Mathematical Methods 2 (PART I)

Lecturer: Dr. D.J. Miller  
Room 535, Kelvin Building  
d.miller@physics.gla.ac.uk

Location: Room 312, Kelvin Building

Recommended Text: Boas, 3rd Edition
Outline

1. Curvilinear coordinate systems

2. Partial Differential Equations in cylindrical and spherical polar coordinates

3. Legendre Polynomials and Bessel Functions

4. Hermite and Laguerre Polynomials

5. Gamma and Beta Functions, and Stirling’s approximation
1. Curvilinear coordinate systems

1.1 Revision of vector calculus with Cartesian coordinates

Consider a 3-dimensional vector space.

Any point in the space can be written in terms of three **coordinates** $x_1$, $x_2$ and $x_3$, and three **basis vectors** $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$.

Sometimes the coordinates are written as $x$, $y$ and $z$, and the unit vectors as $\mathbf{e}_x$, $\mathbf{e}_y$ and $\mathbf{e}_z$. (I will use both notations, but avoid $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$).

Any **vector** $\mathbf{A}$ in this space, can be written in terms of these unit vectors as,

$$\mathbf{A} = \sum_{i=1}^{3} A_i \mathbf{e}_i.$$

I will sometimes assume the **Einstein Summation convention** and omit the summation sign $\Sigma$ when I have **two** repeated indices (unless otherwise specified), e.g.

$$\mathbf{A} = A_i \mathbf{e}_i.$$
These unit vectors are **orthonormal** (orthogonal and of unit length) if

\[ e_i \cdot e_j = \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}. \]

Kronecker delta

The **position vector** \( \mathbf{r} \) is given by \( \mathbf{r} = x_i \mathbf{e}_i \).

The **scalar product** of two vectors \( \mathbf{A} \) and \( \mathbf{B} \) is

\[ \mathbf{A} \cdot \mathbf{B} = A_i B_i. \]

The **vector product** of two vectors \( \mathbf{A} \) and \( \mathbf{B} \) is

\[ \mathbf{A} \times \mathbf{B} = \epsilon_{ijk} A_i B_j \mathbf{e}_k, \]

where \( \epsilon_{ijk} \) is the **Levi Civita symbol**, which is +1 for an even permutation of 1, 2 and 3 and -1 for an odd permutation, and zero if any of the indices are the same, e.g. \( \epsilon_{123} = 1, \epsilon_{132} = -1, \epsilon_{112} = 0 \).
For example, the z-component is:

\[ [A \times B]_z = [A \times B]_3 = \epsilon_{ij3} A_i B_j = (\epsilon_{123} A_1 B_2 + \epsilon_{213} A_2 B_1) \]
\[ = (A_x B_y - A_y B_x) \]

The **gradient operator** \( \nabla \) is given by

\[ \nabla = e_i \frac{\partial}{\partial x_i} = e_x \frac{\partial}{\partial x} + e_y \frac{\partial}{\partial y} + e_z \frac{\partial}{\partial z} \]

From this, and the definitions above, follow the **gradient** of a scalar field \( \phi (\mathbf{r}) \),

\[ \text{grad } \phi (\mathbf{r}) = \nabla \phi (\mathbf{r}) = e_i \frac{\partial \phi (\mathbf{r})}{\partial x_i}, \]

and the **divergence** and **curl** of a vector field \( \mathbf{A}(\mathbf{r}) \),

\[ \text{div } \mathbf{A}(\mathbf{r}) = \nabla \cdot \mathbf{A}(\mathbf{r}) = \frac{\partial A_i(\mathbf{r})}{\partial x_i}, \]
\[ \text{curl } \mathbf{A}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}) = \epsilon_{ijk} \frac{\partial A_j(\mathbf{r})}{\partial x_i} e_k. \]
Exercise: Using the Einstein summation convention, prove

\[ A \cdot B \times C = C \cdot A \times B, \]
\[ A \times (B \times C) = B (A \cdot C) - C (A \cdot B) \]

(you will need \( \epsilon_{ijk} \epsilon_{ipq} = \delta_{jp} \delta_{kq} - \delta_{jq} \delta_{kp} \) for this one), and

\[ \nabla(fg) = f \nabla g + g \nabla f \]
\[ \nabla \cdot (fA) = f \nabla \cdot A + A \cdot \nabla f \]
\[ \nabla \times (fA) = f \nabla \times A - A \times \nabla f \]
\[ \nabla \cdot (A \times B) = B \cdot \nabla \times A - A \cdot \nabla \times B \]
\[ \nabla \times (A \times B) = B \cdot \nabla A - A \cdot \nabla B - B \nabla \cdot A + A \nabla \cdot B \]
1.2 Curvilinear coordinates in physics problems

Key Point: Understand the importance of curvilinear coordinates in solving physics problems

Very often, physical systems are described by classical (or quantum) field theories. We have a field, e.g. \( \psi(r) \), which obeys a **differential equation** over all space, e.g. the Schrödinger Equation

\[
\frac{-\hbar^2}{2m} \nabla^2 \psi = E \psi
\]

The field is constrained by the differential equation and by **boundary conditions**.

- The differential equation is independent of coordinate system (though may look very different in different coordinate systems)
- The boundary condition is often very much simpler in one particular choice of coordinates, making the solution simpler in these coordinates.
- Use symmetries of the boundary conditions (incl. the position of sources/sinks) to choose your coordinate system.
Field \( \psi(r) \) \hspace{1cm} \text{Differential Equation}

General Solution

Boundary Conditions

Specific Solution

coordinate system

scenario independent

scenario dependent
Example: Spherical Polar Coordinates

Describe the position of a point in space using the distance from the origin, $r$, and two angles, $\theta$ and $\phi$.

\[
\begin{aligned}
x &= r \sin \theta \cos \phi \\
y &= r \sin \theta \sin \phi \\
z &= r \cos \theta 
\end{aligned}
\]

This is useful in problems with spherical symmetry.

e.g. Consider a hollow sphere or radius $R$ kept at a constant temperature $T_0$. The temperature inside the sphere obeys Laplace’s equation,

\[
\nabla^2 T(r, \theta, \phi) = 0
\]

which is coordinate system independent.

However, the boundary condition is much more easily expressed in spherical polar coordinates:

\[
T(R, \theta, \phi) = T_0
\]
Example: Cylindrical Coordinates

Describe the position of a point in space using the distance along the $z$-axis, the distance from the $z$-axis, $r$, and an angle, $\theta$.

![Diagram of cylindrical coordinates]

\[
\begin{align*}
x & = r \cos \theta \\
y & = r \sin \theta \\
z & = z
\end{align*}
\]

This is useful in problems with cylindrical symmetry.

e.g. Consider a wire with a uniform charge density $\rho_0$. The electric potential generated by the charge distribution is given by Poisson’s equation,

\[
\nabla^2 \phi(r, \theta, z) = -\frac{\rho(r, \theta, z)}{\varepsilon_0}
\]

which is coordinate system independent (and becomes Laplace’s equation away from the charge).

However, the charge density is much more easily expressed in cylindrical polar coordinates (with the wire running along the $z$-axis):

\[
\rho(0, \theta, z) = \rho_0
\]
1.3 Unit vectors and scale factors

Key Point: Write down the definition of basis vectors and scale factors for general curvilinear coordinates

In Cartesian coordinates, if I change the $x$-coordinate of the position vector $\mathbf{r}$ by an amount $dx$, then the object has moved a distance $dx$.

If I change all of the coordinates (infinitesimally) at once, I move $\mathbf{r}$ a distance $d\mathbf{r}$ where

$$ds^2 = d\mathbf{r} \cdot d\mathbf{r} = dx^2 + dy^2 + dz^2$$

using Pythagoras’ theorem. $d\mathbf{r}$ is know as the infinitesimal line element.

This may seem obvious, but the analogue is not true in general curvilinear coordinates.
e.g. Imagine changing $\theta$ by an amount $d\theta$ in cylindrical coordinates:

The distance moved is

$$2r \sin \left(\frac{d\theta}{2}\right) \approx rd\theta$$

for $d\theta$ small.

(The $z$-direction is out of the slide.)

- **How far we move** depends on the value of the coordinate $r$.

  How far we move for a particular coordinate shift is known as a **scale factor**.

- Also notice that **the direction we move** depends on the coordinate $\theta$.

  The direction we move for a particular coordinate shift is given by the **basis vector**.
Imagine a general coordinate system described by $q_i \ (i=1,2,3)$ and related to Cartesians via

$$x_i = f_i(q_1, q_2, q_3)$$

As we change the coordinate $q_i$, the position vector $r$ will move:

$$\frac{\partial r}{\partial q_i} = h_{qi} \varepsilon_{qi}$$

(no sum over $i$)

The **scale factor** is the magnitude of the vector $\frac{\partial r}{\partial q_i}$, i.e.

$$h_{qi} = \left| \frac{\partial r}{\partial q_i} \right|$$

The **basis vector** is the unit vector in the direction of $\frac{\partial r}{\partial q_i}$, i.e.

$$\varepsilon_{qi} = \frac{1}{h_{qi}} \frac{\partial r}{\partial q_i}$$

(no sum)
As before, the basis vectors are **orthogonal** if \( e_q_i \cdot e_q_j = \delta_{i,j} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \).

Let’s call \( ds_i \) the distance moved by changing the coordinate \( q_i \) by an amount \( dq_i \):  

\[
ds_i = h_{q_i} dq_i \quad \text{(no sum)}
\]

For orthogonal coordinates, we can use Pythagoras’ theorem again to write the total displacement from altering all three coordinates:  

\[
ds^2 = ds_1^2 + ds_2^2 + ds_3^2 = h_{q_1}^2 dq_1^2 + h_{q_2}^2 dq_2^2 + h_{q_3}^2 dq_3^2
\]

More formally, the change in the position vector is  

\[
dr = \sum_i \frac{\partial r}{\partial q_i} dq_i = \sum_i h_{q_i} e_{q_i} dq_i
\]

So,  

\[
ds^2 \equiv dr \cdot dr = \sum_i \frac{\partial r}{\partial q_i} dq_i = \sum_{i,j} h_{q_i} h_{q_j} e_{q_i} \cdot e_{q_j} dq_i dq_j = \sum_i h_{q_i}^2 dq_i^2
\]
More generally, one may define the metric of the space $g_{ij}$ according to

$$ds^2 = \sum_{i,j} g_{ij} dq_i dq_j = \left( \begin{array}{ccc} dq_1 & dq_2 & dq_3 \end{array} \right) \left( \begin{array}{ccc} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{array} \right) \left( \begin{array}{c} dq_1 \\ dq_2 \\ dq_3 \end{array} \right)$$

So, in our case we have

$$g_{ij} = h_{q_i} h_{q_j} c_{q_i} \cdot c_{q_j} = \begin{cases} h_i^2 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}$$

but this can in principle be more complicated.

The **volume element** is given by

$$dV = ds_1 \, ds_2 \, ds_3 = h_{q_1} h_{q_2} h_{q_3} \, dq_1 \, dq_2 \, dq_3$$
Key Point: Derive the scale factors and unit vectors for various coordinate systems

\[ \frac{\partial r}{\partial q_i} = h_{q_i} \mathbf{e}_{q_i} \]

(no sum)

Example: Cartesian Coordinates (trivial!)

The position vector is \( \mathbf{r} = x \mathbf{e}_x + y \mathbf{e}_y + z \mathbf{e}_z \)

So,

\[ \frac{\partial r}{\partial x} = \mathbf{e}_x, \quad \frac{\partial r}{\partial y} = \mathbf{e}_y, \quad \frac{\partial r}{\partial z} = \mathbf{e}_z. \]

These are already unit vectors, so are the basis vectors and the scale factors are,

\[ h_x = h_y = h_z = 1. \]

The volume element is \( dV = h_x \, dx \, h_y \, dy \, h_z \, dz = dx \, dy \, dz \), and the square of the infinitesimal line element is \( ds^2 = dx^2 + dy^2 + dz^2 \)
**Example:** Spherical Polar Coordinates

They are related to Cartesians by:

\[
\begin{align*}
x & = r \sin \theta \cos \phi \\
y & = r \sin \theta \sin \phi \\
z & = r \cos \theta
\end{align*}
\]

and the position vector is \( \mathbf{r} = x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z \)

\( (\mathbf{r} = r\mathbf{e}_r \text{ but since } \mathbf{e}_r \text{ changes with } \theta \text{ and } \phi, \text{ it is more convenient to use } \mathbf{e}_x, \mathbf{e}_y \text{ and } \mathbf{e}_z. ) \)

So,

\[
\begin{align*}
\frac{\partial \mathbf{r}}{\partial r} & = \frac{\partial x}{\partial r} \mathbf{e}_x + \frac{\partial y}{\partial r} \mathbf{e}_y + \frac{\partial z}{\partial r} \mathbf{e}_z = \sin \theta \cos \phi \mathbf{e}_x + \sin \theta \sin \phi \mathbf{e}_y + \cos \theta \mathbf{e}_z \\
\frac{\partial \mathbf{r}}{\partial \theta} & = \frac{\partial x}{\partial \theta} \mathbf{e}_x + \frac{\partial y}{\partial \theta} \mathbf{e}_y + \frac{\partial z}{\partial \theta} \mathbf{e}_z = r \cos \theta \cos \phi \mathbf{e}_x + r \cos \theta \sin \phi \mathbf{e}_y - r \sin \theta \mathbf{e}_z \\
\frac{\partial \mathbf{r}}{\partial \phi} & = \frac{\partial x}{\partial \phi} \mathbf{e}_x + \frac{\partial y}{\partial \phi} \mathbf{e}_y + \frac{\partial z}{\partial \phi} \mathbf{e}_z = -r \sin \theta \sin \phi \mathbf{e}_x + r \sin \theta \cos \phi \mathbf{e}_y
\end{align*}
\]
Normalize these vectors to find the basis vectors and scale factors:

\[
\left| \frac{\partial r}{\partial r} \right| = \sqrt{\sin^2 \theta \cos^2 \phi + \sin^2 \theta \sin^2 \phi + \cos^2 \theta} = 1
\]

\[
\left| \frac{\partial r}{\partial \theta} \right| = \sqrt{r^2 \cos^2 \theta \cos^2 \phi + r^2 \cos^2 \theta \sin^2 \phi + r^2 \sin^2 \theta} = r
\]

\[
\left| \frac{\partial r}{\partial \phi} \right| = \sqrt{r^2 \sin^2 \theta \sin^2 \phi + r^2 \sin^2 \theta \cos^2 \phi} = r \sin \theta
\]

So, we have **scale factors:** \( h_r = 1 \), \( h_\theta = r \), \( h_\phi = r \sin \theta \).

