# Lecture 9

## Numerical Techniques: Differential Equations - Legendre Polynomials & Hermite Polynomials

### Quantum Harmonic Oscillator

IKC-MH.55 *Scientific Computing with Python* at December 22, 2023

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# Contents

# Partial Differential Equations; heat & temperature I

- Consider a straight rod along which there is a uniform flow of heat.
  - Let $u(x, t)$ denote the temperature of the rod at time $t$ and location $x$..
  - Let $q(x, t)$ denote the rate of heat flow.
- The expression $\partial q/\partial x$ denotes the rate at which the rate of heat flow changes per unit length and therefore measures the rate at which heat is accumulating at a given point $x$ at time $t$.
- If heat is accumulating, the temperature at that point is rising, and the rate is denoted by $\partial u/\partial t$.

1 The principle of conservation of energy leads to $\partial q/\partial x = k\partial u/\partial t$, where k is the specific heat of the rod.

- This means that the rate at which heat is accumulating at a point is proportional to the rate at which the temperature is increasing.

# Partial Differential Equations; heat & temperature II

2 A second relationship between $q$ and $u$ is obtained from Newton's law of cooling, which states that $q = K(\partial u/\partial x)$.

- Elimination of $q$ between these equations leads to

$$\frac{\partial^2 u}{\partial x^2} = (k/K)\frac{\partial u}{\partial t}$$

the partial differential equation for one-dimensional heat flow.

- The partial differential equation for heat flow in three dimensions takes the form

$$\boxed{\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial yx^2} = (k/K)\frac{\partial u}{\partial t}}$$

- Often written as

$$\boxed{\nabla^2 u = (k/K)\frac{\partial u}{\partial t}}$$

where the symbol $\nabla$, called del or nabla, is known as the Laplace operator.

# Partial Differential Equations III

- Another example to PDEs for dealing with wave propagation problem:

$$\nabla^2 u = (1/c^2)\frac{\partial^2 u}{\partial t^2}$$

  where c is the speed at which the wave propagates.
- PDEs are harder to solve than ordinary differential equations (ODEs).
- However, the PDEs associated with wave propagation and heat flow can be reduced to a system of ODEs through a process known as ***separation of variables***.
- These ODEs depend on the choice of coordinate system, which in turn is influenced by the physical configuration of the problem.
- The solutions of these ODEs form the majority of the ***special functions*** of mathematical physics.

# Special Functions

- In the broad sense, a set of several classes of functions that arise in the solution of both theoretical and applied problems in various branches.
- In the narrow sense, the special functions of mathematical physics, which arise when solving PDEs by the method of separation of variables.
- Special functions can be defined by means of power series, generating functions, infinite products, repeated differentiation, integral representations, differential, difference, integral, and functional equations, trigonometric series, or other series in orthogonal functions.
- For example, in solving the equations of heat flow or wave propagation in cylindrical coordinates, the method of separation of variables leads to Bessel's differential equation, a solution of which is the Bessel function, denoted by $J_n(x)$.

# Polynomials

- A polynomial ("many terms") is defined as an expression that consist of variables, coefficients and exponents.
- A polynomial can have:

  • variables (like x and y)
  • constants/coefficients (like 6, -10, or $^{3/2}$)
  • exponents (like the 2 in $y^2$)
  • that can be combined using addition, subtraction, multiplication and division
  • but not division by a variable (so something like 2/x is not correct)
  • a monomial is the product of non-negative powers of variables and will only have one term. 13, 3x, $4y^2$, ...
  • a binomial is the sum of two monomials. 3x + 1, 2x + y, ...
  • a trinomial is the sum of three monomials. $x^2 + 2x + 1$, 2x + 3y + 2, ...
  • can have one or more terms, but not an infinite number of terms.

- The standard form of a polynomial refers to writing a polynomial in the descending power of the variable.

$$2x^3 - 4x^2 + 7x - 4$$

# Legendre's Equation

- The Legendre polynomials $P_\ell(x)$, sometimes called Legendre functions of the first kind, Legendre coefficients, or zonal harmonics are solutions to the Legendre differential equation.
- The Legendre polynomials satisfy the second-order differential equation.

$$(1-x^2)\frac{\mathrm{d}^2y}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}y}{\mathrm{d}x} + \ell(\ell+1)y = 0$$

where $y = P_\ell(x)$

- This equation has two regular singular points $x = \pm 1$ where the leading coefficient $(1-x^2)$ vanishes.
- Solutions of Legendre equations are Legendre polynomials

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^\ell (x^2-1)^\ell$$

# Legendre Polynomials I

- If $\ell$ $(0 \leq \ell \leq \infty)$ is an integer, they are polynomials and make up an infinite set of functions of the variable x.
- We therefore have a function $P_0(x)$, another function $P_\ell(x)$, and an infinite number of additional functions belonging to the set of Legendre polynomials.
- Introduce a (**generating**) function $\Phi(x, h)$ of two variables, known as a generating function for the definition of the Legendre polynomials.

$$\boxed{\Phi(x, h) = (1 - 2xh + h^2)^{-1/2}}$$

• The first variable, x, is the same variable that appears as the argument of the Legendre polynomials.
• The second variable, h, is an auxiliary variable with no particular meaning.

