Spherical Harmonics

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OST FHO Campus Rapperswil

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Goals for Today

Spherical Harmonics

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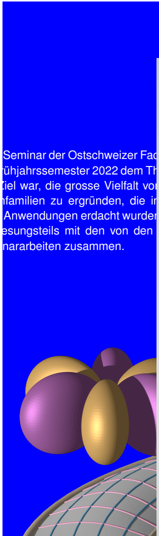
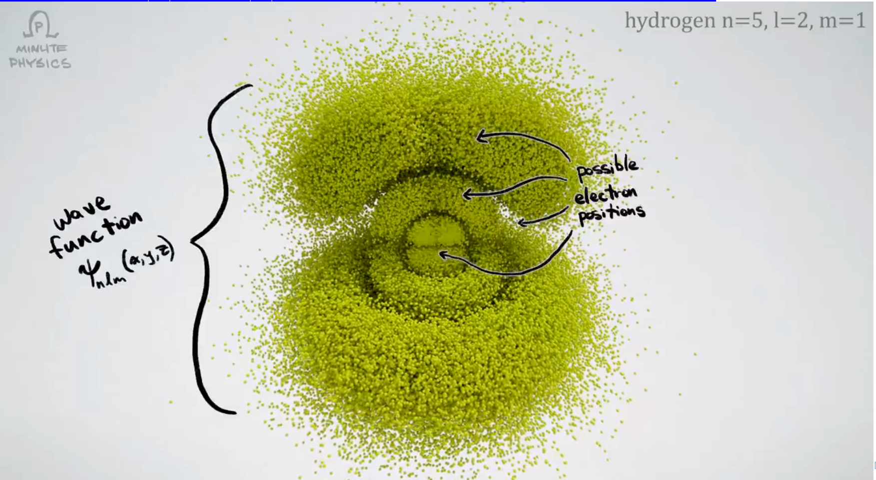
Spherical Harmonics *and* **Electron Orbitals**





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Nice Periodic Functions

Definition

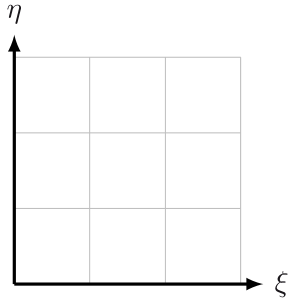
A function

$$f : \mathbb{R}^2 \to \mathbb{C}$$

is a "nice periodic function" when it is

- smooth,
- differentiable,
- (abs.) integrable,
- periodic on $[0,1] \times [0,1]$, i.e.

$$f(\xi, \eta) = f(\xi + 1, \eta) = f(\xi, \eta + 1).$$

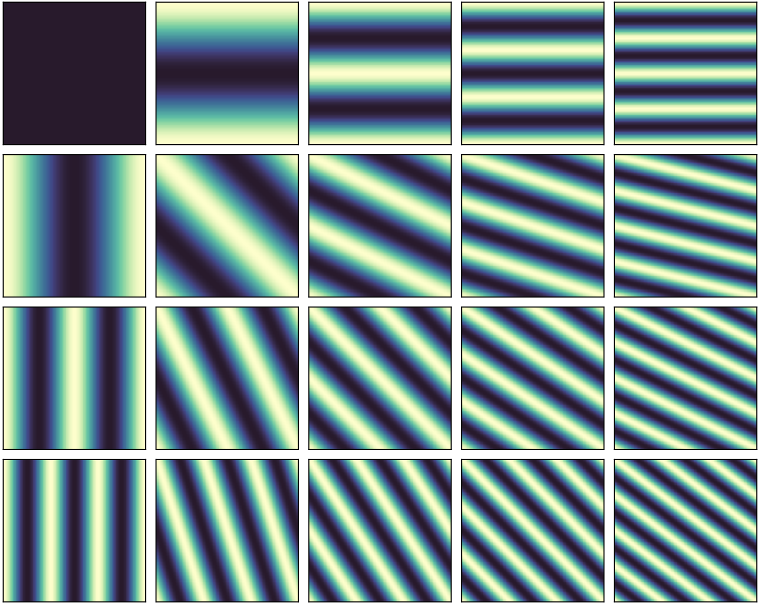


Function Space

Basis Functions

The space of nice periodic functions is spanned by the (also nice) functions

$$B_{m,n}(\xi, \eta) = e^{i2\pi m\xi} e^{i2\pi n\eta}.$$



Inner Product

Definition

Let $f(\xi,\eta)$ and $g(\xi,\eta)$ be nice periodic functions. Their inner product is

$$\langle f, g\rangle = \iint_{[0,1]^2} f(\xi,\eta)\overline{g}(\xi,\eta)\, d\xi d\eta.$$

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Definition

For a nice periodic function $f(\xi, \eta)$: the numbers

$$c_{m,n} = \langle f, B_{m,n} \rangle$$

are the *Fourier coefficients* or *spectrum* of f.