**basis vectors:**

\[
\begin{align*}
e_r &= \sin \theta \cos \phi \, e_x + \sin \theta \sin \phi \, e_y + \cos \theta \, e_z \\
e_\theta &= \cos \theta \cos \phi \, e_x + \cos \theta \sin \phi \, e_y - \sin \theta \, e_z \\
e_\phi &= -\sin \phi \, e_x + \cos \phi \, e_y
\end{align*}
\]

The **volume element** is \( dV = r^2 \sin \theta \, dr \, d\theta \, d\phi \), and the **square of the infinitesimal line element** is \( ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2 \).
We could have derived the scale factors directly from the square of the infinitesimal line element:

\[
\begin{align*}
\text{dx} &= dr \sin \theta \cos \phi + r \cos \theta \, d\theta \cos \phi - r \sin \theta \sin \phi \, d\phi, \\
\text{dy} &= dr \sin \theta \sin \phi + r \cos \theta \, d\theta \sin \phi + r \sin \theta \cos \phi \, d\phi, \\
\text{dz} &= dr \cos \theta - r \sin \theta \, d\theta.
\end{align*}
\]

So, write \( ds^2 = dx^2 + dy^2 + dz^2 \) and plug in \( dx, dy \) and \( dz \) (above). The cross terms vanish and we are left with

\[ ds^2 = dr^2 + r^2 \, d\theta^2 + r^2 \sin^2 \theta \, d\phi^2. \]

The lack of cross-terms tells us the coordinates are orthogonal, and the coefficients of the diagonal terms are the square of the scale factors.

**Exercise:** Find the scale factors, unit vectors, volume element and infinitesimal line element-squared for cylindrical coordinates.
1.3 The Gradient

Key Point: Derive an expression for the gradient in general orthogonal curvilinear co-ordinate systems

The gradient in Cartesian coordinates was: \[ \nabla = e_x \frac{\partial}{\partial x} + e_y \frac{\partial}{\partial y} + e_z \frac{\partial}{\partial z} \]

This tells us how fast a field changes with position, i.e. with respect to the distance moved NOT how much the parameter changes

⇒ We must take into account the scale factors.

For a curvilinear coordinates \( q_i \), recall the distance moved for a change \( dq_i \) was \( ds_i = h_{qi} dq_i \), so the component of the gradient in the direction of \( e_{qi} \) is

\[ \nabla q_i = \frac{\partial}{\partial s_i} = \frac{1}{h_{qi}} \frac{\partial}{\partial dq_i} \] (no sum)

and the gradient is

\[ \nabla = \sum_i e_{qi} \frac{\partial}{\partial s_i} = \sum_i e_{qi} \frac{1}{h_{qi}} \frac{\partial}{\partial q_i} = e_{q1} \frac{1}{h_{q1}} \frac{\partial}{\partial q_1} + e_{q2} \frac{1}{h_{q2}} \frac{\partial}{\partial q_2} + e_{q3} \frac{1}{h_{q3}} \frac{\partial}{\partial q_3} \]
1.5 The Divergence, Curl and Laplacian Operators

Key Point: Derive expressions for div, grad, curl and the Laplacian in general orthogonal curvilinear co-ordinate systems

**Divergence**

We may now use the form of the gradient to derive the divergence $\nabla \cdot A$

\[
\nabla \cdot A = \nabla \cdot \left( \sum_j A_j e_{qj} \right)
\]

$e_{qj}$ changes with coordinates, so we need to differentiate it too!

Before going any further we need to work out $\nabla \cdot e_{qj}$

Back to our definition of the gradient, acting on $q_j$:

\[
\nabla q_j = \sum_i e_{qi} \frac{1}{h_{qi}} \frac{\partial q_j}{\partial q_i} = \sum_i e_{qi} \frac{1}{h_{qi}} \delta_{ij} = e_{qj} \frac{1}{h_{qj}}
\]

\[\Rightarrow e_{qj} = h_{qj} \nabla q_j\]
Our unit vectors form a right-handed set, so \( \mathbf{e}_q \times \mathbf{e}_2 = \mathbf{e}_3 \)

\[
\Rightarrow \nabla q_1 \times \nabla q_2 = \frac{\mathbf{e}_3}{h_{q_1} h_{q_2}}
\]

But the divergence of the left-hand-side of this equation is zero:

\[
\nabla \cdot (\nabla q_1 \times \nabla q_2) = \nabla q_2 \cdot (\nabla \times \nabla q_1) - \nabla q_1 \cdot (\nabla \times \nabla q_2) = 0
\]

\[
\Rightarrow \nabla \cdot \left( \frac{\mathbf{e}_3}{h_{q_1} h_{q_2}} \right) = 0
\]

I can repeat this argument for cyclic permutations

\[
\Rightarrow \nabla \cdot \left( \frac{\mathbf{e}_1}{h_{q_2} h_{q_3}} \right) = \nabla \cdot \left( \frac{\mathbf{e}_2}{h_{q_3} h_{q_1}} \right) = \nabla \cdot \left( \frac{\mathbf{e}_3}{h_{q_1} h_{q_2}} \right) = 0
\]

This allows us to rearrange our equation in a nicer way.
\[ \nabla \cdot A = \nabla \cdot \left( \sum_j A_j e_{q_j} \right) \]

these have no divergence so can be pulled in front of the \( \nabla \)

\[ = \nabla \cdot \left( [h_{q_2} h_{q_3} A_1] \left( \frac{e_{q_1}}{h_{q_2} h_{q_3}} \right) + [h_{q_3} h_{q_1} A_2] \left( \frac{e_{q_2}}{h_{q_3} h_{q_1}} \right) + [h_{q_1} h_{q_2} A_3] \left( \frac{e_{q_3}}{h_{q_1} h_{q_2}} \right) \right) \]

\[ = \left( \frac{e_{q_1}}{h_{q_2} h_{q_3}} \right) \cdot \nabla \left( h_{q_2} h_{q_3} A_1 \right) + \left( \frac{e_{q_2}}{h_{q_3} h_{q_1}} \right) \cdot \nabla \left( h_{q_3} h_{q_1} A_2 \right) + \left( \frac{e_{q_3}}{h_{q_1} h_{q_2}} \right) \cdot \nabla \left( h_{q_1} h_{q_2} A_3 \right) \]

But \( e_{q_i} \cdot \nabla = \frac{1}{h_{q_i}} \frac{\partial}{\partial q_i} \), so finally we have,

\[ \nabla \cdot A = \frac{1}{h_{q_1} h_{q_2} h_{q_3}} \left( \frac{\partial}{\partial q_1} \left( h_{q_2} h_{q_3} A_1 \right) + \frac{\partial}{\partial q_2} \left( h_{q_3} h_{q_1} A_2 \right) + \frac{\partial}{\partial q_3} \left( h_{q_1} h_{q_2} A_3 \right) \right) \]
Curl

Curl works in much the same way. We may use the result we obtained earlier:

$$\nabla q_j = \epsilon q_j \frac{1}{h q_j} \Rightarrow \nabla \times \nabla q_j = \nabla \times \left( \frac{\epsilon q_j}{h q_j} \right) = 0$$

since, again, the left-hand-side is zero.

$$\nabla \times A = \nabla \times \left( \sum_j A_j \epsilon q_j \right)$$

$$= \nabla \times \left( \left[ h q_1 A_1 \right] \frac{\epsilon q_1}{h q_1} + \left[ h q_2 A_2 \right] \frac{\epsilon q_2}{h q_2} + \left[ h q_3 A_3 \right] \frac{\epsilon q_3}{h q_3} \right)$$

$$= - \left( \frac{\epsilon q_1}{h q_1} \right) \nabla (h q_2 A_1) - \left( \frac{\epsilon q_2}{h q_2} \right) \nabla (h q_2 A_2) - \left( \frac{\epsilon q_3}{h q_3} \right) \nabla (h q_3 A_3)$$

Remember that $$\nabla = \frac{\epsilon q_1}{h q_1} \frac{\partial}{\partial q_1} + \frac{\epsilon q_2}{h q_2} \frac{\partial}{\partial q_2} + \frac{\epsilon q_3}{h q_3} \frac{\partial}{\partial q_3}$$

so I will pick up contributions for $$[\nabla \times A]_1$$ from the terms linked by the arrows.
\[ [\nabla \times A]_1 = -\frac{1}{h_{q_2} h_{q_3}} \frac{\partial}{\partial q_3} (h_{q_2} A_2) + \frac{1}{h_{q_2} h_{q_3}} \frac{\partial}{\partial q_2} (h_{q_3} A_3) \]

Similarly for the other terms.

We can write this as a determinant:

\[
\nabla \times A = \frac{1}{h_{q_1} h_{q_2} h_{q_3}} \begin{vmatrix}
    h_{q_1} e_{q_1} & h_{q_2} e_{q_1} & h_{q_3} e_{q_1} \\
    \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\
    h_{q_1} A_1 & h_{q_2} A_2 & h_{q_3} A_3 
\end{vmatrix}
\]
Laplacian

The laplacian is $\nabla \cdot \nabla = \nabla^2$, so we can fairly easily insert our expression for the gradient into the expression we derived for the divergence:

$$\nabla^2 = \frac{1}{h_{q_1} h_{q_2} h_{q_3}} \left( \frac{\partial}{\partial q_1} (h_{q_2} h_{q_3} \nabla_1) + \frac{\partial}{\partial q_2} (h_{q_3} h_{q_1} \nabla_2) + \frac{\partial}{\partial q_3} (h_{q_1} h_{q_2} \nabla_3) \right)$$

but $\nabla_i = \frac{1}{h_{q_i}} \frac{\partial}{\partial q_i}$

So,

$$\nabla^2 = \frac{1}{h_{q_1} h_{q_2} h_{q_3}} \left( \frac{\partial}{\partial q_1} \begin{bmatrix} h_{q_2} h_{q_3} \\ h_{q_1} \end{bmatrix} \frac{\partial}{\partial q_1} + \frac{\partial}{\partial q_2} \begin{bmatrix} h_{q_3} h_{q_1} \\ h_{q_2} \end{bmatrix} \frac{\partial}{\partial q_2} + \frac{\partial}{\partial q_3} \begin{bmatrix} h_{q_1} h_{q_2} \\ h_{q_3} \end{bmatrix} \frac{\partial}{\partial q_3} \right)$$

remember both of these derivatives are acting on **everything** to the right (despite the brackets)
Key Point: Apply these expressions to various coordinate systems, including spherical polar coordinates and cylindrical coordinates.

Example: Spherical Polar Coordinates: \( h_r = 1, \ h_\theta = r, \ h_\phi = r \sin \theta \)

\[
\nabla = e_r \frac{\partial}{\partial r} + e_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + e_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}
\]

\[
\nabla \cdot \mathbf{A} = \frac{1}{r^2 \sin \theta} \left( \frac{\partial}{\partial r} \left( r^2 \sin \theta A_r \right) + \frac{\partial}{\partial \theta} \left( r \sin \theta A_\theta \right) + \frac{\partial}{\partial \phi} \left( r A_\phi \right) \right)
\]

\[
\nabla \times \mathbf{A} = \frac{1}{r^2 \sin \theta} \begin{vmatrix}
 e_r & e_\theta & r \sin \theta e_\phi \\
 \frac{\partial}{\partial r} & \frac{\partial}{\partial \theta} & \frac{\partial}{\partial \phi} \\
 A_r & r A_\theta & r \sin \theta A_\phi
\end{vmatrix}
\]

\[
\nabla^2 = \frac{1}{r^2 \sin \theta} \left( \frac{\partial}{\partial r} \left[ r^2 \sin \theta \frac{\partial}{\partial r} \right] + \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial}{\partial \theta} \right] + \frac{\partial}{\partial \phi} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right] \right)
\]
Exercise: Find the gradient, divergence, curl and Laplacian for cylindrical coordinates.

Exercise: Using spherical polar coordinates, show that

\[ \nabla f(r) = e_r \frac{df}{dr} \]
\[ \nabla \cdot (f(r) e_r) = \frac{2}{r} f(r) + \frac{df}{dr} \]
\[ \nabla \times (f(r) e_r) = 0 \]

and apply these results to show

\[ \nabla r = e_r \]
\[ \nabla \cdot r = 3 \]
\[ \nabla \times r = 0 \]
2. Partial Differential Equations in cylindrical and spherical polar coordinates

2.1 Common Differential Equations

Key Point: Write down Laplace’s equation, Poisson’s equation, the Diffusion equation, the Wave equation, the Helmholtz equation and Schrödinger’s equation.

We have already seen that physical systems are often described by scalar and vector fields in space and time, that obey particular differential equations involving the operators of the previous section.

Laplace’s Equation:

\[ \nabla^2 \phi(r) = 0 \]

Used in electromagnetism, gravitation, hydrodynamics, heat flow, etc, when there are no sources or sinks.

Pierre-Simon, Marquis de Laplace, 1749-1827
Poisson’s Equation:

\[ \nabla^2 \phi(r) = f(r) \]

Used in electromagnetism, gravitation, hydrodynamics, heat flow, etc, with sources or sinks.

**Example:** Maxwell’s equations include

\[ \nabla \cdot \mathbf{E} = \rho(r)/\varepsilon_0 \]

where \( \mathbf{E} \) is the electric field, \( \rho(r) \) is the charge density (at position \( r \)) and \( \varepsilon_0 \) is the permittivity of free space.

In electrostatics, we can write the electric field as the gradient of a potential, \( \mathbf{E} = -\nabla \phi \)

and the equation becomes

\[ \nabla^2 \phi(r) = -\rho(r)/\varepsilon_0 \]

i.e. Poisson’s equation.