# Legendre Polynomials II

- Think of $\Phi$ as a function of a single variable h ($\Phi = \Phi(h)$) and expand as a Taylor expansion in powers of h

$$\begin{aligned} \Phi(h) &= \Phi(0) + \left.\frac{d\Phi}{dh}\right|_{h=0} h + \frac{1}{2!}\left.\frac{d^2\Phi}{dh^2}\right|_{h=0} h^2 + \frac{1}{3!}\left.\frac{d^3\Phi}{dh^3}\right|_{h=0} h^3 + \dots \\ &= \sum_{\ell=0}^{\infty} \frac{1}{\ell!}\left.\frac{d^\ell\Phi}{dh^\ell}\right|_{h=0} h^\ell \end{aligned}$$

- Restore the x-dependence of the generating function. This doesn't change the general appearance of the Taylor expansion but written as partial derivatives instead of total derivatives.

$$\Phi(x,h) = \sum_{\ell=0}^{\infty} \frac{1}{\ell!}\left.\frac{\partial^\ell\Phi}{\partial h^\ell}\right|_{h=0} h^\ell = \sum_{\ell=0}^{\infty} P_\ell(x) h^\ell$$

- Right hand side of this equation is the formal definition of the Legendre polynomials. They are identified as the coefficients in the Taylor expansion of the generating function about $h = 0$.

# Legendre Polynomials III

- Let us use this equation to calculate the first few polynomials.

  • For $\ell = 0$ we are instructed to take no derivatives, and to evaluate the generating function at $h = 0$. This gives $P_0(x) = 1$; the zeroth polynomial is actually a constant.
  • Moving on to $\ell = 1$, we must differentiate $\Phi$ once with respect to h. Evaluating this at $h = 0$ and dividing by $1! = 1$ gives $P_1(x) = x$.
  • For $\ell = 2$ we differentiate $\Phi$ twice. Evaluating this at $h = 0$ and dividing by $2! = 2$ produces $P_2(x) = 1/2(3x^2 - 1)$. We can just keep going like this, and generate any number of polynomials.
- When $\ell$ is even, $P_\ell(x)$ contains only even powers of x, starting with $x^\ell$ and ending with $x^0$.
- When $\ell$ is odd, $P_\ell(x)$ contains only odd powers of x, starting with $x^\ell$ and ending with $x$.
- $P_\ell(x)$ is an even function of $x$ when $\ell$ is even, and an odd function of $x$ when $\ell$ is odd.

# Legendre Polynomials IV

- The first few Legendre polynomials are given by

$$
\begin{aligned}
P_0 &= 1 \\
P_1 &= x \\
P_2 &= \frac{1}{2}(3x^2 - 1) \\
P_3 &= \frac{1}{2}(5x^3 - 3x) \\
P_4 &= \frac{1}{8}(35x^4 - 30x^2 + 3) \\
P_5 &= \frac{1}{8}(63x^5 - 70x^3 + 15x) \\
P_6 &= \frac{1}{16}(231x^6 - 315x^4 + 105x^2 - 5)
\end{aligned}
$$

- Recursion relation:

$$
\boxed{P_\ell(x) = \frac{1}{\ell}[(2\ell - 1)xP_{\ell-1}(x) - (\ell - 1)P_{\ell-2}(x)]}
$$

# Legendre Polynomials V

**Example py-file:** The program to find first 6 Legendre polynomials: myLegendre.py

```
P_0= 1
P_1= x
P_2= 3*x**2/2 - 1/2
P_3= 5*x**3/2 - 3*x/2
P_4= 35*x**4/8 - 15*x**2/4 + 3/8
P_5= 63*x**5/8 - 35*x**3/4 + 15*x/8
P_6= 231*x**6/16 - 315*x**4/16 + 105*x**2/16 - 5/16

1 x  --> P1
     2
1.5 x - 0.5  --> P2
     3
2.5 x - 1.5 x  --> P3
       4              3        2
4.375 x + 4.857e-16 x - 3.75 x + 2.429e-16 x + 0.375  --> P4
       5       3              2
7.875 x - 8.75 x - 4.372e-16 x + 1.875 x  --> P5
       6         4              3         2
14.44 x - 19.69 x + 1.603e-15 x + 6.562 x - 0.3125  --> P6
```

**Figure:** First 6 Legendre Polynomials $P_\ell(x)$ with Recursion Relation: $P_\ell(x) = \frac{1}{\ell}[(2\ell - 1)xP_{\ell-1}(x) - (\ell - 1)P_{\ell-2}(x)]$.

