PDEs and Coordinate Systems

	Cartesian	(Cylindrical) Polar	Spherical Polar
Hyperbolic	1D string 2D membrane 3D volume	Circular membrane Wave in cylinder	Wave in sphere
Elliptic	Laplace in square Laplace in cube	Laplace in cylinder	Laplace in sphere Sphere in E-field
Parabolic	Diffusion in square Diffusion in cube	Diffusion in cylinder	Diffusion in sphere
Schrödinger*	Particle in line Particle in rectangle Particle in cuboid	Particle in a circle Particle in a cylinder	Particle in sphere Particle in hemisphere

PDEs and Coordinate Systems

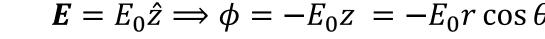
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Conducting Sphere in a Uniform E-field

 $\rightarrow E_0$

- Field satisfies $\nabla^2 \phi = 0$, $E = -\nabla \phi$
- E-field at infinity,

$$E = E_0 \hat{z} \Longrightarrow \phi = -E_0 z = -E_0 r \cos \theta$$



• Axisymmetric solution, no φ dependence, m=0

$$\Rightarrow \phi = \sum_{l=0}^{\infty} (A_l r^l + B_l r^{-l-1}) P_l^0(\cos \theta) \quad \text{wlog } A_0 = 0 \text{ (constant)}$$

- As $z \to \infty$, require $\phi = -E_0 r \cos \theta = -E_0 r P_1^0 (\cos \theta)$
 - $\Rightarrow A_l = 0 \text{ for } l > 1, A_1 = -E_0$
- At r=a, need $\phi=$ constant, so $A_la^l+B_la^{-l-1}=0$ for all l $\Rightarrow B_l = 0 \text{ for } l > 1$, $A_1 a + B_1 a^{-2} = 0$, so $B_1 = E_0 a^3$
- Solution for r > a is

$$\phi = -E_0 r \cos \theta \left(1 - \frac{a^3}{r^3} \right)$$

Induced dipole moment

Laplace's Equation in Polar Coordinates

• In 2D (i.e. Laplace in a circle)

$$r(rR')' - m^2R = 0$$

$$\Rightarrow r^2R'' + rR' - m^2R = 0$$

$$\Rightarrow R(r) = r^{\pm m}$$

• True, but there is another solution in the case m=0:

$$r^{2}R'' + rR' = 0$$

$$\Rightarrow rR'' + R' = (rR')' = 0$$

$$\Rightarrow rR' = \text{constant}, a$$

$$\Rightarrow R(r) = a \log r + b$$
Additional department of the properties of

Additional solution to the problem — dominant solution as $r \to \infty$

Special Functions in Physics

Harmonic Oscillator

$$y'' + k^2 y = 0$$

all

Bessel

$$x^2y'' + xy' + (x^2 - v^2)y = 0$$

polar, cyl. polar, sph. polar

• Legendre (m = 0)

$$(1 - x^2)y'' - 2xy' + l(l+1)y = 0$$

spherical polar

• Legendre (general)

$$(1-x^2)y'' - 2xy' + \left[l(l+1) - \frac{m^2}{1-x^2}\right]y = 0$$

spherical polar

Hermite

$$y'' - 2xy' + 2ny = 0$$

QM harmonic oscillator

Laguerre

$$xy'' - (1 - x)y' + ny = 0$$

QM hydrogen atom

Second-Order Linear (Ordinary) Differential Equations

General form of SOLDE

$$y'' + P(x)y' + Q(x)y = 0$$

• Some definitions, at some point x_0

$$P(x_0)$$
 and $Q(x_0)$ finite $\Rightarrow x = x_0$ is an ordinary point $P(x_0)$ or $Q(x_0)$ infinite $(x - x_0)P(x_0)$, $(x - x_0)^2Q(x_0)$ finite $\Rightarrow x = x_0$ is a regular singular point otherwise, $x = x_0$ is an essential singularity

- All of the equations just cited fall into the first two categories
 - all points are ordinary or regular singular
- Why worry about singular points?
 - they tell us about whether we can construct a power series solution

Series Solutions to SOLDEs

• In the vicinity of some point (here x=0), seek a power-series solution of the form (power series with an x^k multiplier)

$$y(x) = x^k \sum_{i=0}^{\infty} a_i x^i$$

- Notes: k and a_i are formally undetermined, no constraint on k, $a_0 \neq 0$.
- Basic approach: assume convergence and substitute the series into the ODE, then compare powers of x.
- Start with the equation of the <u>Harmonic Oscillator</u> as a familiar starting point:

$$y'' + y = 0$$

In our terminology, P(x) = 0, Q(x) = 1

- Note that x = 0 is an ordinary point.
- Solutions cos x and sin x and their series are all well known.