If we have no charge (i.e. no sources) then this reduces to Laplace’s equation:

\[ \nabla^2 \phi(r) = 0 \]
Diffusion Equation

\[ \nabla^2 \phi(r,t) = \frac{1}{\alpha} \frac{\partial \phi(r,t)}{\partial t} \]

diffusivity (sometimes called the ‘diffusion coefficient’)
[Boas calls this \( \alpha^2 \)]

Used for heat flow, diffusion of materials, etc., when there are no sources.

For systems which have reached equilibrium (i.e. don’t change with time) the time derivative term vanishes and we have Laplace’s equation again.

**Example:** Imagine heat flowing in a metal, where the temperature is a function of position \( r \) and time \( t \), i.e. \( T(r,t) \). The heat energy contained in a small volume \( V \) is

\[ Q = \int_V \rho c_p T(r,t) \, d^3r \]

density
specific heat capacity

The rate at which heat transfers from one volume to another depends on the temperature gradient, the area in contact and the heat conductivity of the material.
The rate at which heat transfers from one volume to another is proportional to the temperature gradient, the area in contact and the thermal conductivity of the material. For a boundary of area \( A \),

\[
\frac{dQ}{dt} = \int_A k \, d\sigma \cdot \nabla T(r, t)
\]

Gauss’ theorem relates an integral over the boundary to an integral over the volume:

\[
\int_A F \cdot d\sigma = \int_V \nabla \cdot F \, d^3r
\]

Applying this to the above (and assuming \( k \) is constant)

\[
\frac{dQ}{dt} = \int_V \nabla \cdot [k \nabla T(r, t)] \, d^3r = \int_V k \nabla^2 T(r, t) \, d^3r
\]

Equating with the expression for \( Q \) (and assuming \( \rho \) and \( c_p \) are constant too)

\[
\frac{dQ}{dt} = \int_V \rho c_p \frac{\partial T(r, t)}{\partial t} \, d^3r = \int_V k \nabla^2 T(r, t) \, d^3r
\]

\[
\Rightarrow \nabla^2 T(r, t) = \frac{\rho c_p}{k} \frac{\partial T(r, t)}{\partial t}
\] (since the volume was arbitrary)
Wave Equation

\[ \nabla^2 \phi(r, t) = \frac{1}{v^2} \frac{\partial^2 \phi(r, t)}{\partial t^2} \]

This is a very important equation since it governs the motions of waves, e.g. vibrating strings, vibrations in solids, sound waves, water waves, electromagnetic waves.

It is so significant that the operator

\[ \Box^2 \equiv \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \]

has a special name, the d’Alembertian, and a special symbol (where c is the speed of light).

The equation \( (\Box^2 - m^2) \phi = 0 \) is known as the Klein-Gordon equation and is very important in particle physics.
**Example:** Maxwell’s equations (again!) in vacuum are

\[ \nabla \times E = -\frac{\partial B}{\partial t} \]
\[ \nabla \times B = \mu_0 \varepsilon_0 \frac{\partial E}{\partial t} \]
\[ \nabla \cdot E = 0 \]
\[ \nabla \cdot B = 0 \]

Taking the curl of the first one and inserting the second

\[ \nabla \times (\nabla \times E) = -\frac{\partial}{\partial t} \nabla \times B = -\mu_0 \varepsilon_0 \frac{\partial^2 E}{\partial t^2} \]

But

\[ \nabla \times (\nabla \times E) = \nabla (\nabla \cdot E) - \nabla^2 E \]

\[ \Rightarrow \nabla^2 E = \varepsilon_0 \mu_0 \frac{\partial^2 E}{\partial t^2} \]

Measuring \( \varepsilon_0 \) and \( \mu_0 \) tells us that electric fields are waves travelling with speed

\[ c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} = 299\,792\,458\,\text{ms}^{-1} \]
The + sign is the Helmholtz equation, while the – sign is the time-independent diffusion equation.

Both of these equations are special cases of the wave equation and time-dependent diffusion equation, when the dependence on time has been factored out.
Schrödinger Equation

This comes in both time-dependent and time-independent forms.

The time-dependent Schrödinger Equation:

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = i\hbar \frac{\partial \psi}{\partial t} \]

The time-independent Schrödinger Equation:

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi \]

These govern the wave-function of a particle state in non-relativistic quantum mechanics. It is simply a relation between energy and momentum in an operator form.

Energy operator: \( \hat{E} = i\hbar \frac{\partial}{\partial t} \)

Momentum operator: \( \hat{p} = -i\hbar \nabla \)

\[ \frac{\hat{p}^2}{2m} \psi + V\psi = \hat{E} \psi \]

kinetic energy

potential energy

total energy
2.2 The method of separation of variables

These equations have multiple dimensions in them. One useful method of solving them is to separate the differential equation into separate differential equations for each dimension.

Removing the time dependence

Consider the (time-dependent) diffusion equation:

\[ \nabla^2 \phi(r, t) = \frac{1}{\alpha} \frac{\partial \phi(r, t)}{\partial t} \]

Let’s look for solutions of the form

\[ \phi(r, t) = \Phi(r) T(t) \]

There might not be a solution of this form, and often there will be solutions not of this form, so this is not necessarily going to work, but there is no harm in trying!

\[ T(t) \nabla^2 \Phi(r) = \frac{1}{\alpha} \Phi(r) \frac{dT(t)}{dt} \quad \Rightarrow \quad \frac{1}{\Phi(r)} \nabla^2 \Phi(r) = \frac{1}{\alpha \frac{1}{T(t)} \frac{dT(t)}{dt}} \]

no \( t \) dependence

no \( r \) dependence
So (if our original assumption about $\phi(r)$ was true) both sides must just be equal to a constant:

$$
\frac{1}{\Phi(r)} \nabla^2 \Phi(r) = \frac{1}{\alpha T(t)} \frac{dT(t)}{dt} = k^2
$$

an arbitrary constant (no $t$ or $r$ dependence)

Now we have two separate equations:

$$
\frac{dT(t)}{dt} = \alpha k^2 T(t)
$$

$$
\nabla^2 \Phi(r) = k^2 \Phi(r)
$$

the time-independent diffusion equation

We can now solve each of these separately and cobble them together at the end.
Key Point: Apply the method of separation of variables to Laplace’s Equation in spherical and cylindrical coordinates

We may decompose Laplace’s equation ($\nabla^2 \varphi = 0$) into three equations in a similar way. (I will use $\varphi$ rather than $\phi$ for the field to avoid confusion with the coordinate.)

Laplace’s equation in spherical polar coordinates is:

$$\frac{1}{r^2 \sin \theta} \left( \frac{\partial}{\partial r} \left[ r^2 \sin \theta \frac{\partial \varphi(r, \theta, \phi)}{\partial r} \right] + \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial \varphi(r, \theta, \phi)}{\partial \theta} \right] + \frac{\partial}{\partial \phi} \left[ \frac{1}{\sin \theta} \frac{\partial \varphi(r, \theta, \phi)}{\partial \phi} \right] \right) = 0$$

We rewrite our $\varphi$ as a product of three functions, each depending on one coordinate:

$$\varphi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi)$$

Now divide by $R(r) \Theta(\theta) \Phi(\phi)$ to give

$$\frac{1}{R \theta \phi} \left( \Theta \Phi \frac{\partial}{\partial r} \left[ r^2 \sin \theta \frac{dR}{dr} \right] + R \Phi \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{d\Theta}{d\theta} \right] + R \Theta \frac{\partial}{\partial \phi} \left[ \frac{1}{\sin \theta} \frac{d\Phi}{d\phi} \right] \right) = 0$$

$$\Rightarrow \frac{1}{R \partial r} \left[ r^2 \sin \theta \frac{dR}{dr} \right] + \frac{1}{\Theta \partial \theta} \left[ \sin \theta \frac{d\Theta}{d\theta} \right] + \frac{1}{\Phi \partial \phi} \left[ \frac{1}{\sin \theta} \frac{d\Phi}{d\phi} \right] = 0$$
\[
\frac{1}{R} \frac{\partial}{\partial r} \left[ r^2 \sin \theta \frac{dR}{dr} \right] + \frac{1}{\Theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{d\Theta}{d\theta} \right] + \frac{1}{\Phi} \frac{\partial}{\partial \phi} \left[ \frac{1}{\sin \theta} \frac{d\Phi}{d\phi} \right] = 0
\]

(Same as on previous slide)

\[
\rightarrow \quad \sin^2 \theta \frac{1}{R} \frac{d}{dr} \left[ r^2 \frac{dR}{dr} \right] + \sin \theta \frac{1}{\Theta} \frac{d}{d\theta} \left[ \sin \theta \frac{d\Theta}{d\theta} \right] = -\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2}
\]

no \( \phi \) dependence

no \( r \) or \( \theta \) dependence

So, just like for the time separation, each side **must** be constant, say \( m^2 \).

\[
\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = -m^2
\]

and

\[
\sin^2 \theta \frac{1}{R} \frac{d}{dr} \left[ r^2 \frac{dR}{dr} \right] + \sin \theta \frac{1}{\Theta} \frac{d}{d\theta} \left[ \sin \theta \frac{d\Theta}{d\theta} \right] = m^2
\]

We can repeat this procedure to separate the \( r \) and \( \theta \) equations

\[
\frac{1}{R} \frac{d}{dr} \left[ r^2 \frac{dR}{dr} \right] = -\frac{1}{\sin \theta} \frac{1}{\Theta} \frac{d}{d\theta} \left[ \sin \theta \frac{d\Theta}{d\theta} \right] + \frac{m^2}{\sin^2 \theta} = k
\]
Finally, we have a set of three equations, one for each coordinate:

**The equation for \( R(r) \)**

\[
\frac{d}{dr} \left[ r^2 \frac{dR(r)}{dr} \right] - kR(r) = 0 \quad \Rightarrow r^2 \frac{d^2R(r)}{dr^2} + 2r \frac{dR(r)}{dr} - kR(r) = 0
\]

Since the coefficients are polynomials of \( r \), try a solution of the form \( R(r) = r^n \)

\[
\Rightarrow r^2 n(n - 1)r^{n-2} + 2nr^{n-1} - kr^n = 0
\]

\[
\Rightarrow n(n - 1) r^n + 2nr^n - kr^n = 0
\]

\[
\Rightarrow n(n + 1) - k = 0
\]

\( k \) was an arbitrary constant, so I can write it however I like. It is more convenient to write \( k = l(l + 1) \)

\[
\Rightarrow n(n + 1) = l(l + 1) \quad \Rightarrow n = l \text{ or } -l - 1
\]

The general solution is

\[
R(r) = Ar^l + Br^{-l-1}
\]

where \( A \) and \( B \) are independent of \( r \).
The equation for $\Phi(\phi)$

\[ \frac{d^2 \Phi(\phi)}{d\phi^2} = -m^2 \Phi(\phi) \]

Since the coefficient is a constant, the solution must have a form $\Phi(\phi) = e^{\alpha \phi}$

\[ \Rightarrow \alpha^2 \Phi(\phi) = -m^2 \Phi(\phi) \quad \Rightarrow \alpha = \pm im \]

The general solution is $\Phi(\phi) = A e^{im\phi} + B e^{-im\phi}$ or (usually) more conveniently

\[ \Phi(\phi) = A' \sin m\phi + B' \cos m\phi \]

where $A'$ and $B'$ are constant

Notice that $m$ must be an integer since $\Phi(\phi + 2\pi) = \Phi(\phi)$.

(this is where the “quantum” of “quantum mechanics” comes from!)
The equation for $\Theta(\theta)$

$$
\sin \theta \frac{d}{d\theta} \left[ \sin \theta \frac{d \Theta(\theta)}{d\theta} \right] - m^2 \Theta(\theta) + l(l+1) \sin^2 \theta \Theta(\theta) = 0
$$

This one is a little bit too hard for now. The solution is an Associated Legendre Polynomial.

We will study these functions in detail later (section 3). For now, we will just write the general solution as

$$
\Theta(\theta) = A P_l^m(\cos \theta)
$$

where $A$ is a constant.

The $l$ and $m$ here are labels corresponding to the differential equation. We saw earlier that $m$ must be an integer. The associated Legendre function similarly insist that $l \geq 0$, and $|m| \leq l$. 
The general solution to \( \nabla^2 \varphi(r, \theta, \phi) = 0 \) is therefore

\[
\varphi(r, \theta, \phi) = \sum_{m=0}^{l} \sum_{l=0}^{\infty} \left[ A_{lm} r^l \sin(m\phi) + B_{lm} r^l \cos(m\phi) 
+ C_{lm} r^{-l-1} \sin(m\phi) + D_{lm} r^{-l-1} \cos(m\phi) \right] P_l^m(\cos \theta)
\]

\( A_{lm}, B_{lm}, C_{lm} \) and \( D_{lm} \) are constants, which are determined by the boundary conditions of the physical problem.

The functions \( Y_l^m(\theta, \phi) = N e^{im\phi} P_l^m(\cos \theta) \) with \( l \geq 0 \) and \( |m| \leq l \), which give the angular dependence are known as spherical harmonics \((N \text{ is a normalization constant})\)
Key Point: Apply boundary conditions to general solutions to provide solutions to physical problems.

A physical example

The surface of a metal sphere, or radius $r_0$ is held at an electrostatic potential of $\varphi_0 \cos \theta$, where $\theta$ is the polar angle. Find the electrostatic potential inside and outside the sphere, assuming no other sources of electric charge.

There are no sources, other than the sphere, so the electrostatic potential obeys Laplace’s equation away from the sphere. We can solve Laplace’s equation to provide a general solution.

The boundary conditions are

\[ \varphi(r_0, \theta, \phi) = \varphi_0 \cos \theta \]

\[ \lim_{r \to \infty} \varphi(r, \theta, \phi) = 0 \]

\[ \varphi(r, \theta, \phi) \text{ should be finite everywhere} \]

These are most easily expressed in spherical polar coordinates, so that is the coordinate system we should use.