# Legendre Polynomials VI

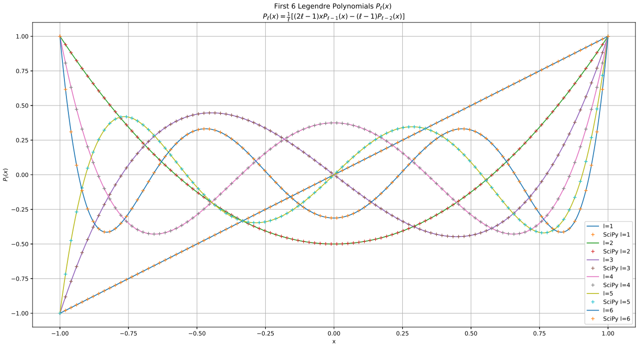



**Figure:** Plot of first 6 $P_\ell(x)$.

# Hermite's Equation

- The Hermite polynomials $H_k(x)$ are solutions to the Hermite differential equation of the form

$$a(x)y'' + b(x)y' + c(x)y = 0$$

where $a(x) = 1$, $b(x) = -2x$ and $c(x) = 2k$ (positive integer parameter k)

$$\boxed{\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + 2ky = 0}$$

- $y_k$ is a solution of the Hermite equation. Therefore, defining $H^k(x) = y_k$.
- A natural one to define Hermite polynomials is through the so-called Rodrigues'formula:

$$\boxed{H_k(x) = (-1)^k e^{x^2} \frac{d^k}{dx^k}\left[e^{-x^2}\right]}$$

# Hermite Polynomials I

- The first few Hermite polynomials are given by

$$\begin{aligned}
H_0 &= 1 \\
H_1 &= 2x \\
H_2 &= 4x^2 - 2 \\
H_3 &= 8x^3 - 12x \\
H_4 &= 16x^4 - 48x^2 + 12 \\
H_5 &= 32x^5 - 160x^3 + 120x \\
H_6 &= 64x^6 - 480x^4 + 720x^2 - 120
\end{aligned}$$

- Recursion relation:

$$\boxed{H_{k+1}(x) = 2xH_k(x) - 2kH_{k-1}(x)}$$

# Hermite Polynomials II

**Example py-file:** The program to find first 6 Hermite polynomials: myHermite.py

```
P_0= 1
P_1= x
P_2= 3*x**2/2 - 1/2
P_3= 5*x**3/2 - 3*x/2
P_4= 35*x**4/8 - 15*x**2/4 + 3/8
P_5= 63*x**5/8 - 35*x**3/4 + 15*x/8
P_6= 231*x**6/16 - 315*x**4/16 + 105*x**2/16 - 5/16

1 x  --> P1
     2
1.5 x - 0.5  --> P2
     3
2.5 x - 1.5 x  --> P3
       4              3        2
4.375 x + 4.857e-16 x - 3.75 x + 2.429e-16 x + 0.375  --> P4
       5        3              2
7.875 x - 8.75 x - 4.372e-16 x + 1.875 x  --> P5
       6         4             3         2
14.44 x - 19.69 x + 1.603e-15 x + 6.562 x - 0.3125  --> P6
```

**Figure:** First 6 Hermite Polynomials $H_k(x)$ with Recursion Relation: $H_{k+1}(x) = 2xH_k(x) - 2kH_{k-1}(x)$.

# Hermite Polynomials III

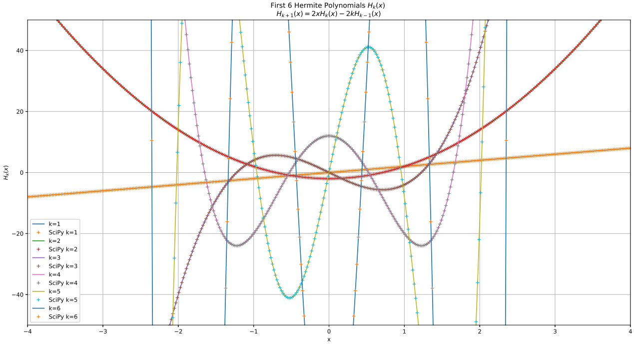



**Figure:** Plot of first 6 $H_k(x)$.

# Quantum Harmonic Oscillator I

- The quantum harmonic oscillator as analog of the classical one is often used as an approximate model for the behavior of some quantum systems.
- It is one of the few quantum-mechanical systems for which an exact, analytical solution is known.
- The Hamiltonian for a particle of mass $m$ moving in one dimension in a potential $V(x) = 1/2kx^2$ is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

  where $\hat{x}$ is the position operator, and $\hat{p}$ is the momentum operator (given by $\hat{p} = -i\hbar\partial/\partial x$ in the coordinate basis).
- The first term in the Hamiltonian represents the kinetic energy of the particle, and the second term represents its potential energy, as in Hooke's law.