Fourier Series

Theorem

For nice periodic functions:

$$f(\xi, \eta) = \sum_{m \in \mathbb{Z}} \sum_{n \in \mathbb{Z}} c_{m,n} B_{m,n}(\xi, \eta)$$

where

$$c_{m,n} = \langle f, B_{m,n} \rangle.$$

Why exponentials?

Why $B_{m,n} = e^{i2\pi m\xi} e^{i2\pi n\eta}$***?***

Because ∇^2

The Problem

Eigenvalue Problem

$$\nabla^2 f(\xi,\eta) = \frac{\partial^2 f}{\partial \xi^2} + \frac{\partial^2 f}{\partial \eta^2} = \lambda f(\xi,\eta)$$

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Eigenvalue Problem

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Solution

Separation ansatz:

$$f(\xi, \eta) = M(\xi) N(\eta)$$

Resulting ODEs:

$$\frac{d^2 M}{d\xi^2} = \kappa M(\xi), \qquad \frac{d^2 N}{d\eta^2} = (\lambda - \kappa) N(\eta)$$

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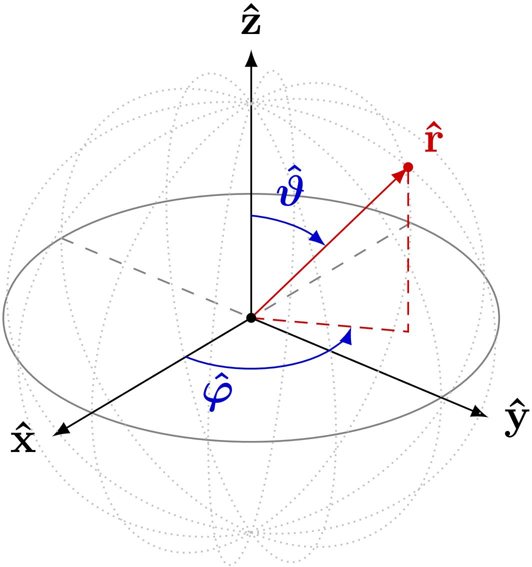
Spherical Coordinates



Variables

$$r \in \mathbb{R}^+$$
$$\vartheta \in [0, \pi]$$
$$\varphi \in [0, 2\pi)$$

To cartesian

$$x = r \cos\varphi \sin\vartheta$$
$$y = r \sin\varphi \sin\vartheta$$
$$z = r \cos\vartheta$$

Spherical Laplacian

Cartesian Laplacian

$$\nabla^2 := \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2}$$

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Cartesian Laplacian

$$\nabla^2 := \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2}$$

Spherical Laplacian

$$\nabla^2 := \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right]$$

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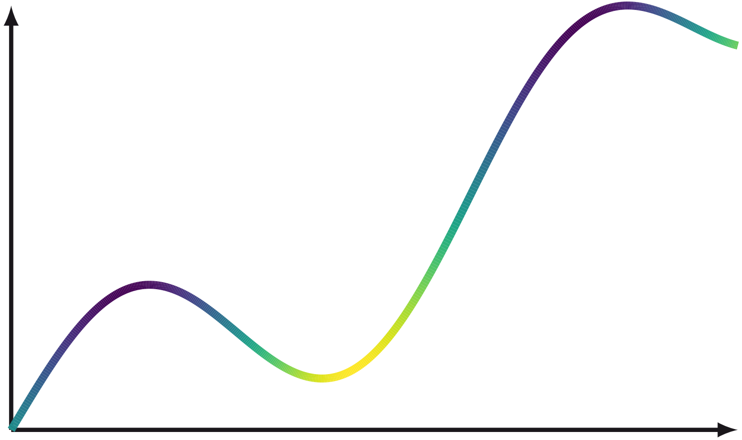
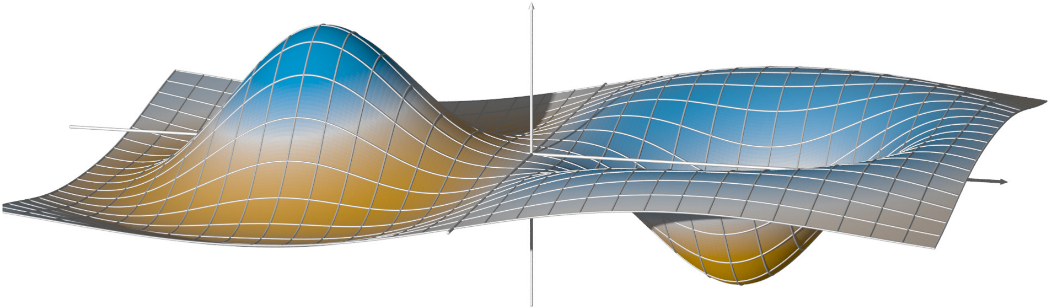
Surface Spherical Laplacian