We apply the boundary conditions to the general solution to obtain a specific solution.
The general solution to $\nabla^2 \varphi(r, \theta, \phi) = 0$ is, from before:

$$
\varphi(r, \theta, \phi) = \sum_{m=0}^{l} \sum_{l=0}^{\infty} \left[ A_{lm} r^l \sin(m\phi) + B_{lm} r^l \cos(m\phi) \right. \\
\left. + C_{lm} r^{-l-1} \sin(m\phi) + D_{lm} r^{-l-1} \cos(m\phi) \right] P^m_l(\cos \theta)
$$

Apply boundary conditions:

Inside the sphere:

$$R(r) \propto r^{-l-1} \text{ would give infinity at } r = 0 \quad \text{so} \quad C_{lm} = D_{lm} = 0.$$ 

So,

$$\varphi(r, \theta, \phi) = \sum_{m=0}^{l} \sum_{l=0}^{\infty} \left[ A_{lm} \sin(m\phi) + B_{lm} \cos(m\phi) \right] r^l P^m_l(\cos \theta)$$

The boundary condition $\varphi(r_0, \theta, \phi) = \phi_0 \cos \theta$ has no $\phi$ dependence.

$$\Rightarrow \quad A_{lm} = B_{lm} = 0 \quad \text{for} \quad m > 0$$
The first few Legendre polynomials (associated Legendre polynomials with $m = 0$) are

\[
\begin{align*}
P_0(x) &= 1 \\
P_1(x) &= x \\
P_2(x) &= \frac{1}{2}(3x^2 - 1) \\
P_3(x) &= \frac{1}{2}(5x^3 - 3x)
\end{align*}
\]

(You will get to derive these later!)

**Exercise:** Show that the above functions with $x = \cos \theta$ are solutions of

\[
\sin \theta \frac{d}{d\theta} \left[ \sin \theta \frac{dP_l(\cos \theta)}{d\theta} \right] + l(l+1) \sin^2 \theta P_l(\cos \theta) = 0
\]

But

\[
\varphi(r_0, \theta, \phi) = \sum_{l=0}^{\infty} B_{l0} r_0^l P_l(\cos \theta) = \varphi_0 \cos \theta
\]

so, since the other Legendre polynomials are higher powers of $x$, $l = 1$, and the electrostatic potential is

\[
\varphi(r, \theta, \phi) = \varphi_0 \frac{r}{r_0} \cos \theta \\
\text{ (for } r < r_0)\]
More formally,
\[ \varphi(r_0, \theta, \phi) = \sum_{l=0}^{\infty} B_{l0} r_0^l P_l(\cos \theta) = \varphi_0 \cos \theta \]

\[ \Rightarrow \sum_{l=0}^{\infty} B_{l0} r_0^l \int_{-1}^{1} P_k(\cos \theta) P_l(\cos \theta) \, d\cos \theta = \varphi_0 \int_{-1}^{1} \cos \theta P_k(\cos \theta) \, d\cos \theta \]

\[ = \varphi_0 \int_{-1}^{1} P_1(\cos \theta) P_k(\cos \theta) \, d\cos \theta \]

We can then use the **orthogonality relation** for Legendre polynomials (which I will prove later in the course):

\[ \int_{-1}^{1} P_l(\cos \theta) P_k(\cos \theta) \, d\cos \theta = \frac{2}{2l + 1} \delta_{lk} \]

\[ \Rightarrow \sum_{l=0}^{\infty} B_{l0} r_0^l \frac{2}{2l + 1} \delta_{lk} = \varphi_0 \frac{2}{3} \delta_{1k} \quad \Rightarrow B_{k0} r_0^k \frac{2}{2k + 1} = \varphi_0 \frac{2}{3} \delta_{1k} \]

So \( B_{10} = \varphi_0 \frac{1}{r_0} \) and \( B_{k0} = 0 \) for \( k \neq 1 \)
Outside the sphere

\[ R(r) \propto r^l \text{ would give infinity at } r \to \infty \text{ so } A_{lm} = B_{lm} = 0. \]

we need \( \phi \) to drop to zero infinitely far from the sphere, since this is what we would have if we removed the sphere.

The same arguments for the angular dependence hold as for inside, so

\[ \varphi(r, \theta, \phi) = \varphi_0 \left( \frac{r_0}{r} \right)^2 \cos \theta \quad (r > r_0) \]

**Exercise**: A conducting sphere of radius \( r_0 \) is placed in an originally uniform electric field \( E \), and maintained at zero potential.

Show that the potential outside the sphere is

\[ \varphi(r, \theta, \phi) = |E| \left( r - \frac{r_0^3}{r^2} \right) \cos \theta, \]

where the line \( \theta = 0 \) is aligned with the direction of \( E \).
Laplace’s Equation is separable in all the following coordinate systems, with solutions written in terms of the functions shown:

<table>
<thead>
<tr>
<th>Coordinate System</th>
<th>Functions in solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cartesian</td>
<td>exponential functions, trigonometric functions, hyperbolic functions</td>
</tr>
<tr>
<td>circular cylindrical</td>
<td><strong>Bessel functions</strong>, exponential functions, trigonometric functions</td>
</tr>
<tr>
<td>conical</td>
<td>ellipsoidal harmonics, powers</td>
</tr>
<tr>
<td>ellipsoidal</td>
<td>ellipsoidal harmonics</td>
</tr>
<tr>
<td>elliptic cylindrical</td>
<td>Mathieu functions, trigonometric functions</td>
</tr>
<tr>
<td>oblate spheroidal</td>
<td><strong>Legendre polynomial</strong>, trigonometric functions</td>
</tr>
<tr>
<td>parabolic</td>
<td><strong>Bessel functions</strong>, trigonometric functions</td>
</tr>
<tr>
<td>parabolic cylindrical</td>
<td>parabolic cylinder functions, <strong>Bessel functions</strong>, trigonometric functions</td>
</tr>
<tr>
<td>paraboloidal</td>
<td>trigonometric functions</td>
</tr>
<tr>
<td>prolate spheroidal</td>
<td><strong>Legendre polynomial</strong>, trigonometric functions</td>
</tr>
<tr>
<td>spherical</td>
<td><strong>Legendre polynomial</strong>, power, trigonometric functions</td>
</tr>
</tbody>
</table>
Separation of variables in cylindrical coordinates

**Exercise**: Use the method of separation of variables to find a general solution to Laplace’s equation in cylindrical polar coordinates.

You may write your solution in terms of **Bessel functions** $J_n(kr)$, which are the solutions of the differential equation

$$r \frac{d}{dr} \left[ r \frac{dJ_n(kr)}{dr} \right] + (k^2 r^2 - n^2) J_n(kr) = 0$$

($k$ and $n$ constants)

Although $J_{-n}(kr)$ is clearly also a solution to the radial equation (since the equation only involves $n^2$) it is not an independent solution for $n$ an integer, since

$$J_{-n}(kr) = (-1)^n J_n(kr)$$
2.3 Spherical harmonics and the Schrödinger Equation.

Key Point: Define spherical harmonics and understand their role in the solution of Schrödinger’s equation.

Recall the time independent Schrödinger equation:

\[-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi\]

In Spherical coordinates, this becomes

\[-\frac{\hbar^2}{2m} \frac{1}{r^2 \sin \theta} \left( \frac{\partial}{\partial r} \left[ r^2 \sin \theta \frac{\partial \psi}{\partial r} \right] + \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial \psi}{\partial \theta} \right] + \frac{\partial}{\partial \phi} \left[ \frac{1}{\sin \theta} \frac{\partial \psi}{\partial \phi} \right] \right) + (V - E)\psi = 0\]

In principle, $V$ is a function of $r$, $\theta$ and $\phi$, but often it is only a function of $r$.

We can separate this into equations for each of the coordinates as we did before, but this time, let’s just separate into a radial and angular part.
\[ \psi(r, \theta, \phi) = R(r) Y(\theta, \phi) \]

\[
\begin{align*}
\rightarrow \quad & \quad \frac{1}{R} \frac{d}{dr} \left[ r^2 \frac{dR}{dr} \right] - \frac{2m}{\hbar^2} (V(r) - E) r^2 = -\frac{1}{\sin \theta} \frac{1}{Y} \left[ \sin \theta \frac{\partial Y}{\partial \theta} \right] - \frac{1}{\sin^2 \theta} Y \frac{\partial^2 Y}{\partial \phi^2} = l(l+1) \\
\end{align*}
\]

We can’t solve the radial equation without knowing \( V(r) \), but we can solve the angular part (since we have explicitly required the potential to have no angular dependence).

Radial:
\[
\frac{d}{dr} \left[ r^2 \frac{dR(r)}{dr} \right] - \frac{2m}{\hbar^2} (V(r) - E) r^2 R(r) - l(l+1) R(r) = 0 
\]
(for later use)

Angular:
\[
\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right] + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} + l(l+1) Y(\theta, \phi) = 0
\]

The solutions to this angular part are the **spherical harmonics** (as we saw earlier):

\[ Y_l^m(\theta, \phi) = N e^{im\phi} P_l^m(\cos \theta) \]
The constant $N$ is fixed by requiring an orthogonality condition:

$$
\int_0^\theta \int_0^{2\pi} Y_l^m(\theta, \phi) Y_{l'}^{m'}(\theta, \phi) \sin \theta \, d\theta \, d\phi = \delta_{ll'} \delta_{mm'} \quad \Rightarrow \quad N = \sqrt{\frac{(2l + 1)(l - m)!}{4\pi (l + m)!}}
$$

measure $\, ds_\theta \, ds_\phi$

**What is the physical significance of $l$ and $m$?**

Angular momentum is defined by $\hat{L} = r \times \hat{p}$

In quantum mechanics, the momentum operator is $\hat{p} = -i\hbar \nabla$, so angular momentum is

$$
\hat{L} = -i\hbar \, r \times \nabla
$$

In spherical coordinates, this is

$$
\hat{L} = -i\hbar \left[ e_\phi \frac{\partial}{\partial \theta} - e_\theta \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right]
$$
Hopefully, you know by now that the important operators in quantum mechanical discussions of angular momentum are $\hat{L}^2$ and $\hat{L}_z$. What are these in spherical polars?

\[
\hat{L}^2 = -\hbar^2 \left[ e_\phi \frac{\partial}{\partial \theta} - e_\theta \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right] \cdot \left[ e_\phi \frac{\partial}{\partial \theta} - e_\theta \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right]
\]

\[
= -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]
\]

and

\[
\hat{L}_z = e_z \cdot \hat{L} = -i\hbar \frac{\partial}{\partial \phi}
\]

(After some algebra – remember to differentiate the basis vectors too!)

**Exercise:** Prove the above results for $\hat{L}^2$ and $\hat{L}_z$
Let’s apply these operators to the spherical harmonics:

\[ \hat{L}^2 Y_l^m(\theta, \phi) = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial Y_l^m(\theta, \phi)}{\partial \theta} \right] + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y_l^m(\theta, \phi)}{\partial \phi^2} \right] = l(l + 1)\hbar \ Y_l^m(\theta, \phi) \]

and

\[ \hat{L}_z Y_l^m(\theta, \phi) = -i\hbar \frac{\partial Y_l^m(\theta, \phi)}{\partial \phi} = -i\hbar N \frac{\partial e^{im\phi}}{\partial \phi} \ P_l^m(\theta) \]

\[ = -i\hbar N \im e^{im\phi} \ P_l^m(\theta) = m\hbar \ Y_l^m(\theta, \phi) \]

So \( Y_l^m(\theta, \phi) \) is the angular part of a state with angular momentum of magnitude \( \sqrt{l(l + 1)\hbar} \) and z-component \( m\hbar \).
3. Legendre Polynomials and Bessel Functions

3.1 Legendre Polynomials and the Coulomb potential

Key Point: Define Legendre polynomials from a generating function

The Legendre polynomials may be defined by

\[ g(t, x) = \frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n \]

One can then find expressions for the Legendre polynomials by expanding the root in powers of \( t \), and equating coefficients.
Equating powers of $t$:

\[
(1-2xt+t^2)^{-1/2} = 1 + \frac{1}{2}(2xt-t^2) + \frac{3}{8}(2xt-t^2)^2 + \frac{5}{12}(2xt-t^2)^3 + \frac{35}{128}(2xt-t^2)^4 + \mathcal{O}(t^5)
\]

\[
\Rightarrow \sum_{n=0}^{\infty} P_n(x)t^n = t^0 + xt^1 + \frac{1}{2}(3x^2-1)t^2 + \frac{1}{2}(5x^3-3)t^3 + \frac{1}{8}(35x^4-30x^2+3)t^4 + \mathcal{O}(t^5)
\]

You can have fun working out the next few (they get harder) but it is rather tedious…

Note that these are not the associated Legendre polynomials we saw in the spherical harmonics. They are only ‘ordinary’ Legendre polynomials, that is associated Legendre polynomials with $m=0$, i.e. $P_n(x) = P^0_n(x)$. 

58
Notice that the value at $x = \pm 1$ is rather simple:

$$g(t, \pm 1) = \frac{1}{\sqrt{1 \mp 2t + t^2}} = \frac{1}{\sqrt{(1 \mp t)^2}} = \frac{1}{1 \mp t} = 1 \pm t + t^2 \pm t^3 + \ldots = \sum_{n=0}^{\infty} (-1)^n t^n$$

But,

$$g(t, \pm 1) = \sum_{n=0}^{\infty} P_n(\pm 1) t^n$$

so,

\[
P_n(1) = 1 \quad \text{for all Legendre polynomials}
\]

\[
P_n(-1) = (-1)^n = \begin{cases} 1 & \text{for } n \text{ even} \\ -1 & \text{for } n \text{ odd} \end{cases}
\]

Also,

$$g(-t, -x) = \frac{1}{\sqrt{1 - 2(-x)(-t) + (-t)^2}} = \frac{1}{\sqrt{1 - 2xt + t^2}} = g(t, x)$$

Equating powers of $t$:

$$P_n(-x) = (-1)^n P_n(x)$$
Key Point: Expand the Coulomb potential in Legendre polynomials

There is an interesting direct physical interpretation of Legendre polynomials.

