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$\boxed{\text{834 Lecture 17}}$

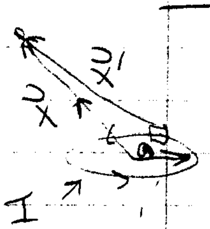
Lecture Plan:

- Laplace equation with spherical symmetry example (142)-(144)
- Spherical harmonics and general expansion (148)-(149)
- If time permits: undetermined coefficients (138), Gaussian quadrature

Before class:

- Start up 834 page + Mathematica
  - legendre_polynomial_1.nb
  - spherical_harmonics_1.nb
  - gauss_quad_test_1.nb

On board:



- For PS#9 2b) (static) magnetic vector potential $\vec{A}(\vec{x}) = \frac{\mu_0}{4\pi}\int \frac{\vec{J}(\vec{x}')}{|\vec{x}-\vec{x}'|} d^3x'$
  - $\vec{J}$ is current density $\Rightarrow$ current/area
  - What coordinate system? (Remember what expansion you have!)
  - What symmetries are there? So what does $\vec{A}$ depend on?
  - Use the symmetry to make $\vec{A}$ point in a simple direction so that only the magnitude matters.
- PS#9 1: basic expansion, like today
- For PS#9 3: What are the symmetries? What do they imply for what $T(\vec{x},t)$ depends on? What are the implicit assumptions in this problem?
  Do separation of variables for t and whatever dependence of x, y, z or r, θ, φ or ρ, φ, z.
- Try PS#9 4, 5 if you have time: good supplements!

- Separation of variables in spherical coordinates for $\nabla^2\Phi$ (eg. from (142)+)

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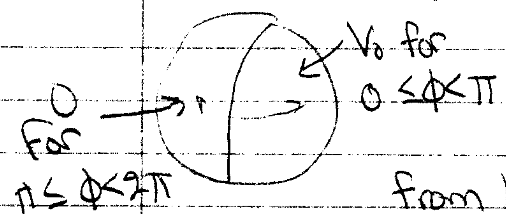
As an example of how the expansion works when we don't have azimuthal symmetry (ϕ-independent), let's consider the same split conducting sphere, but now turned on its side:



This example is considered in detail in Lea Example 8.3, including showing that it reproduces the same answer from before when the coordinates are transformed appropriately. We will focus on the set up.

There is now a ϕ dependence, so we will start with the general expansion for a solution to $\nabla^2 \Phi = 0$:

$$\Phi(r,\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(A_{lm} r^l + \underbrace{\cancel{B_{lm}}}_{\to 0 \text{ because finite at } r=0} r^{-(l+1)} \right) Y_{lm}(\theta,\varphi)$$

Goal: use the boundary condition to find the A_{lm}'s.

Given: $$\Phi(r=a,\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{lm}\, a^l\, Y_{lm}(\theta,\varphi) = \begin{cases} V_0 & \text{if } 0 \le \varphi < \pi \\ 0 & \text{if } \pi \le \varphi < 2\pi \end{cases}$$

Plan: Project out A_{lm} using the orthonormality of the Y_{lm}'s

$\Rightarrow$ multiply by $Y^*_{l'm'}(\theta,\varphi)$ and integrate $\int d\Omega = \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi$

$$\Rightarrow \int d\Omega \, \underset{\wedge}{Y^*_{l'm'}(\theta,\phi)}\, \Phi(r=a,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{lm}\, a^l \int d\Omega \, \underbrace{Y^*_{l'm'}(\theta,\varphi) Y_{lm}(\theta,\varphi)}_{\delta_{l'l}\delta_{m'm}}$$

$$= A_{l'm'}\, a^{l'}$$

$$= \int_0^{\pi} \sin\theta \, d\theta \int_0^{\pi} d\phi \; V_0 \, Y^*_{l'm'}(\theta,\varphi)$$

$\leftarrow$ not 2π!

what would we get if the ϕ integral was 0 to 2π? $\rightarrow$

so we're basically done. Let's expose the θ,φ dependence:

drop primes

$$A_{lm} = \frac{V_0}{a^l} \sqrt{\frac{(2l+1)}{4\pi}} \sqrt{\frac{(l-m)!}{(l+m)!}} \int_{-1}^{1} P_l^m(x)\, dx \underbrace{\int_0^{\pi} e^{-im\phi}\, d\phi}_{\text{for } m>0,\ \left(\frac{1-(-1)^m}{im}\right)}$$

$\leftarrow$ zero unless m is odd

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Let's look at $A_{\ell m}$ for $m=0$, which we need to treat separately.

