pole in the upper half complex plane at $z = i \, a$. The residue at the pole is

$$R = \frac{1}{2 \, i \, a} \left(\ln \, a \, + \, i \, \frac{\pi}{2} \right) \tag{1651}$$

Hence, the contour integration is evaluated as

$$2 \int_0^\infty d\rho \, \frac{\ln \rho}{\rho^2 \, + \, a^2} \, + \, i \, \pi \, \frac{\pi}{2 \, a} \, = \, \frac{\pi}{a} \left(\ln \, a \, + \, i \, \frac{\pi}{2} \right) \tag{1652}$$

Thus, we have the final result

$$\int_0^\infty dx \, \frac{\ln x}{x^2 \, + \, a^2} \, = \, \frac{\pi}{2 \, a} \left(\ln \, a \right) \tag{1653}$$

where $a > 0$.

Example:

Prove that

$$\int_0^\infty dx \left(\frac{\ln^2 x}{1 \, + \, x^2} \right) \, = \, \frac{\pi^2}{8} \tag{1654}$$

Example:

Show that

$$\int_0^\infty dx \left(\frac{1}{1 \, + \, x^n} \right) \, = \, \frac{\left(\frac{\pi}{n} \right)}{\sin \left(\frac{\pi}{n} \right)} \tag{1655}$$

by integrating over a contour composed of the real axis an arc at infinity of length $R \left(\frac{2 \, \pi}{n} \right)$, and a straight line back to the origin.

The segment of the contour at infinity vanishes. The two straight line segments are evaluated as

$$\int_0^\infty dx \left(\frac{1}{1 \, + \, x^n} \right) \, - \, \exp \left[\, i \, \frac{2 \, \pi}{n} \, \right] \int_0^\infty ds \left(\frac{1}{1 \, + \, s^n} \right) \tag{1656}$$

where

$$z \, = \, s \, \exp \left[\, i \, \frac{2 \, \pi}{n} \, \right] \tag{1657}$$

along the second segment. The contour integral is equal to the residue of the pole at

$$z = \exp \left[i \frac{\pi}{n} \right] \tag{1658}$$

which is enclosed by the contour. The residue has the value

$$R = \frac{1}{n z^{n-1}} = - \frac{1}{n} \exp \left[i \frac{\pi}{n} \right] \tag{1659}$$

Thus, we have

$$\left(1 - \exp \left[i \frac{2 \pi}{n} \right] \right) \int_0^\infty dx \left(\frac{1}{1 + x^n} \right) = - \frac{2 \pi i}{n} \exp \left[i \frac{\pi}{n} \right] \tag{1660}$$

which on dividing by the prefactor can be re-written as

$$\int_0^\infty dx \left(\frac{1}{1 + x^n} \right) = \frac{\left(\frac{\pi}{n} \right)}{\sin \left(\frac{\pi}{n} \right)} \tag{1661}$$

as was to be shown.

15.5 The Poisson Summation Formula

The sum

$$\sum_{n=0}^{\infty} f(n) \tag{1662}$$

can be evaluated as a contour integration using the Poisson summation formula. The method is based on the fact that the function

$$\frac{\exp \left[i 2 \pi z \right] + 1}{\exp \left[i 2 \pi z \right] - 1} = \frac{1}{i \tan \pi z} \tag{1663}$$

has simple poles at $z = n$ for positive and negative integer values of n, with residues

$$R_n = \frac{1}{\pi i} \tag{1664}$$

The summation can be written as a contour integration, where the contour encircles the poles and avoids the singularities of $f(z)$. Thus, the summation can be expressed as

$$\sum_{n=0}^{\infty} f(n) = \frac{1}{2 i} \oint_C dz \frac{1}{\tan \pi z} f(z) \tag{1665}$$

and the contour can be deformed as convenient. If the contour at infinity vanishes, the integration can be evaluated along the imaginary axis.

Example:

Express the sum

$$\sum_{n=1}^{\infty} \frac{1}{n^m} \tag{1666}$$

for $m \geq 2$, as an integral.