Consider a point charge $q$ on the $z$-axis, a distance $a$ from the origin. The electrostatic potential at a point $r$ will be:

$$\varphi(r) = \frac{1}{4\pi\varepsilon_0} \frac{q}{d} = \frac{1}{4\pi\varepsilon_0} \frac{q}{|r - ae_z|}$$

$$= \frac{1}{4\pi\varepsilon_0} \frac{q}{\sqrt{(r - ae_z) \cdot (r - ae_z)}}$$

$$= \frac{1}{4\pi\varepsilon_0} \frac{q}{\sqrt{r^2 - 2ra \cos \theta + a^2}}$$

$$= \frac{q}{4\pi\varepsilon_0r} \left[ 1 - 2\frac{a}{r} \cos \theta + \left(\frac{a}{r}\right)^2 \right]^{-1/2} = \frac{q}{4\pi\varepsilon_0r} \sum_{n=0}^{\infty} P_n(\cos \theta) \left(\frac{a}{r}\right)^n$$

The Coulomb potential is written as a series in Legendre polynomials.
We can add an extra charge \(-q\) a distance \(a\) on the opposite side of the origin and see what happens. Now,

\[
\varphi(r) = \frac{1}{4\pi\varepsilon_0} \frac{q}{d_1} - \frac{1}{4\pi\varepsilon_0} \frac{q}{d_2} = \frac{1}{4\pi\varepsilon_0} \frac{q}{|r - ae_z|} - \frac{1}{4\pi\varepsilon_0} \frac{q}{|r + ae_z|}
\]

\[
= \frac{q}{4\pi\varepsilon_0 r} \left( \left[ 1 - 2\frac{a}{r} \cos \theta + \left(\frac{a}{r}\right)^2 \right]^{-1/2} - \left[ 1 + 2\frac{a}{r} \cos \theta + \left(\frac{a}{r}\right)^2 \right]^{-1/2} \right)
\]

\[
= \frac{q}{4\pi\varepsilon_0 r} \sum_{n=0}^{\infty} \left( P_n(\cos \theta) \left(\frac{a}{r}\right)^n - P_n(\cos \theta) \left(-\frac{a}{r}\right)^n \right)
\]

\[
= \frac{2q}{4\pi\varepsilon_0 r} \left( P_1(\cos \theta) \frac{a}{r} + P_3(\cos \theta) \left(\frac{a}{r}\right)^3 + \ldots \right)
\]

For \(r\) large enough, \(\varphi(r) \approx \frac{2qa}{4\pi\varepsilon_0 r^2} P_1(\cos \theta)\)

This is the potential from an electric dipole and \(2qa\) is known as the electric dipole moment.
Any charge distribution will produce an electrostatic potential described by a power series with terms like

\[ \frac{q}{4\pi \epsilon_0 r} P_n(\cos \theta) \left( \frac{a}{r} \right)^n \]

If the leading term is proportional to

\[ \frac{1}{r} P_0(\cos \theta) \left( \frac{a}{r} \right)^0 = \frac{1}{r} \]

then the charge distribution is known as a monopole,

\[ \frac{1}{r} P_1(\cos \theta) \left( \frac{a}{r} \right)^1 = \frac{a}{r^2} \cos \theta \]

.. dipole,

\[ \frac{1}{r} P_2(\cos \theta) \left( \frac{a}{r} \right)^2 = \frac{a^2}{2r^3} \left( 3 \cos^2 \theta - 1 \right) \]

.. quadrupole,

\[ \frac{1}{r} P_3(\cos \theta) \left( \frac{a}{r} \right)^3 = \frac{a^3}{2r^4} \left( 5 \cos^3 \theta - 3 \cos \theta \right) \]

.. octupole.

Sometimes these names are used to identify the individual terms, e.g. the term containing \( \frac{a}{r^2} \cos \theta \) is known as the “dipole term”.
3.2 Recurrence relations for Legendre polynomials and the Legendre equation

Key Point: Derive recurrence relations from the Legendre polynomial generating function.

Let's take the derivative of the generating function \( g(t, x) = \frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n \)

\[
\frac{\partial g(t, x)}{\partial t} = \frac{x - t}{(1 - 2xt + t^2)^{3/2}} = \sum_{n=0}^{\infty} P_n(x) nt^{n-1}
\]

But

\[
\frac{x - t}{(1 - 2xt + t^2)^{3/2}} = \frac{x - t}{1 - 2xt + t^2} \frac{1}{\sqrt{1 - 2xt + t^2}} = \frac{x - t}{1 - 2xt + t^2} \sum_{n=0}^{\infty} P_n(x) t^n
\]

\[
\Rightarrow (1 - 2xt + t^2) \sum_{n=0}^{\infty} P_n(x) nt^{n-1} = (x - t) \sum_{n=0}^{\infty} P_n(x) t^n
\]

\[
\Rightarrow \sum_{n=0}^{\infty} P_n(x) nt^{n-1} - 2x \sum_{n=0}^{\infty} P_n(x) nt^n + \sum_{n=0}^{\infty} P_n(x) nt^{n+1} = x \sum_{n=0}^{\infty} P_n(x) t^n - \sum_{n=0}^{\infty} P_n(x) t^{n+1}
\]

(all we have done here is expand the brackets)
\[ \sum_{n=0}^{\infty} P_n(x)nt^{n-1} - 2x \sum_{n=0}^{\infty} P_n(x)nt^n + \sum_{n=0}^{\infty} P_n(x)nt^{n+1} = x \sum_{n=0}^{\infty} P_n(x)t^n - \sum_{n=0}^{\infty} P_n(x)t^{n+1} \]

Relabelling:

\[ \Rightarrow \sum_{n=-1}^{\infty} P_{n+1}(x)(n+1)t^n - 2x \sum_{n=0}^{\infty} P_n(x)nt^n + \sum_{n=1}^{\infty} P_{n-1}(x)(n-1)t^n = x \sum_{n=0}^{\infty} P_n(x)t^n - \sum_{n=1}^{\infty} P_{n-1}(x)t^n \]

Equate powers of \( t^n \) for \( n \geq 1 \):

\[ \Rightarrow P_{n+1}(x)(n+1) - 2x P_n(x)n + P_{n-1}(x)(n-1) = x P_n(x) - P_{n-1}(x) \]

\[ \Rightarrow (2n+1)x P_n(x) = (n+1)P_{n+1}(x) + n P_{n-1}(x) \quad (n \geq 1) \]

This is the most efficient way to calculate the polynomials using a computer. Since we know \( P_0 \) and \( P_1 \) we can calculate \( P_2 \) and then \( P_3 \) etc.

**Exercise**: Use this result to verify the first five Legendre polynomials given earlier.
We could have taken the derivative with respect to $x$ instead:

\[
\frac{\partial g(t, x)}{\partial x} = \frac{t}{(1 - 2xt + t^2)^{3/2}} = \sum_{n=0}^{\infty} P_n'(x)t^n
\]

but

\[
\frac{t}{(1 - 2xt + t^2)^{3/2}} = \frac{t}{1 - 2xt + t^2} \cdot \frac{1}{\sqrt{1 - 2xt + t^2}} = \frac{t}{1 - 2xt + t^2} \sum_{n=0}^{\infty} P_n(x)t^n
\]

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

\[
\Rightarrow P_{n+1}'(x) + P_{n-1}'(x) = 2x P_n'(x) + P_n(x)
\]

\[
(n \geq 1)
\]

**Exercise:** Use the two results

\[
(2n+1)x P_n(x) = (n+1) P_{n+1}(x) + n P_{n-1}(x),
\]

and

\[
P_{n+1}'(x) + P_{n-1}'(x) = 2x P_n'(x) + P_n(x),
\]

to show that

\[
P_{n+1}'(x) - P_{n-1}'(x) = (2n + 1) P_n(x).
\]
Key Point: Derive the Legendre equation using recurrence relations.

**Exercise:** Show that the generating function satisfies the differential equation

$$
\frac{\partial}{\partial x} \left[ (1 - x^2) \frac{\partial}{\partial x} g(x, t) \right] + t \frac{\partial^2}{\partial t^2} [tg(x, t)] = 0.
$$

Then we have

$$
\sum_{n=0}^{\infty} t^n \frac{d}{dx} \left[ (1 - x^2) \frac{d}{dx} P_n(x) \right] + \sum_{n=0}^{\infty} t P_n(x) \frac{d^2}{dt^2} \left[ t^{n+1} \right] = 0
$$

$$
\Rightarrow \sum_{n=0}^{\infty} t^n \frac{d}{dx} \left[ (1 - x^2) \frac{d}{dx} P_n(x) \right] + \sum_{n=0}^{\infty} P_n(x) n(n+1) t^n = 0
$$

Since $t$ is arbitrary we may compare power of $t$ again:

$$
\Rightarrow \frac{d}{dx} \left[ (1 - x^2) \frac{d}{dx} P_n(x) \right] + n(n+1) P_n(x) = 0
$$

This is the **Legendre equation.**
3.3 Orthogonality and Completeness of the Legendre Polynomials

Key Point: Know that the Legendre Polynomials are orthogonal and complete

We can use the Legendre equation to show that the Legendre polynomials are orthogonal.

\[
\frac{d}{dx} \left[ (1 - x^2) \frac{d}{dx} P_n(x) \right] + n(n + 1) P_n(x) = 0
\]

\[
\Rightarrow \quad P_m(x) \frac{d}{dx} \left[ (1 - x^2) \frac{d}{dx} P_n(x) \right] - P_n(x) \frac{d}{dx} \left[ (1 - x^2) \frac{d}{dx} P_m(x) \right]
\]

\[
= -P_m(x) n(n + 1) P_n(x) + P_n(x) m(m + 1) P_m(x)
\]

Now integrate this over \(x\) from -1 to 1. We integrate the left-hand-side by parts.

\[
\int_{-1}^{1} P_m(x) \frac{d}{dx} \left[ (1 - x^2) \frac{d}{dx} P_n(x) \right] \, dx = \left[ u \frac{d}{dx} v \right]_{-1}^{1} - \int_{-1}^{1} \frac{d}{dx} u \ v \ dx
\]

\[
= \left[ P_m(x) (1 - x^2) \frac{d}{dx} P_n(x) \right]_{-1}^{1} - \int_{-1}^{1} \frac{d}{dx} P_m(x) \ (1 - x^2) \frac{d}{dx} P_n(x) \, dx
\]

zero

\[
\Rightarrow \quad [m(m + 1) - n(n + 1)] \int_{-1}^{1} P_n(x) P_m(x) \, dx = 0
\]
For \( n \neq m \) this tells us that \( \int_{-1}^{1} P_n(x)P_m(x) \, dx = 0 \), i.e. they are orthogonal over \([-1,1]\).

For \( n = m \) we need to go back to the generating function.

\[
\sum_{n=0}^{\infty} P_n(x)t^n \sum_{m=0}^{\infty} P_m(x)t^m = \frac{1}{1 - 2xt + t^2}
\]

Now integrate over \( x \):

\[
\int_{-1}^{1} \frac{1}{1 - 2xt + t^2} \, dx = \left[ -\frac{1}{2t} \log (1 - 2xt - t^2) \right]_{-1}^{1} = \frac{1}{t} \log \left( \frac{1 + t}{1 - t} \right) = 2 \sum_{n=0}^{\infty} \frac{t^{2n}}{2n + 1}
\]

\[
\int_{-1}^{1} \sum_{n=0}^{\infty} P_n(x)t^n \sum_{m=0}^{\infty} P_m(x)t^m \, dx = \sum_{n=0}^{\infty} \int_{-1}^{1} [P_n(x)]^2 t^{2n} \, dx \quad \text{(orthogonality for } n \neq m \text{)}
\]

Equating powers of \( t \):

\[
\int_{-1}^{1} [P_n(x)]^2 \, dx = \frac{2}{2n + 1}
\]
Putting these together we have the orthogonally and normalization condition

$$\int_{-1}^{1} P_n(x) P_m(x) \, dx = \frac{2}{2n + 1} \delta_{nm}$$

The Legendre polynomials are also “complete” – we can write any (continuous) function as a sum over Legendre polynomials. (This is just like a Fourier series being a sum over sines and cosines.)

Let’s write

$$f(x) = \sum_{n=0}^{\infty} c_n P_n(x)$$

where \(c_n\) are constants. Now,

$$\int_{-1}^{1} f(x) P_m(x) \, dx = \sum_{n=0}^{\infty} c_n \int_{-1}^{1} P_n(x) P_m(x) \, dx = \sum_{n=0}^{\infty} c_n \frac{2}{2m + 1} \delta_{nm} = c_m \frac{2}{2m + 1}$$

So,

$$f(x) = \sum_{n=0}^{\infty} \left( n + \frac{1}{2} \right) \left( \int_{-1}^{1} f(y) P_m(y) \, dy \right) P_n(x)$$

**Exercise:** Write the Dirac delta function \(\delta(1 - x)\) as a sum over Legendre Polynomials.
3.4 Series expansion and Rodrigues’ Formula

Key Point: Use Rodrigues’ formula to generate the Legendre Polynomials

We can find a series expansion of the polynomials by making a binomial expansion of the generating function.

\[ g(t, x) = (1 - 2xt + t^2)^{-1/2} = \sum_{n=0}^{\infty} \frac{(2n)!}{2^n (n!)^2} (2xt - t^2)^n = \sum_{n=0}^{\infty} \sum_{m=0}^{n} (-1)^m \frac{(2n)!}{2^{2n} n! m! (n - m)!} (2x)^{n-m} t^{n+m} \]

\[ = \sum_{n=0}^{\infty} \sum_{m=0}^{n/2} (-1)^m \frac{(2n - 2m)!}{2^{2n-2m} (n - m)! m! (n - 2m)!} (2x)^{n-2m} t^n \]

(To do this yourself, you will need to know things like \( \frac{1}{2}! \) (see the later discussion of the Gamma function), and be able to rearrange the order of summation.)