For $\ell=0, m=0$, $Y^*_{00} = \frac{1}{\sqrt{4\pi}}$

$$\Rightarrow A_{00} = V_0 \underbrace{\int_{-1}^{1} dx}_{2} \underbrace{\int_0^{\pi} d\phi}_{\pi} \frac{1}{\sqrt{4\pi}} = \frac{V_0}{\sqrt{\pi}} \quad \text{(typo in Lea!)}$$

Suppose $m=0$ but $\ell \neq 0$? Recall $P_\ell^{m=0}(x) = P_\ell(x)$ Legendre polynomial

$$\Rightarrow \int_{-1}^{1} P_\ell^0(x)\,dx = \int_{-1}^{1} P_\ell(x)\,dx = \int_{-1}^{1} P_\ell(x) \underbrace{P_0(x)}_{=1} dx = 2\delta_{\ell 0}$$

So only $\ell=0$ when $m=0$.

When $m \neq 0$, $\left(\frac{1-(-1)^m}{im}\right) = 0$ unless m is odd. But if m is odd and ℓ even, then P_ℓ^m is odd, so integrates to zero.

$\Rightarrow$ besides the $\ell=0, m=0$ term, the expansion is over ℓ odd, m odd.

We are left with an integral $I_{\ell m}$:

$$\left.\begin{aligned} I_{\ell m} \equiv \int_{-1}^{1} P_\ell^m(x)\,dx &= \pi P_{\ell+1}(0) P_\ell^m(0) \frac{m}{\ell}(-1)^{(m+1)/2} \\ &= -m\pi \frac{(\ell-2)!!}{(\ell+1)!!} \frac{(\ell+m-1)!!}{(\ell-m)!!} \end{aligned}\right\} \ \ell, m \text{ odd; see Lea}$$

$$\Rightarrow \Phi(r,\theta,\varphi) = V_0 \left[\frac{1}{2} + \sum_{\substack{\ell=1 \\ \text{odd}}}^{\infty} \sum_{\substack{m=-\ell \\ \text{odd}}}^{\ell} \left(\frac{r}{a}\right)^{\ell} \underbrace{\frac{(2\ell+1)}{4\pi} \frac{(\ell-m)!}{(\ell+m)!} I_{\ell m} \frac{2}{im} P_\ell^m(x) e^{im\phi}}_{I_{\ell m} \sqrt{\frac{(2\ell+1)}{4\pi}} \sqrt{\frac{(\ell-m)!}{(\ell+m)!}} \frac{2}{im} Y_{\ell m}(\theta,\varphi)} \right.$$

Not immediately obvious, but this is real.

First terms $V_0 = \left[\frac{1}{2} + \frac{r}{a} \frac{3}{4} \sin\theta \sin\phi + \frac{7}{128} \left(\frac{r}{a}\right)^3 \left[3(5\cos^2\theta - 1) \sin\theta \sin\phi + 5 \sin^3\theta \sin 3\phi \right] + \ldots \right]$

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cf. the 8.2 example result:

$$\Phi(r,\theta,\varphi) = \frac{V_0}{2}\left[1 - \sum_{l=1}^{\infty} \frac{2l+1}{l} P_{l+1}(0)\left(\frac{r}{a}\right)^l P_l(\cos\gamma)\right]$$

should be the same potential ⇒ shown in Lec.

- What if the equation is not Laplace's equation.
Eg. the wave equation in spherical coordinates:

$$\nabla^2 F - \frac{1}{c^2}\frac{\partial^2 F}{\partial t^2} = 0$$

First Fourier transform in time ⇒ $k^2 = \frac{\omega^2}{c^2}$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial F}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 F}{\partial\phi^2} + k^2 F = 0$$

What if a time-independent Schrödinger equation with $V(r)$?
Same except $k^2F \to V(r)F - EF$ [where $F \to \Psi(r,\theta,\varphi)$]

- Separate yet again as $F = R(r)\Theta(\theta)\Phi(\phi)$
⇒ θ and ϕ equations will be the same!

- But r equation will depend on wave equation vs. S-eqn vs ...
wave equation: $\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + k^2r^2 - l(l+1) = 0$.

This can be converted to Bessel's equation and we read off that

$R(r) = \frac{J_{l+1/2}(kr)}{\sqrt{r}}$ ⇒ this combination called "spherical Bessel function": $j_l(z) = \sqrt{\frac{\pi}{2z}}\, J_{l+1/2}(z)$
(and independent solution not regular at origin)

$j_l(z) \propto z^l$ for small z, satisfies recursion relations. Trig functions!