One can express the sum as a contour integrations around all the positive poles of $\cot \pi z$,

$$\sum_{n=0}^{\infty} \frac{1}{n^m} = \frac{1}{2\,i} \oint_C dz \, \frac{1}{\tan \pi z} \, \frac{1}{z^m} \tag{1667}$$

The function $f(z)$ has no poles except the simple pole at $z = 0$, so the contour of integration can be deformed. The integrations can be deformed from C to C' which is an integration along both sides of the positive real axis, running from 1 to ∞. The small anti-parallel segments cancel, so the infinite number of circles of C have been joined into the closed contour C'. The contour can then be furthered deformed to an integral parallel to the imaginary axis

$$z = \frac{1}{2} + i\,y \tag{1668}$$

and a semi-circle at infinity. The contour at infinity vanishes as $m \geq 2$. Hence we have

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{1}{n^m} &= \frac{i}{2} \int_{-\infty}^{\infty} dy \, \tanh \pi y \, \frac{1}{(\frac{1}{2} + i\,y)^m} \\ &= \frac{i}{2} \int_0^{\infty} dy \, \tanh \pi y \left[\frac{1}{(\frac{1}{2} + i\,y)^m} - \frac{1}{(\frac{1}{2} - i\,y)^m} \right] \\ &= \int_0^{\infty} dy \, \tanh \pi y \, \operatorname{Im} \left[\frac{1}{(\frac{1}{2} - i\,y)^m} \right] \end{aligned} \tag{1669}$$

Thus, for example with $m = 2$ one has

$$\sum_{n=0}^{\infty} \frac{1}{n^2} = \int_0^{\infty} dy \, \tanh \pi y \, \frac{y}{(\frac{1}{4} + y^2)^2} \tag{1670}$$

Example:

Evaluate

$$\sum_{n=-\infty}^{\infty} \frac{(- 1)^n}{(a + n)^2} \tag{1671}$$

where a is a non-integer number.

This can be evaluated as a contour integral

$$\sum_{n=0}^{\infty} \frac{(- 1)^n}{(a + n)^2} = \frac{1}{2 i} \oint_C dz \; \csc \pi \, z \, \frac{1}{(a + z)^2} \tag{1672}$$

in which the contour runs on both sides of the real axis, but does not enclose the double pole at $z = - a$. The function $\csc \pi \, z$ has poles at $z = \pi \, n$ and has residues

$$\frac{1}{\pi} \, (- 1)^n \tag{1673}$$

The contour can be deformed to infinity, and an excursion that excludes the double pole. The excursion circles the double pole in a clockwise direction. The contribution from the contour at infinity vanishes. Thus, we find that the sum is equal to a contribution from the clockwise contour around the double pole. The residue at the double pole $z = - a$ is

$$- \pi \, \csc \pi \, a \quad \cot \pi \, a \tag{1674}$$

Hence, we have evaluated the sum as

$$\sum_{n=0}^{\infty} \frac{(- 1)^n}{(a + n)^2} = \pi^2 \csc \pi \, a \quad \cot \pi \, a \tag{1675}$$

Example:

Evaluate the sum

$$\sum_{n=1}^{\infty} \frac{2 \, x}{x^2 + n^2 \, \pi^2} \tag{1676}$$

Let

$$f(z) = \sum_{n=1}^{\infty} \frac{2 \, x}{x^2 + z^2 \, \pi^2} \tag{1677}$$

then

$$\sum_{n=-\infty}^{\infty} \frac{2\,x}{(\,x^2 \,+\, n^2\,\pi^2\,)} \;=\; \frac{1}{2\,\pi\,i} \oint_C dz\, \cot\pi\,z\;f(z) \;-\; \sum_{\text{poles of } f(z)} Res\left[\,\pi\,\cot\pi\,z\;f(z)\,\right] \tag{1678}$$

where C is a closed contour enclosing the real axis and the poles of $f(z)$. The contour integral vanishes as the contour is deformed to infinity since $|\,f(z)\,| \to 0$. Hence, as the poles of $f(z)$ are located at

$$z \;=\; \pm\,i\,\frac{x}{\pi} \tag{1679}$$

and the residues are $\coth x$, one has

$$\sum_{n=-\infty}^{\infty} \frac{2\,x}{(\,x^2 \,+\, z^2\,\pi^2\,)} \;=\; 2\,\coth x \tag{1680}$$

or

$$\coth\,x \;-\; \frac{1}{x} \;=\; \sum_{n=1}^{\infty} \frac{2\,x}{x^2 \,+\, n^2\,\pi^2} \tag{1681}$$

On integrating this relation from $x \;=\; 0$ to $x \;=\; \theta$ one obtains

$$\ln\,\sinh\theta \;-\; \ln\theta \;=\; \sum_{n=1}^{\infty} \ln\left(\,1 \;+\; \frac{\theta^2}{n^2\,\pi^2}\,\right) \tag{1682}$$

or

$$\frac{\sinh\theta}{\theta} \;=\; \prod_{n=1}^{\infty}\left(\,1 \;+\; \frac{\theta^2}{n^2\,\pi^2}\,\right) \tag{1683}$$

On analytically continuing this to complex θ, such that $\theta \;=\; i\,\varphi$ one obtains a formulae for $\sin\varphi$ as a product

$$\sin\varphi \;=\; \varphi\,\prod_{n=1}^{\infty}\left(\,1 \;-\; \frac{\varphi^2}{n^2\,\pi^2}\,\right) \tag{1684}$$

in which the zeroes appear explicitly.