But \( g(t, x) = \sum_{n=0}^{\infty} P_n(x) t^n \), so,

\[ P_n(x) = \sum_{m=0}^{n/2} (-1)^m \frac{(2n - 2m)!}{2^m m! (n - m)! (n - 2m)!} x^{n-2m} \]
We can use this to derive Rodrigues’ formula by using 

\[ \left( \frac{d}{dx} \right)^n x^{2n-2m} = \frac{(2n-2m)!}{(n-2m)!} x^{n-2m} \]

\[
P_n(x) = \sum_{m=0}^{n/2} (-1)^m \frac{(2n - 2m)!}{2^m m!(n - m)!} x^{n-2m}
\]

\[
= \sum_{m=0}^{n/2} (-1)^m \frac{1}{2^m m!(n - m)!} \left( \frac{d}{dx} \right)^n x^{2n-2m}
\]

\[
= \frac{1}{2^n n!} \left( \frac{d}{dx} \right)^n \sum_{m=0}^{n} \frac{(-1)^m n!}{m!(n - m)!} x^{2n-2m}
\]

\[
\left( \frac{d}{dx} \right)^n x^{2n-2m} = 0 \quad \text{for} \ m > n/2
\]

\[
(x^2 - 1)^n
\]

\[
P_n(x) = \frac{1}{2^n n!} \left( \frac{d}{dx} \right)^n (x^2 - 1)^n
\]

This is Rodrigues’ formula.

**Exercise:** Use Rodrigues’ formula to verify the first 5 Legendre Polynomials.
3.5 Associated Legendre Polynomials

Key Point: Understand how associated Legendre polynomials are related to “ordinary” Legendre polynomials.

Associate Legendre polynomials \( P_n^m(x) \) are obtained from normal Legendre polynomials \( P_n(x) \) by differentiating \( m \) times with respect to \( x \):

\[
P_n^m(x) = (1 - x^2)^{m/2} \frac{d^m}{dx^m} P_n(x)
\]

Exercise: Show that the above definition of \( P_n^m(x) \) are solutions of the associated Legendre equation,

\[
\frac{d}{dx} \left[ (1 - x^2) \frac{dP_n^m(x)}{dx} \right] + n(n+1) P_n^m(x) - \frac{m^2}{1 - x^2} P_n^m(x) = 0
\]

You may assume that \( P_n(x) \) are solutions of the “ordinary” Legendre equation.
3.6 Bessel Functions

Key Point: Understand the importance of Bessel functions to the solution of Laplace’s equation in cylindrical coordinates.

The radial part of Laplace’s equation in cylindrical coordinates is

\[ r \frac{d}{dr} \left( r \frac{dJ_\nu(kr)}{dr} \right) + (k^2 r^2 - \nu^2) J_\nu(kr) = 0 \quad (k \text{ and } \nu \text{ constants}) \]

The solutions to this equation are known as Bessel functions (they are also solutions to the Helmholtz equation in spherical coordinates).

Just like the Legendre polynomials, they have a generating function, a differential equation (above), recurrence relations, a series expansion and orthogonality relations.

We don’t have time to go into detail here, so I will just state them without proof.
Generating function:
\[ g(x, t) = e^{x/2}{t^2-1} = \sum_{\nu=-\infty}^{\infty} J_\nu(x)t^\nu \]

Series expansion:
\[ J_\nu(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(m+n)!} \left( \frac{x}{2} \right)^{m+2\nu} \]

Bessel functions with negative (integer) index are related to those with positive integer index by
\[ J_{-\nu}(x) = (-1)^\nu J_\nu(x) \]

Recurrence relations:
\[ J_{\nu-1}(x) + J_{\nu+1}(x) = \frac{2\nu}{x} J_\nu(x) \quad \text{(diff. } g \text{ with respect to } t) \]
\[ J_{\nu-1}(x) - J_{\nu+1}(x) = 2J'_\nu(x) \quad \text{(diff. } g \text{ with respect to } x) \]

**Exercise:** Derive the two recurrence relations.
Integral representation for $n \geq 0$: \[ J_\nu(x) = \frac{1}{\pi} \int_0^\pi \cos(\nu \theta - x \sin \theta) \, d\theta \]

The values of $x$ for which $J_\nu(x)$ vanishes are called the zeros (or roots) and are often denoted $\alpha_{\nu m}$, where $m$ denotes which zero we are concerned with, i.e. $J_\nu(\alpha_{\nu m}) = 0$.

Orthogonality uses these zeros: \[ \int_0^{r_0} J_\nu \left( \alpha_{\nu n} \frac{r}{r_0} \right) J_\nu \left( \alpha_{\nu m} \frac{r}{r_0} \right) r \, dr = \frac{r_0^2}{2} \left[ J_{\nu+1}(\alpha_{\nu n}) \right]^2 \delta_{nm} \]

In general, $\nu$ does not have to be an integer and $x$ does not have to be real.

The Bessel functions are related to Neumann and Hankel functions.
4. Hermite and Laguerre polynomials

4.1 Hermite polynomials from a generating function

We will see that Hermite polynomials are solutions to the radial part of the Schrödinger Equation for the simple harmonic oscillator.

**Key Point: Derive Hermite’s equation and the Hermite recurrence relations from the generating function.**

Just like Legendre polynomials and Bessel functions, we may define Hermite polynomials $H_n(x)$ via a generating function.

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

We could, of course, use this to derive the individual polynomials, but this is very tedious. It is better to derive recurrence relations.
Differentiate with respect to $t$:

$$\frac{\partial}{\partial t} g(x, t) = (-2t + 2x) e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} H_n(x) \frac{t^{n-1}}{n!}$$

Expand the terms, and put the generating function in again:

$$-2 \sum_{n=0}^{\infty} H_n(x) \frac{t^{n+1}}{n!} + 2x \sum_{n=0}^{\infty} H_n(x) \frac{t^{n}}{n!} = \sum_{n=1}^{\infty} H_n(x) \frac{t^{n-1}}{(n-1)!}$$

Relabel:

$$-2 \sum_{n=1}^{\infty} nH_{n-1}(x) \frac{t^{n}}{n!} + 2x \sum_{n=0}^{\infty} H_n(x) \frac{t^{n}}{n!} = \sum_{n=0}^{\infty} H_{n+1}(x) \frac{t^{n}}{n!}$$

Equating coefficients of $t^n$:

$$\Rightarrow \quad H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad (n \geq 1)$$
\[ g(x, t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \]

Differentiate with respect to \( x \):

\[ \frac{\partial}{\partial x} g(x, t) = 2t e^{-t^2+2tx} = \sum_{n=0}^{\infty} H'_n(x) \frac{t^n}{n!} \]

Stick in \( g \):

\[ 2 \sum_{n=0}^{\infty} H_n(x) \frac{t^{n+1}}{n!} = \sum_{n=1}^{\infty} H'_n(x) \frac{t^n}{n!} \]

Relabel:

\[ 2 \sum_{n=1}^{\infty} H_{n-1}(x) \frac{t^{n}}{(n-1)!} = \sum_{n=1}^{\infty} H'_n(x) \frac{t^n}{n!} \]

Equating coefficients of \( t^n \):

\[ \Rightarrow \quad H'_n(x) = 2n H_{n-1}(x) \quad (n \geq 1) \]
We can use these recurrence relations to derive the Hermite differential equation (much easier than Legendre’s!).

\[
\begin{align*}
H_{n+1}(x) &= 2xH_n(x) - 2nH_{n-1}(x) \\
H'_n(x) &= 2nH_{n-1}(x)
\end{align*}
\]

\[
\Rightarrow \quad H_{n+1}(x) = 2xH_n(x) - H'_n(x)
\]

Differentiate with respect to \(x\):

\[
H'_{n+1}(x) = 2H_n(x) + 2xH'_n(x) - H''_n(x)
\]

\[
2(n + 1)H_n(x) = 2H_n(x) + 2xH'_n(x) - H''_n(x)
\]

\[
\Rightarrow \quad H''_n(x) - 2xH'_n(x) + 2nH_n(x) = 0
\]

This is Hermite’s equation.
Key Point: Use a generating function and recurrence relations to find the first few Hermite polynomials.

Generating function:

\[
\sum_{n=0}^{\infty} \frac{H_n(x)t^n}{n!} = e^{-t^2+2tx}
\]

\[\Rightarrow H_0(x) + H_1(x)t + O(t^2) = 1 - t^2 + 2tx + O(t^2) \Rightarrow \begin{cases} 
  t^0: & \Rightarrow H_0(x) = 1 \\
  t^1: & \Rightarrow H_1(x) = 2x 
\end{cases}\]

Now use the recurrence relation,

\[H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)\]

\[H_2(x) = 2xH_1(x) - 1 \times 2H_0(x) = 4x^2 - 2\]

\[H_3(x) = 2xH_2(x) - 2 \times 2H_1(x) = 8x^3 - 4x - 8x = 8x^3 - 12x\]

\[H_4(x) = 2xH_3(x) - 3 \times 2H_2(x) = 16x^4 - 24x^2 - (24x^2 - 12) = 16x^4 - 48x^2 + 12\]
4.2 Properties of Hermite polynomials

Symmetry about $x=0$:

$$g(-x, -t) = e^{-(t)^2 + 2(-t)(-x)} = e^{-t^2 + 2tx} = g(x, t)$$

$$\Rightarrow \sum_{n=0}^{\infty} H_n(-x) \frac{(-t)^n}{n!} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!}$$

$$\Rightarrow H_n(-x) = (-1)^n H_n(x)$$

(just like for Legendre polynomials)

There also exists a specific series form:

$$H_n(x) = \sum_{m=0}^{n/2} (-1)^m (2x)^{n-2m} \frac{n!}{(n-2m)!m!}$$

**Exercise**: Use this series to verify the first few Hermite polynomials.
Exercise:

Writing \( g(x, t) = e^{x^2} e^{-(t-x)^2} \) show that

\[
H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \left( e^{-x^2} \right)
\]

This is Rodrigues’ equation for Hermite polynomials.

\[
\begin{align*}
\text{Hint: work out } & \left. \frac{\partial^n g}{\partial t^n} \right|_{t=0} \\
\text{and observe that } & \frac{\partial}{\partial t} e^{-(t-x)^2} = -\frac{\partial}{\partial x} e^{-(t-x)^2}
\end{align*}
\]
Key Point: Write down the Hermite polynomial orthogonality condition.

Starting from Hermite’s equation: \[ H''_n(x) - 2xH'_n(x) + 2nH_n(x) = 0 \]

\[ \Rightarrow \frac{d}{dx} \left( e^{-x^2} \frac{d}{dx} H_n(x) \right) + 2n e^{-x^2} H_n(x) = 0 \]

we proceed much the same way as we did for Legendre polynomials.

\[ \Rightarrow H_m(x) \frac{d}{dx} \left[ e^{-x^2} \frac{d}{dx} H_n(x) \right] - H_n(x) \frac{d}{dx} \left[ e^{-x^2} \frac{d}{dx} H_m(x) \right] \]

\[ = -H_m(x) 2n e^{-x^2} H_n(x) + H_n(x) 2m e^{-x^2} H_m(x) \]

Integrate this over \( x \) from \(-\infty\) to \( \infty \), integrating the left-hand-side by parts.

\[ \int_{-\infty}^{\infty} H_m(x) \frac{d}{dx} \left[ e^{-x^2} \frac{d}{dx} H_n(x) \right] dx = \left[ H_m(x) e^{-x^2} \frac{d}{dx} H_n(x) \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \left[ \frac{d}{dx} H_m(x) \right] e^{-x^2} \frac{d}{dx} H_n(x) dx \]

zero \hspace{1cm} \text{symmetric in } n \leftrightarrow m

\[ \Rightarrow 2(m-n) \int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = 0 \]
We say that Hermite polynomials are orthogonal on the interval $[-\infty, \infty]$ with a weighting $e^{-x^2}$

\[
\int_{-\infty}^{\infty} g^2(x, t)e^{-x^2} \, dx = \int_{-\infty}^{\infty} e^{-2t^2+4tx-x^2} \, dx = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{t^{n+m}}{n!m!} \int_{-\infty}^{\infty} H_n(x)H_m(x)e^{-x^2} \, dx
\]

\[
\int_{-\infty}^{\infty} e^{-(x-2t)^2} e^{2t^2} \, dx = e^{2t^2} \int_{-\infty}^{\infty} e^{-x^2} \, dx = e^{2t^2} \sqrt{\pi}
\]

\[
\sum_{n=0}^{\infty} \frac{t^{2n}}{(n!)^2} \int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2} \, dx = \left( \int_{-\infty}^{\infty} e^{-x^2} \, dx \right)^2 = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy e^{-x^2-y^2} = \int_{0}^{2\pi} d\theta \int_{0}^{\infty} dr \, r e^{-r^2} = 2\pi \left[ -\frac{1}{2} e^{-r^2} \right]_0^\infty = \pi
\]

Equating powers of $t^{2n}$ gives \[
\int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2} \, dx = 2^n \sqrt{\pi} n!
\]

\[
\Rightarrow \quad \int_{-\infty}^{\infty} H_n(x)H_m(x) e^{-x^2} \, dx = 2^n \sqrt{\pi} n! \delta_{nm}
\]
Exercise: For a continuous function, I can write \( f(x) = \sum_{n=0}^{\infty} c_n H_n(x) \). Show that

\[
c_n = \frac{1}{2^n \sqrt{\pi} n!} \int_{-\infty}^{\infty} f(x) H_n(x) e^{-x^2} \, dx
\]

Sometimes people remove the weighting by redefining the function: \( \varphi_n(x) \equiv e^{-x^2/2} H_n(x) \)

\[
\Rightarrow \int_{-\infty}^{\infty} \varphi_n(x) \varphi_m(x) \, dx = 2^n \sqrt{\pi} n! \delta_{nm}
\]

Now this looks like a “traditional” orthogonality relation.

\[
H_n(x) = e^{x^2/2} \varphi_n(x) \quad \Rightarrow \quad H'_n(x) = x e^{x^2/2} \varphi_n(x) + e^{x^2/2} \varphi'_n(x)
\]

\[
\Rightarrow \quad H''_n(x) = e^{x^2/2} \varphi''_n(x) + 2x e^{x^2/2} \varphi'_n(x) + (1 + x^2) \varphi_n(x)
\]

Then Hermite’s equation \( H''_n(x) - 2x H'_n(x) + 2n H_n(x) = 0 \) becomes

\[
\varphi''_n(x) + (1 - x^2 + 2n) \varphi_n(x) = 0
\]
4.3 Hermite polynomials and the Quantum Harmonic Oscillator

Key Point: Solve the quantum harmonic oscillator in terms of Hermite polynomials.