$j_0(z) = \frac{\sin z}{z}$, $j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}$, $j_2(z) = \left(\frac{3}{z^3} - \frac{1}{z}\right)\sin z - \frac{3}{z^2}\cos z$

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In the problem set, you find an expansion for $\frac{1}{|\vec{x}-\vec{x}'|}$:

$$\frac{1}{|\vec{x}-\vec{x}'|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{lm}(\theta,\phi) Y^*_{lm}(\theta',\phi')$$

could be

$\frac{r}{r'}$ or $\frac{r'}{r}$ ⟸ depends on whether $r > r' \Rightarrow \frac{r'^l}{r^{l+1}}$, $r < r' \Rightarrow \frac{r^l}{r'^{l+1}}$

angles of $\vec{x}$

angles of $\vec{x}'$

- Useful for EM problems: electrostatics, magnetostatics

- Another very useful expansion is of a plane wave:

$$\langle \vec{r} | \vec{k} \rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} = \frac{1}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} i^l j_l(kr)(2l+1) P_l(\cos\theta)$$

cf. fourier transform

or $$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr) Y^*_{lm}\underbrace{(\theta_k,\phi_k)}_{\Omega_k} Y_{lm}\underbrace{(\theta_r,\phi_r)}_{\Omega_r}$$

seperate out the l dependence

⟹ "partial wave expansion", eg. for central potential in quantum mechanics.

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Orthogonal Polynomials

- orthogonal on $[a,b]$ with weight function $w(x)$
- satisfy recursion relations
- have a generating functional and Rodrigues-type formula

Common examples

	a	b	$w(x)$	normalization
Legendre	-1	1	1	$\int_{-1}^{1} [P_n(x)]^2 dx = \frac{2}{n+1}$
Hermite	$-\infty$	∞	e^{-x^2}	$\int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2} dx = 2^n \pi^{1/2} n!$
Laguerre	0	∞	$x^{\nu} e^{-x}$	$\int_0^{\infty} [L_n(x)]^2 e^{-x} dx = 1$
Chebyshev	-1	1	$\frac{1}{\sqrt{1-x^2}}$	$\int_{-1}^{1} \frac{[T_n(x)]^2}{(1-x^2)^{1/2}} = \begin{cases} \pi/2 & n \neq 0 \\ \pi & n = 0 \end{cases}$

other spellings are common!

- Call them generically $p_n(x)$ with weight $w(x)$ on $[a,b]$.
- We've encountered them as solutions to differential equations, but an alternative construction, up to normalization, is to require

unique given $w(x)$ and $[a,b]$

$$\int_a^b w(x)\, x^k\, p_n(x)\, dx = 0 \text{ for all } 0 \le k < n, \text{ with } p_0(x) = 1.$$

so $p_1(x)$ from $\int_a^b w(x) x^0 (x+b)\, dx = 0$, $\Rightarrow b \Rightarrow p_1(x)$ $\quad$ $p_2(x)$ from $\int_{-1}^{1} w(x) \begin{Bmatrix} x^0 \\ x^1 \end{Bmatrix} (x^2 + bx + c)\, dx = 0$ $\Rightarrow b, c \Rightarrow p_2(x)$

and so on. For $w(x) = 1$, $a = -1$, $b = 1$, generates Legendre polynomials with leading coefficient $= 1$: $p_0(x) = 1$, $p_1(x) = x$, $p_2(x) = x^2 - \frac{1}{3}x, \ldots$

If $p_{-1}(x)=0$, $p_0(x)=1$, $\Rightarrow$ $p_{j+1}(x)=(x-a_j)p_j(x)-b_j p_{j-1}(x)$ $j=0,1,2,\ldots$
where $a_j=\frac{\langle p_j|x|p_j\rangle}{\langle p_j|p_j\rangle}$, $b_j=\frac{\langle p_j|p_j\rangle}{\langle p_{j-1}|p_{j-1}\rangle}$ and $\langle p_i|p_j\rangle=\int_a^b w(x)p_i(x)p_j(x)$

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How can we use these to do approximate calculations of integrals? (called numerical quadrature).

- We can transform $\int_a^b f(x)\,dx$, possibly after breaking it into pieces, into an integral from -1 to 1.

$$\Rightarrow I=\int_{-1}^{1} f(x)\,dx$$

- We want a quadrature rule with N points:

$$I \doteq \sum_{i=1}^{N} f(x_i)\, w_i$$

where $\{x_i, w_i\}$ are fixed (ie. don't change for different $f(x)$).