Differential equation:

$$y'' + y = 0$$
(solutions $y = \cos x$, $\sin x$)

Substitute the assumed solution

$$y(x) = x^k \sum_{i=0}^{\infty} a_i x^i = \sum_{i=0}^{\infty} a_i x^{k+i}$$

into the equation

$$y' = \sum_{i=0}^{\infty} a_i(k+i)x^{k+i-1}$$

$$y'' = \sum_{i=0}^{\infty} a_i(k+i)(k+i-1)x^{k+i-2}$$

$$\Rightarrow \sum_{i=0}^{\infty} a_i(k+i)(k+i-1)x^{k+i-2} + \sum_{i=0}^{\infty} a_ix^{k+i} = 0$$

- Equation must be satisfied by the coefficient of every power of x.
- Start by rewriting to equalize the powers of x in both sums.

$$\sum_{i=0}^{\infty} a_i(k+i)(k+i-1)x^{k+i-2} + \sum_{i=0}^{\infty} a_i x^{k+i} = 0$$

• Write j = i - 2 in the first sum, j = i in the second

$$\Rightarrow \sum_{j=-2}^{\infty} a_{j+2}(k+j+2)(k+j+1)x^{k+j} + \sum_{j=0}^{\infty} a_j x^{k+j} = 0$$

$$\Rightarrow a_0 k(k-1)x^{k-2} + a_1(k+1)kx^{k-1}$$

$$+ \sum_{j=0}^{\infty} \left[a_{j+2}(k+j+2)(k+j+1) + a_j \right] x^{k+j} = 0$$

• Equation must be satisfied term by term, and $a_0 \neq 0$, so

$$x^{k-2}$$
 $a_0k(k-1)=0 \implies k=0 \text{ or } 1$ Indicial Equation
$$x^{k-1}$$
 $a_1k(k+1)=0 \implies \text{no new constraint if } k=0$
$$a_1=0 \text{ if } k=1$$

- Indicial equation <u>always</u> gives algebraic constraint on k.
- Second equation may constrain coefficients.
- Note that in either case, the solution is a polynomial in x.
- Now consider the remaining sum:

$$\sum_{j=0}^{\infty} \left[a_{j+2}(k+j+2)(k+j+1) + a_j \right] x^{k+j} = 0$$

• Coefficient of x^{k+j} must be zero, so

$$a_{j+2}(k+j+2)(k+j+1) + a_j$$

A <u>recurrence relation</u> for the coefficients:

$$a_{j+2} = \frac{-1}{(k+j+2)(k+j+1)} a_j$$

Thus,

$$a_{j+2} = \frac{-1}{(k+j+2)(k+j+1)} a_j$$

- Note that even couples with even, odd with odd.
- For k=1, we know $a_1=0$, so the solution consists only of terms <u>odd</u> in x: a_0x , a_2x^3 , a_4x^5 , etc.

$$a_{2n} = \frac{-1}{(2n+1)(2n)} a_{2n-2} = \frac{(-1)^2}{(2n+1)(2n)(2n-1)(2n-2)} a_{2n-4}$$

$$\vdots$$

$$= \frac{(-1)^n}{(2n+1)!} a_0,$$

so
$$y(x) = a_0 \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1} = a_0 \left(x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots \right) = \sin x$$

- If k = 1, the polynomial consists of only <u>odd</u> powers of x.
- If k=0, a_1 , a_3 , a_5 , \cdots are not determined by the recurrence, but conventional to take them to be zero, so the polynomial has only <u>even</u> powers of x.

 (Recall that any linear combination of two solutions is a solution, so this is equivalent to absorbing the odd powers for k=0 into the k=1 solution.)
- For k = 0, we now have

$$a_{2n} = \frac{-1}{(2n)(2n-1)} a_{2n-2} = \frac{(-1)^2}{(2n)(2n-1)(2n-2)(2n-3)} a_{2n-4}$$

$$\vdots$$

$$= \frac{(-1)^n}{(2n)!} a_0,$$

so
$$y(x) = a_0 \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n} = a_0 \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \right) = \cos x$$