Recall our earlier discussion of the time-independent Schrödinger equation. That was in 3-dimensions, but here I will simplify to one dimension again,

$$\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x),$$

where $m$ is the particle mass, and $E$ is its energy.

For the simple harmonic oscillator, $V(x) = \frac{1}{2}m\omega^2x^2$, so the equation becomes

$$\psi''(x) + \left(-\frac{m^2\omega^2}{\hbar^2}x^2 + \frac{2mE}{\hbar^2}\right) \psi(x) = 0$$

Notice that this looks awfully like the equation we just had on the previous slide:

$$\varphi''_n(x) + (1 - x^2 + 2n) \varphi_n(x) = 0$$

Our reweighted Hermite polynomials are solutions of the Quantum Harmonic Oscillator!
Let’s write \( y = ax \) with \( a = \sqrt{\frac{m\omega}{\hbar}} \) so we get

\[
\frac{d^2}{dy^2} \psi \left( \frac{y}{a} \right) + \left( -y^2 + \frac{2mE}{\hbar^2 a^2} \right) \psi \left( \frac{y}{a} \right) = 0
\]

Comparing the two equations, we see that we have solutions,

\[
\psi_n(x) = \sqrt{\frac{a}{2^n n! \sqrt{\pi}}} e^{-a^2 x^2/2} H_n(ax)
\]

where the normalization constant in front ensures that \( \int_{-\infty}^{\infty} |\psi_n(x)|^2 \, dx = 1 \), and, the energy is given by the equation

\[
\frac{2mE}{\hbar^2 a^2} = 1 + 2n \quad \Rightarrow \quad \frac{2E}{\hbar\omega} = 1 + 2n \quad \Rightarrow \quad E = \hbar\omega \left( n + \frac{1}{2} \right)
\]

Have you seen this somewhere before?
You probably solved this elsewhere using ladder operators. This works (in part) because of the Hermite recurrence relation $H'_n(x) = 2nH_{n-1}(x)$.

Writing $\varphi_n(x) = \sqrt{\frac{1}{2^n \sqrt{\pi n!}}} e^{-x^2/2} H_n(x)$ for simplicity (ie. set $a=1$ for now)

Then $\frac{1}{\sqrt{2}} \left( x + \frac{d}{dx} \right) \varphi_n(x) = \sqrt{\frac{1}{2^{n+1} \sqrt{\pi n!}}} \left( x + \frac{d}{dx} \right) e^{-x^2/2} H_n(x)$

$= \sqrt{\frac{1}{2^{n+1} \sqrt{\pi n!}}} \left( xe^{-x^2/2} H_n(x) - xe^{-x^2/2} H_n(x) + e^{-x^2/2} H'_n(x) \right)$

$= \sqrt{\frac{1}{2^{n+1} \sqrt{\pi n!}}} \left( e^{-x^2/2} 2n H_{n-1}(x) \right) = \sqrt{\frac{n}{2^{n-1} \sqrt{\pi (n-1)!}}} \left( e^{-x^2/2} H_{n-1}(x) \right)$

$= \sqrt{n} \varphi_{n-1}(x)$

This is a lowering operator.

Exercise: Use recurrence relations to show that the operator $\frac{1}{\sqrt{2}} \left( x - \frac{d}{dx} \right)$ is a raising operator. Can you show it using the Rodrigues’ equation?
We have seen why \( E = \hbar \omega \left( n + \frac{1}{2} \right) \), and how to move from one energy state to another using ladder operators, but we still have no reason for why \( n \) must be an integer!

Indeed, Hermite’s equation \( H''_n(x) - 2xH'_n(x) + 2nH_n(x) = 0 \) does have solutions for non-integer values of \( n \).

Plugging \( H_n(x) = \sum_{k=0}^{\infty} c_k x^k \) into the equation, one finds a solution

\[
H_n(x) = c_0 \left[ 1 + \frac{2(-n)}{2!} x^2 + \frac{2^2(-n)(2-n)}{4!} x^4 + \ldots \right] \\
+ c_1 \left[ x + \frac{2(1-n)}{3!} x^3 + \frac{2^2(1-n)(3-n)}{5!} x^5 + \ldots \right]
\]

which is valid for non-integer \( n \). (This is known as a Hermite “function”.)

For integer \( n \), this solution (or to be more precise, half of it) will truncate to give Hermite polynomials.

For non-integer \( n \), it does not truncate and one can show that the terms grow like \( x^n e^{x^2/2} \). These solutions do not satisfy the boundary condition \( \psi(x) \to 0 \) as \( x \to \infty \), so must be discarded and the harmonic oscillator is quantized.
4.4 Laguerre polynomials and the hydrogen atom

Key Point: Understand the importance of Laguerre polynomials to the solution of Schrödinger’s equation for the hydrogen atom.

Generating function:

\[
g(x, t) = \frac{e^{-xt/(1-t)}}{1 - t} = \sum_{n=0}^{\infty} L_n(x) t^n
\]

Exercise: Starting from the generating function, prove the two recurrence relations

\[
(n + 1)L_{n+1}(x) = (2n + 1 - x)L_n(x) - nL_{n-1}(x)
\]

\[
xL'_n(x) = nL_n(x) - nL_{n-1}(x)
\]

Also, show \( L_n(0) = 1 \) and find expressions for the first 4 polynomials.
Following a similar method to that used for Legendre and Hermite polynomials, we can show that the Laguerre polynomials are orthogonal over the interval \([0, \infty]\) with a weighting \(e^{-x}\), i.e.

\[
\int_0^\infty L_n(x)L_m(x)e^{-x} \, dx = \delta_{nm}
\]

They satisfy the **Laguerre equation**:

\[
xL''_n(x) + (1-x)L'_n(x) + nL_n(x) = 0
\]

and have a Rodrigues’ formula

\[
L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} \left( x^n e^{-x} \right)
\]

(These results can be proven using similar methods to those used earlier for Legendre and Hermite polynomials. If you are feeling assiduous feel free to do these as an exercise.)
Associated Laguerre polynomials are obtained by differentiating “regular” Laguerre polynomials (just as for Legendre).

\[ L_n^k(x) = (-1)^n \frac{d^k}{dx^k} L_{n+k}(x) \]

**Exercise:** Show that \( L_n^k(x) \) are solutions to the associated Laguerre equation

\[ xL_n^{k\,\prime\prime}(x) + (k + 1 - x)L_n^{k\,\prime}(x) + nL_n^k(x) = 0 \]

These are also orthogonal with

\[ \int_0^\infty L_n^k(x)L_m^k(x)x^k e^{-x} \, dx = \frac{(n + k)!}{n!} \delta_{nm} \]
Recall our investigation of the Schrödinger equation in spherical coordinates with $V = V(r)$.

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

Separating $\psi(r) = R(r)Y^m_l(\theta, \phi)$ resulted in spherical harmonics

$$Y^m_l(\theta, \phi) = \sqrt{\frac{(2l + 1) (l - m)!}{4\pi (l + m)!}} e^{im\phi} P^m_l(\cos \theta)$$

and a radial equation

$$\frac{d}{dr} \left[ r^2 \frac{dR(r)}{dr} \right] - \frac{2m}{\hbar^2} (V(r) - E) r^2 R(r) - l(l+1) R(r) = 0$$

For the hydrogen atom (that is, with $\psi(r)$ the wavefunction for an electron orbiting a proton), the potential is the Coulomb potential,

$$V(r) = \frac{-e^2}{4\pi \varepsilon_0 r}$$
To make the maths a wee bit cleaner, let’s make the following redefinitions:

\[ \rho = \alpha r, \quad \alpha = \sqrt{-\frac{8mE}{\hbar^2}}, \quad \lambda = \frac{me^2}{2\pi \epsilon_0 \alpha \hbar^2}, \quad \chi(\rho) = R(r), \text{ with } E < 0 \]

(we regard \( E = 0 \) at \( \infty \))

Then

\[
\frac{d}{dr} \left[ r^2 \frac{dR(r)}{dr} \right] - \frac{2m}{\hbar^2} \left( \frac{-e^2}{4\pi \epsilon_0 r} - E \right) r^2 R(r) - l(l+1)R(r) = 0
\]

becomes

\[
\frac{d}{d\rho} \left[ \rho^2 \frac{d\chi(\rho)}{d\rho} \right] + \left( \lambda \rho - \frac{1}{4} \rho^2 - l(l+1) \right) \chi(\rho) = 0
\]

which has solutions containing associated Laguerre polynomials,

\[
\chi(\rho) = e^{-\rho^2} \rho^l L^{2l+1}_{\lambda - l - 1}(\rho)
\]
**Exercise:** Plug the above result into the radial equation to recover the associated Laguerre equation for $L(\rho)$.

Just as for the Hermite equation, solutions exist for non-integer $\lambda-l-1$ but these diverge as $r \to \infty$ and must be discarded. The boundary conditions quantize the energy of the Hydrogen atom.

Fixing $\lambda$ to be an integer $n$,

$$E_n = -\frac{\alpha^2 \hbar^2}{8m} = -\frac{e^2}{4\pi \epsilon_0} \frac{1}{2a_0} \frac{1}{n^2}$$

where $a_0 = \frac{4\pi \epsilon_0 \hbar^2}{me^2} = \frac{2}{n\alpha}$ is the Bohr radius.

Also, hydrogen wavefunctions are,

$$\psi_{nlm}(r, \theta, \phi) = N_{nlm} e^{-\alpha r/2} (\alpha r)^l L_{n-l-1}^{2l+1}(\alpha r) Y_l^m(\theta, \phi)$$

where $N_{nlm}$ is a normalization coefficient.
To find the normalization coefficient we need

\[
\int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} |\psi_{nlm}(r, \theta, \phi)|^2 r^2 \sin \theta \, dr \, d\theta \, d\phi = \alpha^{-3} \int_0^{\infty} |\chi(\rho)|^2 \rho^2 d\rho
\]

\[= N_{nlm}^2 \frac{1}{\alpha^3} \int_0^{\infty} e^{-\rho} \rho^{2l+2} L_{n-l-1}^{2l+1}(\rho) L_{n-l-1}^{2l+1}(\rho) \, d\rho = N_{nlm}^2 \frac{2n}{\alpha^3} \frac{(n+l)!}{(n-l-1)!} = 1\]

Notice the 2n here. This is because we don’t quite have the orthogonality condition for the associated Laguerre polynomials we had before - we have an extra power of \( \rho \). This result is most easily proven with a recurrence relation,

\[x L_n^k = (2n+k+1)L_n^k - (n+k)L_{n-1}^k - (n+1)L_{n+1}^k\]

Finally, the electron wavefunction in the hydrogen atom is

\[\psi_{nlm}(r, \theta, \phi) = \left[ \frac{\alpha^3 (n-l-1)!}{2n (n+l)!} \right]^{1/2} (\alpha r)^l e^{-\alpha r / 2} L_{n-l-1}^{2l+1}(\alpha r) Y_l^m(\theta, \phi)\]
5. Gamma and Beta Functions, and Stirling’s approximation

5.1 The Gamma Function

Key Point: write down the three definitions of the gamma function and understand how they are related.

The gamma function $\Gamma(z)$ is often known as the “factorial function”, and is useful because:

- It crops up in many places in its own right (e.g. statistics, field theory)
- It is used in the definitions/relations of many other functions.

It was first written down by Gauss, but was developed by Euler. The notation $\Gamma(z)$ was invented by Legendre.

The first definition (due to Euler) of the gamma function:

$$\Gamma(z) = \lim_{n \to \infty} \frac{1 \cdot 2 \cdot 3 \cdots n}{z(z + 1)(z + 2) \cdots (z + n)} n^z, \quad \Re(z) > 0$$
Using this definition,

\[ \Gamma(z+1) = \lim_{n \to \infty} \frac{1 \cdot 2 \cdot 3 \cdots n}{(z + 1)(z + 2)(z + 3) \cdots (z + n + 1)} n^{z+1} \]

\[ = \lim_{n \to \infty} \frac{n}{(z + n + 1)} \frac{1 \cdot 2 \cdot 3 \cdots n}{z(z + 1)(z + 2) \cdots (z + n)} n^{z} \]

\[ \rightarrow 1 \text{ as } n \to \infty \quad \rightarrow \Gamma(z) \text{ as } n \to \infty \]

So,

\[ \Gamma(z + 1) = z\Gamma(z) \]

Also using this definition,

\[ \Gamma(1) = \lim_{n \to \infty} \frac{1 \cdot 2 \cdot 3 \cdots n}{2 \cdot 3 \cdot 4 \cdots (n + 2)} n^2 = \lim_{n \to \infty} \frac{1}{(n + 1)(n + 2)} n^2 = 1 \]
Now we can use $\Gamma(z + 1) = z\Gamma(z)$ and $\Gamma(1) = 1$ to derive other values for the gamma function:

\[
\begin{align*}
\Gamma(1) &= 1 \\
\Gamma(2) &= 1 \Gamma(1) = 1 \\
\Gamma(3) &= 2 \Gamma(2) = 2 \\
\Gamma(n) &= (n-1)\Gamma(n-1) = (n-1)(n-2)\Gamma(n-2) = \ldots \\
&= (n - 1)(n - 2) \cdots 1 = (n - 1)!
\end{align*}
\]

where $n$ is an integer.

This is why the gamma function is often called the \emph{factorial function}.

Euler’s first definition holds for any $z \in \mathbb{C}$ except $z = 0, -1, -2, \ldots$ for which it diverges.