# Quantum Harmonic Oscillator II

- Then, Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi = E\psi$$

- with the change of variable, $q = (mk/\hbar^2)^{1/4}x$, this equation becomes

$$-\frac{1}{2}\frac{d^2\psi}{dq^2} + \frac{1}{2}q^2\psi = \frac{E}{\hbar\omega}\psi$$

  where $\omega = \sqrt{k/m}$ is the angular frequency of the oscillator.

- This differential equation has an exact solution in terms of a quantum number $\nu = 0, 1, 2, \ldots$:

$$\boxed{\psi(q) = N_\nu H_\nu(q) e^{-q^2/2}}$$

  where $N_\nu = (\sqrt{\pi}2^\nu \nu!)^{-1/2}$ is a normalization constant.

- The function $H_\nu(q)$ is the physicists' Hermite polynomials of order $\nu$, defined by:

$$H_\nu(q) = (-1)^\nu e^{q^2}\frac{d^\nu}{dq^\nu}\left(e^{-q^2}\right)$$

# Quantum Harmonic Oscillator III

- The corresponding energy levels are

$$E_\nu = \hbar\omega\left(\nu + \frac{1}{2}\right) = (2\nu + 1)\frac{\hbar}{2}\omega$$

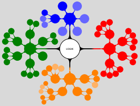
- Recursion formula:

$$\boxed{H_{\nu+1}(q) = 2qH_\nu(q) - 2\nu H_{\nu-1}(q)}$$

with the first two: $H_0 = 1$ and $H_1 = 2q$.

**Example py-file:** The program to find the harmonic oscillator wavefunctions/probability densities for up to 4 vibrational energy levels with the harmonic potential, $V = q^2/2$. QHO.py





# Quantum Harmonic Oscillator IV

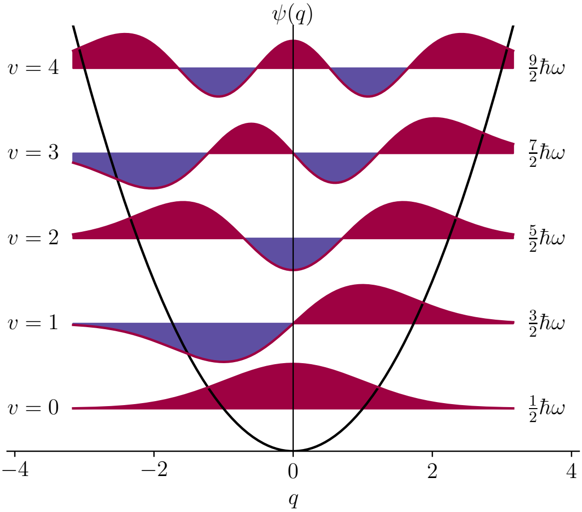



**Figure:** Wavefunction representations for the first 5 bound eigenstates, $\nu = 0 - 4$.

# Quantum Harmonic Oscillator V

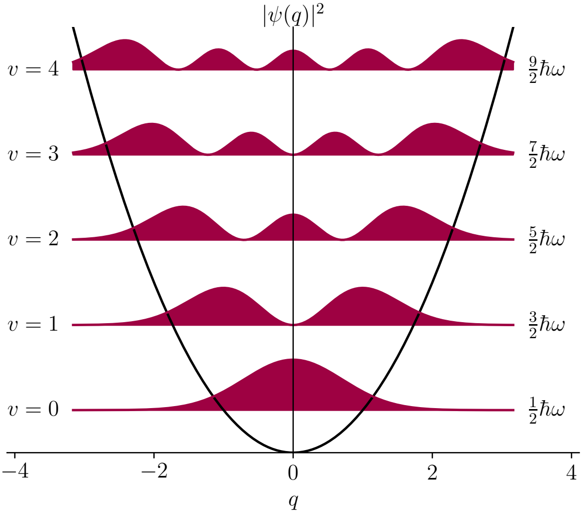



**Figure:** Corresponding probability densities.