15.6 Kramers-Kronig Relations

The Kramers-Kronig relation expresses causality. The response of a system can be expressed in terms of a response function. The response of the system $A(t)$ only occurs after the system has been perturbed by an applied field $B(t')$ at an earlier time t'. The general relation between the response and applied field is given by linear response theory and involves the convolution

$$A(t) \;=\; \int_{-\infty}^{\infty} dt' \; \chi(t-t') \; B(t') \tag{1685}$$

where the response function is defined to be zero for $t' \;>\; t$, i.e.

$$\chi(t) \;=\; 0 \qquad t \;<\; 0 \tag{1686}$$

The response $\chi(t)$ represents the time variation of $A(t)$ if the applied field, $B(t)$, consists of a delta function pulse of strength unity occurring at time $t' \;=\; 0$. When Fourier transformed with respect to time, the linear response relation becomes

$$A(\omega) \;=\; \chi(\omega) \; B(\omega) \tag{1687}$$

which relates the amplitude of a response $A(\omega)$ to the application of a time dependent applied field with frequency ω and amplitude $B(\omega)$. The quantity $\chi(\omega)$ is the response function. Causality leads to the response function being analytic in the upper half complex plane and on the real frequency axis. The response function $\chi(\omega)$ usually satisfies the Kramers-Kronig relations.

Consider a function $\chi(z)$ which is analytic in the upper half complex plane and real on the real axis. Furthermore, we assume that

$$\lim_{|z| \;\rightarrow\infty} \; \chi(z) \;\rightarrow\; 0 \tag{1688}$$

so that the integral on the semi-circle at infinity in the upper half complex plane is zero. The Cauchy integral formula is given by

$$\chi(z_0) \;=\; \frac{1}{2\;\pi\;i} \oint_C dz \; \frac{\chi(z)}{z \;-\; z_0} \tag{1689}$$

if z_0 is in the upper half complex plane. Since the semi-circle at infinity vanishes

$$\chi(z_0) \;=\; \frac{1}{2\;\pi\;i} \int_{-\infty}^{\infty} dz \; \frac{\chi(z)}{z \;-\; z_0} \tag{1690}$$

On varying z_0 from the upper half complex plane to a value ω_0 on the real axis, the integral becomes the sum of the Principal Value and a contour of radius ε around the pole. Hence,

$$\chi(\omega_0) \;=\; \frac{\mathrm{Pr}}{2\;\pi\;i} \int_{-\infty}^{\infty} dz \; \frac{\chi(z)}{z \;-\; \omega_0} \;+\; \frac{\chi(\omega_0)}{2} \tag{1691}$$

or

$$\chi(\omega_0) \;=\; \frac{\mathrm{Pr}}{\pi\;i} \int_{-\infty}^{\infty} dz \; \frac{\chi(z)}{z \;-\; \omega_0} \tag{1692}$$

On taking the real and imaginary part of this equation one has the two equations

$$\text{Real}\ \chi(\omega_0) \ = \ \frac{\Pr}{\pi} \int_{-\infty}^{\infty} d\omega \ \frac{\text{Im}\ \chi(\omega)}{\omega \ - \ \omega_0} \tag{1693}$$

and

$$\text{Im}\ \chi(\omega_0) \ = \ - \ \frac{\Pr}{\pi} \int_{-\infty}^{\infty} d\omega \ \frac{\text{Real}\ \chi(\omega)}{\omega \ - \ \omega_0} \tag{1694}$$

which are the Kramers-Kronig relations.