• Now look at the <u>Legendre equation</u> (just the associated Legendre equation with m=0):

$$(1 - x^2)y'' - 2xy' + l(l+1)y = 0$$

In our terminology, $P(x) = \frac{-2x}{1-x^2}$, $Q(x) = \frac{l(l+1)}{1-x^2}$

- Again, x = 0 is an ordinary point.
- Substitute the assumed solution

$$y(x) = x^k \sum_{i=0}^{\infty} a_i x^i = \sum_{i=0}^{\infty} a_i x^{k+i}$$

with $a_0 \neq 0$ into the equation and again note

$$y' = \sum_{i=0}^{\infty} a_i(k+i)x^{k+i-1}$$

$$y'' = \sum_{i=0}^{\infty} a_i(k+i)(k+i-1)x^{k+i-2}$$

Substitute the assumed solution

$$y(x) = x^k \sum_{i=0}^{\infty} a_i x^i = \sum_{i=0}^{\infty} a_i x^{k+i}$$

into the Legendre ODE: $(1 - x^2)y'' - 2xy' + l(l + 1)y = 0$

Result:

$$(1-x^{2}) \sum_{i=0}^{\infty} a_{i}(k+i)(k+i-1)x^{k+i-2}$$

$$-2x \sum_{i=0}^{\infty} a_{i}(k+i)x^{k+i-1} + l(l+1) \sum_{i=0}^{\infty} a_{i}x^{k+i} = 0$$

$$\Rightarrow \sum_{i=0}^{\infty} a_{i}(k+i)(k+i-1)x^{k+i-2}$$

$$-\sum_{i=0}^{\infty} [(k+i)(k+i-1) + 2(k+i) - l(l+1)]a_{i}x^{k+i} = 0$$

$$\Rightarrow \sum_{j=-2}^{\infty} a_{j+2}(k+j+2)(k+j+1)x^{k+j} \qquad j=i-2$$

$$-\sum_{i=0}^{\infty} a_{i}[(k+j)(k+j+1) - l(l+1)]x^{k+j} = 0$$

$$j=i$$

Combine the sums:

$$a_0 k(k-1) x^{k-2} + a_1(k+1) k x^{k-1}$$

$$+ \sum_{j=0}^{\infty} a_{j+2}(k+j+2)(k+j+1) x^{k+j}$$

$$- \sum_{j=0}^{\infty} a_j [(k+j)(k+j+1) - l(l+1)] x^{k+j} = 0$$

- Expect every coefficient of x^{k+j} to sum to zero individually, and $a_0 \neq 0$
- Leading terms are

$$x^{k-2}$$
 $a_0k(k-1) = 0 \implies k = 0 \text{ or } 1$
 x^{k-1} $a_1k(k+1) = 0 \implies a_1 = 0 \text{ if } k = 1$

• Again, indicial equation gives the allowed values of k, second equation constrains the coefficients.

- In either case, the solution is a Legendre polynomial, $P_l(x)$.
- Now consider the remaining sum.

$$\sum_{j=0}^{\infty} a_{j+2}(k+j+2)(k+j+1)x^{k+j}$$
$$-\sum_{j=0}^{\infty} a_j[(k+j)(k+j+1) - l(l+1)] x^{k+j} = 0$$

• Coefficient of x^{k+j} must be zero, so

$$a_{j+2}(k+j+2)(k+j+1) = a_j[(k+j)(k+j+1) - l(l+1)]$$

- Recurrence relation for the coefficients.
- Again connects even to even, odd to odd.

Recurrence relation is

$$a_{j+2}(k+j+2)(k+j+1) = a_j[(k+j)(k+j+1) - l(l+1)]$$

• In the case k = 1, $a_0 \neq 0$, $a_1 = 0$, so

$$a_{j+2} = \frac{(j+1)(j+2)-l(l+1)}{(j+3)(j+2)} a_j$$

and all even terms are determined (odd terms are zero):

$$\begin{split} a_{2n} &= \frac{(2n)(2n-1)-l(l+1)}{(2n+1)(2n)} a_{2n-2} \\ &\vdots \\ &= \frac{[(2n)(2n-1)-l(l+1)] \left[(2n-2)(2n-3)-l(l+1) \right] \cdots \left[6-l(l+1) \right] \left[-l(l+1) \right]}{(2n+1)!} a_0 \end{split}$$

(recall in this case, a_{2n} is the coefficient of x^{2n+1})

• In the case k=0,

$$a_{j+2} = \frac{j(j+1)-l(l+1)}{(j+2)(j+1)} a_j$$

- Odd terms are undetermined; make the same arguments as before to absorb them into the k=1 solution, so just look at the even terms.
- Then all even terms are determined:

$$a_{2n} = \frac{(2n-2)(2n-1)-l(l+1)}{(2n)(2n-1)} a_{2n-2}$$

$$\cdots = \frac{[(2n-2)(2n-1)-l(l+1)][(2n-4)(2n-3)-l(l+1)]\cdots[6-l(l+1)][-l(l+1)]}{(2n)!} a_0$$

- Note: as before, if k=1, polynomial consists of only <u>odd</u> powers of x.
- If k = 0, polynomial has only <u>even</u> powers of x.