$|\Gamma(z)|$ for $z \in \mathbb{C}$
The second definition (known as Euler’s integral definition) is

\[ \Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt, \quad \Re(z) > 0 \]

Notice that writing \( t = x^2 \),

\[ \Gamma(z) = 2 \int_0^\infty e^{-x^2} x^{2z-1} dx \]

So,

\[ \Gamma \left( \frac{1}{2} \right) = 2 \int_0^\infty e^{-x^2} dx = \sqrt{\pi} \]  
(see slide 81)

To show that this function is the same as that of the first definition, let’s define

\[ \Gamma_n(z) = n^2 \int_0^1 (1 - u)^n u^{z-1} du \]

writing \( t = nu \)

\[ \Gamma_n(z) = \int_0^n \left( 1 - \frac{t}{n} \right)^n t^{z-1} dt \]
Since \[ \lim_{n \to \infty} \left( \frac{1 - \frac{t}{n}}{n} \right)^n = e^{-t} \]

\[
\left\{ \log \left( \frac{1 - \frac{t}{n}}{n} \right)^n = n \log \left( 1 - \frac{t}{n} \right) = n \left( -\frac{t}{n} - \frac{t^2}{2n^2} - \ldots \right) \to -t, \text{ as } n \to \infty \right\}
\]

then,

\[ \lim_{n \to \infty} \Gamma_n(z) = \lim_{n \to \infty} \int_0^n \left( \frac{1 - \frac{t}{n}}{n} \right)^n t^{z-1} dt = \int_0^\infty e^{-t} t^{z-1} dt = \Gamma(z) \]

But \[ \Gamma_n(z) = n^2 \int_0^1 (1 - u)^n u^{z-1} du \] can be solved by (lots of) integration by parts

\[ \Gamma_n(z) = n^2 \int_0^1 (1 - u)^n u^{z-1} du = \left[ n^2(1 - u)^n \frac{1}{z} u^z \right]_0^1 + \frac{n^3(n-1)}{z} \int_0^1 (1 - u)^{n-1} u^z du \]

\[ = \left[ n^2(1 - u)^{n-1} \frac{1}{z(z+1)} u^{z+1} \right]_0^1 + \frac{n^3(n-1)}{z(z+1)} \int_0^1 (1 - u)^{n-2} u^{z+1} du \]

\[ = n^z \frac{n(n-1) \cdots 1}{z(z+1) \cdots (z+n-1)} \int_0^1 u^{z+n-1} du = n^z \frac{n(n-1) \cdots 1}{z(z+1) \cdots (z+n)} \]

\[ \Rightarrow \quad \Gamma(z)|_{\text{second defn}} = \lim_{n \to \infty} \Gamma_n(z) = \Gamma(z)|_{\text{first defn}} \]
The third definition (due to Weierstrass)

\[
\frac{1}{\Gamma(z)} = z e^{\gamma z} \prod_{n=1}^{\infty} \left(1 + \frac{z}{n}\right) e^{-z/n}
\]

\(\gamma\) is the Euler-Mascheroni constant

\[
\gamma = \lim_{n \to \infty} \left( \sum_{k=1}^{n} \frac{1}{k} - \log n \right) = 0.577216\ldots
\]

To prove this is the same function again, write the first definition as a product:

\[
\Gamma(z) = \lim_{n \to \infty} \frac{1 \cdot 2 \cdot 3 \cdots n}{z(z + 1)(z + 2) \cdots (z + n)} n^z = \lim_{n \to \infty} \frac{1}{z} \prod_{k=1}^{n} \left(1 + \frac{z}{k}\right)^{-1} n^z
\]

\[
\Rightarrow \quad \frac{1}{\Gamma(z)} = \lim_{n \to \infty} z \prod_{k=1}^{n} \left(1 + \frac{z}{k}\right) n^{-z} = \lim_{n \to \infty} z \prod_{k=1}^{n} \left(1 + \frac{z}{k}\right) e^{-z \log n}
\]
\[ \frac{1}{\Gamma(z)} = \lim_{n \to \infty} z \prod_{k=1}^{n} \left(1 + \frac{z}{k}\right) e^{-z \log n} = \lim_{n \to \infty} z \prod_{k=1}^{n} \left(1 + \frac{z}{k}\right) e^{-z \log n} e^{-z/k} e^{z/k} \]

\[ \prod_{k=1}^{n} e^{z/k} = \exp \left(\frac{z}{\sum_{k=1}^{n} \frac{1}{k}}\right) \]

\[ \Rightarrow \frac{1}{\Gamma(z)} = \lim_{n \to \infty} z \left[ \prod_{k=1}^{n} \left(1 + \frac{z}{k}\right) e^{-z/k} \right] \exp \left(\frac{z}{\sum_{k=1}^{n} \frac{1}{k}} - \log n\right) \]

\[ \Rightarrow \frac{1}{\Gamma(z)} = z e^{\gamma z} \prod_{k=1}^{\infty} \left(1 + \frac{z}{k}\right) e^{-z/k} \]

which is the Weierstrass definition.

**Exercise**: Using the infinite product representation \( \sin x = x \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2 \pi^2}\right) \), show that

\[ \Gamma(z) \Gamma(1 - z) = \frac{\pi}{\sin z \pi} \]

Hint: do \( \Gamma(z) \Gamma(-z) \) first and then use \( \Gamma(z + 1) = z \Gamma(z) \)
5.2 Stirling’s approximation

Key Point: Use Stirling’s approximation to approximate factorials of large numbers and estimate the error on the approximation.

Very large factorials, such as used in statistical mechanics for the evaluation of entropy, can be difficult (i.e. slow and computationally expensive) to calculate. It is useful to have an analytic approximation. **Stirling’s approximation** is an approximate form of the gamma function for large numbers:

\[
\Gamma(n + 1) = n! \approx \sqrt{2\pi n} \left(\frac{n}{e}\right)^n
\]

**Proof:**

\[
\Gamma(n + 1) = n! = \int_0^\infty e^{-t} t^n dt = \int_0^\infty e^{-t+n \log t} dt
\]

Now

\[
\frac{d}{dt} (-t + n \log t) = \frac{n}{t} - 1 = 0 \quad \Rightarrow \quad t = n
\]

so the exponential is a maximum at \( t = n \). Any other values of \( t \) will give a small contribution (the exponential of a large negative number).
Taylor expand around $t = n$: 

$$n \log t - t = n \log n - n - \frac{(t-n)^2}{2n} + \mathcal{O}\left((t-n)^3\right)$$

Sticking this into our expression:

$$n! \approx \int_0^\infty \exp \left[ n \log n - n - \frac{(t-n)^2}{2n} \right] dt = \sqrt{2n \left(\frac{n}{e}\right)^n} \int_{-\sqrt{n}/2}^{\infty} e^{-x^2} dx$$

where we have written $x = \frac{t-n}{\sqrt{2n}}$.

Now, for large $n$, 

$$\int_{-\sqrt{n}/2}^{\infty} e^{-x^2} dx \approx \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

So, 

$$n! \approx \sqrt{2\pi n} \left(\frac{n}{e}\right)^n$$

We could have gone further with the expansion and found the next term:

$$n! \approx \sqrt{2\pi n} \left(\frac{n}{e}\right)^n \left(1 + \frac{1}{12n} + \frac{1}{288n^2} + \ldots\right)$$
This series converges very quickly. It is useful for calculating things like the entropies, which are logarithms of large factorials.

\[ \log(n!) \approx n \log n - n + \frac{1}{2} \log(2\pi n) \approx n \log n - n \]

<table>
<thead>
<tr>
<th>$n$</th>
<th>$n!$</th>
<th>$\sqrt{2\pi n} \left(\frac{n}{e}\right)^n$</th>
<th>Error</th>
<th>$\log n!$</th>
<th>$n \log n - n$</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.92213</td>
<td>7.779%</td>
<td>0</td>
<td>-1</td>
<td>$\infty$</td>
</tr>
<tr>
<td>10</td>
<td>3628800</td>
<td>3598696</td>
<td>0.830%</td>
<td>15.1</td>
<td>13.0</td>
<td>13.8%</td>
</tr>
<tr>
<td>100</td>
<td>$9 \times 10^{157}$</td>
<td>$9 \times 10^{157}$</td>
<td>0.083%</td>
<td>364</td>
<td>360</td>
<td>0.89%</td>
</tr>
</tbody>
</table>

(Schroeder, *An Introduction to Thermal Physics*, Addison Wesley, 2000.)

**Exercise:** Use Stirling’s approximation to calculate the number of ways in which you can rearrange a deck of standard playing cards (i.e. 52!). Estimate your error by considering the next term in the expansion. How does your calculation and error correspond to the correct result?
5.3 The Beta Function

Key Point: Define the beta function and understand its relation to the gamma function

The beta function can be defined by the integral

\[ B(p, q) = \int_0^1 t^{p-1} (1 - t)^{q-1} dt \]

This integral crops up surprisingly often in physics, so it is useful to know.

It also appears in other forms.

e.g. put \( t = \cos^2 \theta \) \( \Rightarrow \) \( dt = -2 \cos \theta \sin \theta d\theta \), \( t^{p-1} = \cos^{2p-2} \theta \), \( (1-t)^{q-1} = \sin^{2q-2} \theta \)

\[ \Rightarrow B(p, q) = 2 \int_0^{\pi/2} \cos^{2p-1} \theta \sin^{2q-1} \theta d\theta \]
The beta function is related to the gamma function:

$$B(p, q) = \frac{\Gamma(p) \Gamma(q)}{\Gamma(p + q)} = \frac{(p - 1)!(q - 1)!}{(p + q - 1)!}$$

To prove this I will work from the gamma functions backwards.

$$\Gamma(p) \Gamma(q) = \int_0^\infty e^{-u} u^{p-1} du \int_0^\infty e^{-v} v^{q-1} dv$$

$$= 4 \int_0^\infty \int_0^\infty e^{-x^2-y^2} x^{2p-1} y^{2q-1} dx \, dy \quad \text{where} \ u = x^2, \ v = y^2$$

$$= 4 \int_0^{\pi/2} \int_0^{2q-1} e^{-r^2} \cos^{2p-1} \theta \, \sin^{2q-1} \theta \, dr \, d\theta$$

where in the last step I have converted to polar coordinates, \(x = r \cos \theta, \ y = r \sin \theta\).
The $r$ integral should be familiar – it is just the gamma function,

$$\int_0^\infty r^{2p+2q-1} e^{-r^2} dr = \frac{1}{2} \int_0^\infty t^{p+q-1} e^{-t} dt = \frac{1}{2} \Gamma(p+q) \quad (t = r^2)$$

The angular integral should also now be familiar, since it is a beta function:

$$\int_0^{\pi/2} \cos^{2p-1} \theta \sin^{2q-1} \theta d\theta = \frac{1}{2} B(p, q)$$

Putting this together  \( \Gamma(p)\Gamma(q) = \Gamma(p + q)B(p, q) \) which proves the result.
5.3 The simple pendulum at large angles

In the past, you have always assumed that pendulums only have small angle oscillations. But what is the period of oscillation of a pendulum for large angle swings?

Use polar coordinates: \( x = r \cos \theta, \quad y = r \sin \theta \)

Position vector of mass: \( \mathbf{r} = r \mathbf{e}_r \)

\[
\begin{align*}
\dot{\mathbf{r}} &= r \dot{\mathbf{e}}_r = r \frac{d\mathbf{e}_r}{d\theta} \dot{\theta} \\
\ddot{\mathbf{r}} &= r \ddot{\mathbf{e}}_r = r \frac{d^2\mathbf{e}_r}{d\theta^2} \dot{\theta}^2 + r \frac{d\mathbf{e}_r}{d\theta} \ddot{\theta} = -r \mathbf{e}_r \dot{\theta}^2 + r \mathbf{e}_\theta \ddot{\theta}
\end{align*}
\]

The force due to gravity: \( \mathbf{F} = m g \mathbf{e}_x = m g (\cos \theta \mathbf{e}_r - \sin \theta \mathbf{e}_y) \)

Tension in the string: \( \mathbf{T} = -T \mathbf{e}_r \)

\[
\mathbf{F} + \mathbf{T} = m \ddot{\mathbf{r}} \quad \Rightarrow \quad \mathbf{e}_r : \quad -m r \dot{\theta}^2 = m g \cos \theta - T \\
\quad \mathbf{e}_\theta : \quad m r \ddot{\theta} = -m g \sin \theta
\]
I don’t really care about the tension, so the interesting equation is:

\[ \dot{\theta} = -\frac{g}{r} \sin \theta \]

Use a trick:

\[ \frac{d}{dt} \left( \frac{1}{2} \dot{\theta}^2 \right) = \ddot{\theta} \dot{\theta} = -\dot{\theta} \frac{g}{r} \sin \theta \quad \Rightarrow \quad \int d \left( \frac{1}{2} \dot{\theta}^2 \right) = -\int \frac{g}{r} \sin \theta \, d\theta \]

So,

\[ \frac{1}{2} \dot{\theta}^2 = \frac{g}{r} \cos \theta + \text{constant} \]

We can set the constant via a boundary condition: the pendulum is at rest at an angle \( \alpha \)

\[ \Rightarrow \quad \frac{1}{2} \dot{\theta}^2 = \frac{g}{r} (\cos \theta - \cos \alpha) \]

The **period** is the time taken to go from \( \theta = 0 \) back to \( \theta = 0 \) again, or 4 times the time taken to go from \( \theta = 0 \) to \( \theta = \alpha \).

\[ \tau = \int_{0}^{\alpha} \frac{1}{\dot{\theta}} \, d\theta = 4 \int_{0}^{\alpha} \frac{1}{\sqrt{2g \int_{0}^{\alpha} \frac{1}{\sqrt{\cos \theta - \cos \alpha}} \, d\theta}} \, d\theta \]

\[ \frac{1}{\dot{\theta}} \, d\theta = \frac{dt}{d\theta} \, d\theta = dt \]
So the period is \[ \tau = 4 \sqrt{\frac{r}{2g}} \int_0^\alpha \frac{1}{\sqrt{\cos \theta - \cos \alpha}} d\theta \]

This is an **elliptic integral**, and unfortunately we don’t have time to introduce its solutions, the **elliptic functions**.

However, we can now do the special case of \( \alpha = 90^\circ \). Then \( \cos \alpha = 0 \) and the period becomes,

\[ \tau = 4 \sqrt{\frac{r}{2g}} \int_0^{\pi/2} \frac{1}{\sqrt{\cos \theta}} d\theta \]

Recall that \( B(p, q) = 2 \int_0^{\pi/2} \cos^{2p-1} \theta \sin^{2q-1} \theta \, dt \), so,

\[ \tau = \sqrt{\frac{2r}{g}} B\left(\frac{1}{4}, \frac{1}{2}\right) \]