Symmetry Relations

An applied field of frequency ω can usually be expressed in terms of an amplitude $A(\omega)$ or $A(-\omega)$, since for a real field $A(t)$ one has

$$A^*(\omega) \ = \ A(-\omega) \tag{1695}$$

Hence, one expects that the response function may also satisfy

$$\chi^*(\omega) \ = \ \chi(-\omega) \tag{1696}$$

This implies that the real and imaginary parts, respectively, are even and odd as

$$\chi(\omega) \ = \ \text{Real}\ \chi(\omega) \ + \ i\ \text{Im}\ \chi(\omega) \tag{1697}$$

so

$$\chi^*(\omega) \ = \ \text{Real}\ \chi(\omega) \ - \ i\ \text{Im}\ \chi(\omega) \tag{1698}$$

Hence

$$\chi(-\omega) \ = \ \chi^*(\omega) \ = \ \text{Real}\ \chi(\omega) \ - \ i\ \text{Im}\ \chi(\omega) \tag{1699}$$

and thus

$$\begin{aligned} \text{Real}\ \chi(-\omega) \ &= \ \text{Real}\ \chi(\omega) \\ \text{Im}\ \chi(-\omega) \ &= \ - \ \text{Im}\ \chi(\omega) \end{aligned} \tag{1700}$$

These symmetry relations can be used in the Kramers-Kronig relations

$$\begin{aligned} \text{Real}\ \chi(\omega_0) \ &= \ \frac{\Pr}{\pi} \int_{-\infty}^{\infty} d\omega \ \frac{\text{Im}\ \chi(\omega)}{\omega \ - \ \omega_0} \\ &= \ \frac{1}{\pi} \int_0^{\infty} d\omega \ \frac{\text{Im}\ \chi(\omega)}{\omega \ - \ \omega_0} \ - \ \frac{1}{\pi} \int_0^{\infty} d\omega \ \frac{\text{Im}\ \chi(-\omega)}{\omega \ + \ \omega_0} \\ &= \ \frac{1}{\pi} \int_0^{\infty} d\omega \ \frac{\text{Im}\ \chi(\omega)}{\omega \ - \ \omega_0} \ + \ \frac{1}{\pi} \int_0^{\infty} d\omega \ \frac{\text{Im}\ \chi(\omega)}{\omega \ + \ \omega_0} \\ &= \ \frac{2}{\pi} \int_0^{\infty} d\omega \ \frac{\omega\ \text{Im}\ \chi(\omega)}{\omega^2 \ - \ \omega_0^2} \end{aligned} \tag{1701}$$

and similarly for the imaginary part, one can show that

$$\begin{aligned} \text{Im}\ \chi(\omega_0) &= -\ \frac{\text{Pr}}{\pi} \int_{-\infty}^{\infty} d\omega\ \frac{\text{Real}\ \chi(\omega)}{\omega\ -\ \omega_0} \\ &= -\ \frac{2}{\pi} \int_{0}^{\infty} d\omega\ \frac{\omega_0\ \text{Real}\ \chi(\omega)}{\omega^2\ -\ \omega_0^2} \end{aligned} \tag{1702}$$

This representation of the Kramers-Kronig relation is useful as perhaps only either the real or imaginary part of the response function may only be measurable for positive ω.

15.7 Integral Representations

The generating functions can be used to develop an integral representation of the special functions. For example, if

$$g(x,t)\ =\ \sum_n\ f_n(x)\ t^n \tag{1703}$$

then the function $f_n(x)$ can be identified as a contour integral

$$f_n(x)\ =\ \frac{1}{2\ \pi\ i}\ \oint_C\ dt\ g(x,t)\ t^{-(n+1)} \tag{1704}$$

around a contour C running around the origin, but excluding any singularities of $g(x,t)$.

Hence, one can express the Bessel functions as

$$J_n(x)\ =\ \frac{1}{2\ \pi\ i}\ \oint\ dt\ \exp\left[\ \frac{x}{2}\ (\ t\ -\ t^{-1}\ )\ \right]\ t^{-(n+1)} \tag{1705}$$

The Legendre functions can be expressed as

$$P_n(x)\ =\ \frac{1}{2\ \pi\ i}\ \oint\ dt\ \frac{1}{\sqrt{1\ -\ 2\ x\ t\ +\ t^2}}\ t^{-(n+1)} \tag{1706}$$

The Hermite polynomials can be written as

$$H_n(x)\ =\ \frac{1}{2\ \pi\ i}\ \oint\ dt\ \exp\left[\ -\ t^2\ +\ 2\ x\ t\ \right]\ t^{-(n+1)} \tag{1707}$$

and the Laguerre polynomials can be written as

$$L_n(x)\ =\ \frac{1}{2\ \pi\ i}\ \oint\ dt\ \frac{\exp\left[\ -\ \frac{x\ t}{1\ -\ t}\ \right]}{1\ -\ t}\ t^{-(n+1)} \tag{1708}$$