Convergence of the Series

Note that since

$$\frac{a_{j+2}}{a_j} = \frac{(k+j)(k+j+1) - l(l+1)}{(k+j+2)(k+j+1)} \to 1 \text{ as } j \to \infty,$$

Ratio of j+2 and j terms is $\frac{a_{j+2}}{a_j}x^2$

ratio test implies that the series is divergent at $x = \pm 1$.

- The only way the solution can converge everywhere is if terminates.
- Require $a_{j+2} = 0$ for some j

$$\Rightarrow$$
 $(k+j)(k+j+1) - l(l+1) = 0$ for some j

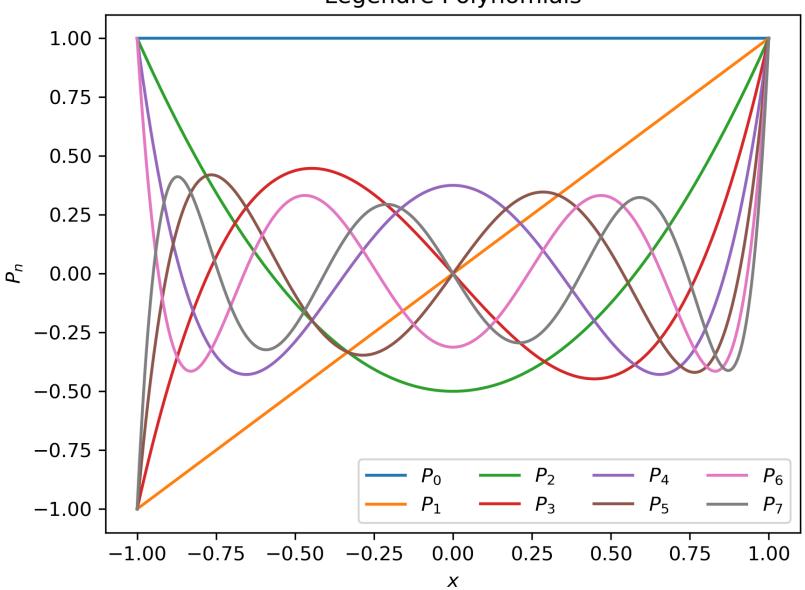
$$\implies l = k + j$$
 for some j

- $\Rightarrow l$ must be an <u>integer</u>
- (Recall $P_l(x) = P_l^0(x)$ previously, $x = \cos \theta$, want solution finite everywhere on the sphere.)

Legendre Polynomials

- *l* must be an integer for convergence
- Even solution (k = 0) stops at j = l
- Odd solution (k = 1) stops at j = l 1 $P_l(x) \text{ is a polynomial of order } l$ $\text{even powers of } x \text{ only if } l \text{ is even:} \qquad 0, 2, 4, ..., l$ $\text{odd powers of } x \text{ only if } l \text{ is odd:} \qquad 1, 3, 5, ..., l$
- Already seen the first few $(P_l = P_l^0)$.
- Convention: $P_l(1) = 1$
- Parity: $P_l(-x) = (-1)^l P_l(x)$
- Standard function in Python and other languages.

Legendre Polynomials



Series Solutions to Bessel's Equation

• The Bessel Equation is:

$$x^2y'' + xy' + (x^2 - m^2)y = 0$$
, $m \text{ integer}$
 $P(x) = \frac{1}{x}$, $Q(x) = 1 - \frac{m^2}{x^2}$