- Suppose $N=3$ and we require $x_0=-1$, $x_1=0$, $x_2=+1$
  On small interval, smooth functions looks like (low-order) polynomials (Taylor expansion!) $\Rightarrow$ approximate as quadratic.
  - equivalent to requiring
    $f(x) = ax^2+bx+c$
    is perfectly integrated for any a, b, c

$$\text{So } \int_{-1}^{1}(ax^2+bx+c)\,dx=\frac{ax^3}{3}+\frac{bx^2}{2}+cx\Big|_{-1}^{1}=\frac{2a}{3}+2c$$

$$\doteq w_1 f(x_1)+w_2 f(x_2)+w_3 f(x_3)$$

With $x_1=-1, x_2=0, x_3=+1$ $\Rightarrow$ $f(-1)=a-b+c$
$f(0)=c$
$f(+1)=a+b+c$

$$\Rightarrow (a-b+c)w_1+c\,w_2+(a+b+c)w_3=2a/3+2c$$

For any a,b,c $\Rightarrow$ so equate a,b,c coefficients

$a(w_0+w_2)=\frac{2a}{3}$, $b(-w_0+w_2)=0$, $c(w_0+w_1+w_2)=2c$ $\Rightarrow$ $w_0=w_2=1/3$, $w_0=w_2$, $w_1=4/3$

$I \doteq \frac{1}{3}f(x_1)+\frac{4}{3}f(x_2)+\frac{1}{3}f(x_3)$ $\Rightarrow$ Simpson's rule.

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Simpson's rule is exact for polynomials of degree 2.

- In general a Taylor series with N equally spaced points yields a rule that integrates a polynomial of degree N or N+1, depending on whether N is odd or even.

Stitch Simpson's together: $\frac{1}{3}f(x_1) + \frac{4}{3}f(x_2) + \frac{2}{3}f(x_3) + \frac{4}{3}f(x_4) + \ldots + \frac{1}{3}f(x_N)$

- How can we do better with an N-point rule?
  - ⇒ let the x_i vary rather than being equally spaced!
  - ⇒ integrate 2N−1 polynomial exactly
  - ⇒ Gaussian quadrature!

- Basic idea: given $w(x)$ and N, construct the orthogonal polynomials $p_0(x), \ldots p_N(x)$.

- Now consider all $h(x)$ polynomials of degree 2N−1 or less
  - Divide $h(x)$ by $p_N(x)$
    - ⇒ $q(x)$ and remainder $r(x)$ ⇒ both of degree less than N so both orthogonal to $p_N(x)$

$$\Rightarrow h(x) = q(x)p_N(x) + r(x) \quad \text{uniquely}$$

$$\int_a^b w(x)h(x)\,dx = \int_a^b w(x)\underbrace{q(x)p_N(x)}_{0}\,dx + \int_a^b w(x)r(x)\,dx$$

integration rule

$$\doteq \sum_{i=1}^{N} w_i h(x_i) = \sum_{i=1}^{N} w_i q(x_i)p_N(x_i) + \sum_{i=1}^{N} w_i r(x_i)$$

choose the x_i at N zeros of p_N ⇒ this term is zero!

use freedom of N w_i's so this term integrated exactly

correct answer for ⇒ first N (0 to N−1) $p_i(x)$'s

$$\begin{pmatrix} p_0(x_1) & \cdots & p_0(x_N) \\ p_1(x_1) & & \vdots \\ & \ddots & \vdots \\ p_{N-1}(x_1) & \cdots & p_{N-1}(x_N) \end{pmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_N \end{bmatrix} = \begin{bmatrix} \int_a^b w(x)p_0(x)\,dx \\ 0 \\ \vdots \\ 0 \end{bmatrix} \Leftarrow \text{solve for } w_i\text{'s!}$$

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Example problems:

Consider $I = \int_0^3 (1+t)^{1/2}\, dt = 4.666\overline{6}$

We can always switch to $[-1,1]$ using

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{a+b}{2}\right)dx \doteq \frac{b-a}{2}\sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

So for I, switch to $x = -1 + \frac{2}{3}t \Rightarrow I = \frac{3}{2}\int_{-1}^{1}\left(\frac{3}{2}x + \frac{5}{2}\right)^{1/2} dx$

See gauss_quad_test_1.nb for these tests.

$N=3$ Simpson's rule yields $I_{simpsons} = 4.66228 = 10^{-3}$ relative error

$N=3$ Gauss-Legendre nodes and weights are
$x_1 = -x_3 = -0.774597$, $x_2 = 0$; $w_1 = w_3 = 0.555556$, $w_2 = 0.888889$
yields $I_{Gauss\,Legendre} = 4.66683 \Rightarrow 0.3 \times 10^{-4}$ relative error
$\Rightarrow \hat{\approx} 30$ times more accurate with same # of evaluations!

Try on $N=3$ Gauss-Laguerre integration with $\int_0^\infty (x^2+3x+5)e^{-x}dx = 10$
Perfect! Also for $x^4 - 2x^3 + 4x^2 + 3x + 5$.
Pretty good for $\int_0^\infty \sin x\, e^{-x} dx$. Fails for $x^6 - 2x^3 + 4x^2 + 3x + 5$
↖ order is greater than $2 \cdot 3 - 1 = 5$