- Now x = 0 is a <u>regular singular point</u>.
- Substitute the assumed solution

$$y(x) = x^{k} \sum_{i=0}^{\infty} a_{i} x^{i} = \sum_{i=0}^{\infty} a_{i} x^{k+i}$$

$$\Rightarrow \sum_{i=0}^{\infty} a_{i} (k+i) (k+i-1) x^{k+i}$$

$$+ \sum_{i=0}^{\infty} a_{i} (k+i) x^{k+i} + \sum_{i=0}^{\infty} a_{i} x^{k+i+2} = 0$$

$$-m^{2} \sum_{i=0}^{\infty} a_{i} (k+i) x^{k+i} = 0$$

• Indicial equation: $a_0[(k(k-1)+k-m^2]=0 \implies k^2=m^2$, $k=\pm m$

Leading term is x^k

Series Solutions to Bessel's Equation

• Indicial equation:
$$a_0[(k(k-1)+k-m^2]=0 \implies k^2=m^2, \ k=\pm m$$

$$x^{k+1}: \qquad a_1[(k+1)k+k+1-m^2]=0$$

$$\implies a_1(k+1+m)(k+1-m)=0$$

$$\implies a_1=0$$

• General term for k = +m is

$$a_{i}[(m+i)(m+i-1) + (m+i) - m^{2}] + a_{i-2} = 0$$

$$a_{i}[(m+i)^{2} - m^{2}] + a_{i-2} = 0$$

$$\Rightarrow a_{i} = \frac{-1}{i(i+2m)} a_{i-2} \text{ "etc."}$$

• Solution is $J_m(x)$

Series Solutions to Bessel's Equation

- Expect a second-order differential equation to have two linearly independent solutions.
- If m is <u>not</u> an integer, turns out that $J_{-m}(x)$ is <u>independent</u> of $J_m(x)$.
- But if m is an <u>integer</u> (as in the case of separation in cylindrical polars), can show (see R&H 9.5.2) that

$$J_{-m}(x) = (-1)^m J_m(x)$$

- The two solutions for k do <u>not</u> necessarily yield independent solutions to the problem.
- But sometimes they do: e.g. $\sin x$ and $\cos x$...
- How do we know when we actually have two independent solutions?

Fuch's Theorem

- Classifies behavior of SOLDE solutions.
- Expand about an ordinary point or a regular singular point
 - \Rightarrow indicial equation has ≥ 1 solutions
 - if roots of indicial equation are equal, then they provide only 1 solution
 - if roots of indicial equation differ by a non-integer, then they represent
 2 independent solutions
 - if roots of indicial equation differ by an integer, then the larger of the two gives a solution; the lower may or may not — <u>must check</u>
- Expand about an essential singularity ⇒ all bets are off!
- SOLDEs of interest all fall into the former category

Second Solutions

- Expect all SOLDEs to have 2 independent solutions.
- Power series development gives us a first solution in all cases.
- Some SOLDEs naturally generate 2 independent series solutions.
- Others do not.
- How can we determine if two solutions are independent?
- How can we generate a second solution, given a first series solution?
- Wronskian development shows the way

Wronskians

- Suppose we have 2 solutions y_1 and y_2
- Define Wronskian:

$$W(x) = y_1 y_2' - y_1' y_2$$

Then

$$W = 0 \iff \frac{y_1'}{y_1} = \frac{y_2'}{y_2}$$

$$\Leftrightarrow \frac{d(\log y_1)}{dx} = \frac{d(\log y_2)}{dx}$$

$$\Leftrightarrow \log y_1 = \log y_2 + \log A$$

$$\Leftrightarrow y_1 = Ay_2$$

• Non-zero Wronskian means <u>linear independence</u>.

Second Solutions

Can use the Wronskian to develop a second solution given the first:

$$y_1'' + P(x)y_1' + Q(x)y_1 = 0$$
$$W(x) = y_1y_2' - y_1'y_2$$

Then

$$W' = y_1'y_2' + y_1y_2'' - y_1''y_2 - y_1'y_2'$$

$$= y_1(-Py_2' - Qy_2) - y_2(-Py_1' - Qy_1)$$

$$= -P(x)(y_1y_2' - y_1'y_2)$$

$$= -P(x)W$$

• Simple differential equation for W: $W(x) = W(x_0)e^{-\int_{x_0}^x P(x')dx'}$

Second Solutions

But we can also write

$$W(x) = y_1 y_2' - y_1' y_2 = y_1^2 \frac{d}{dx} \left(\frac{y_2}{y_1} \right)$$

SO

$$\frac{d}{dx}\left(\frac{y_2}{y_1}\right) = \frac{e^{-\int_{x_0}^x P(x')dx'}}{y_1^2}$$

$$\Rightarrow y_2(x) = y_1(x) \int_{x_0}^{x} \frac{e^{-\int_{x_0}^{x''} P(x')dx'}}{y_1^2(x'')} dx''$$

• Can <u>always</u> generate a second solution.