$$\nabla_s^2 := r^2 \nabla^2 - \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)$$

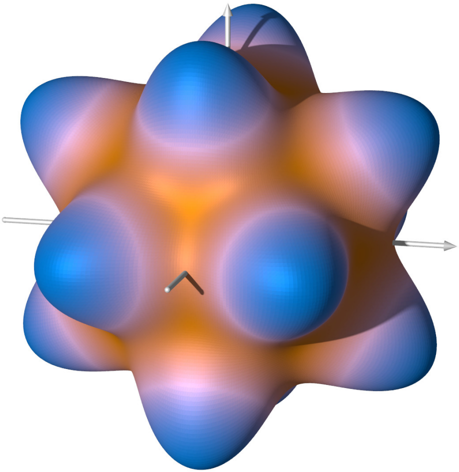
Geometrical Intuition



Geometrical Intuition

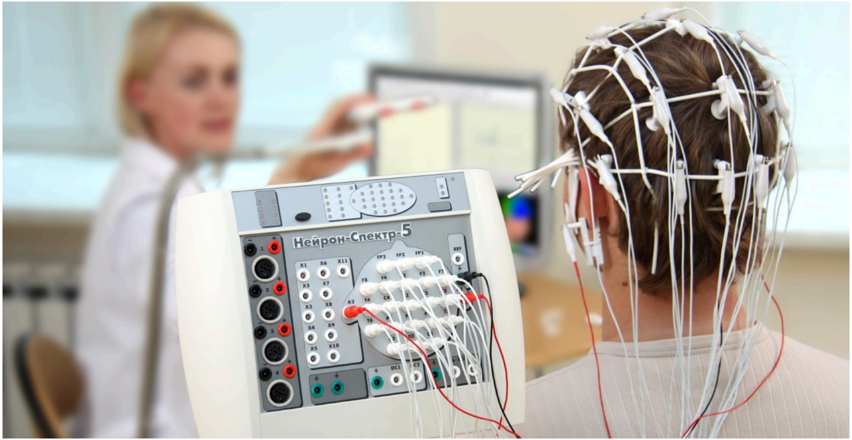


Geometrical Intuition



Where is ∇_s^2 useful?

To do brain scans, apparently [2]



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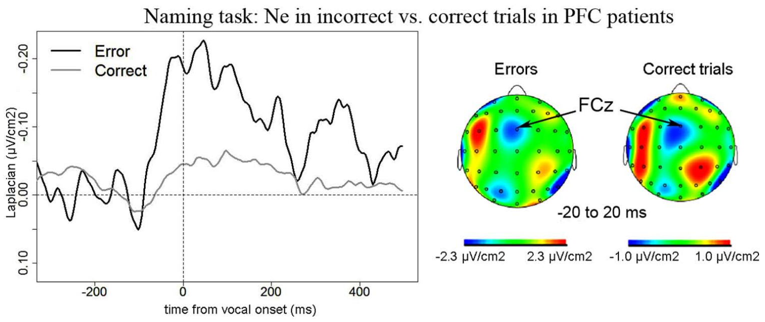

FIGURE 2 | EEG activity in PFC patients in the Naming task after surface Laplacian transformation, recorded at FCz for errors (black line) and correct trials (gray line). Zero of time represents vocal onset. The cartographies were made on a 40-ms time-window centered on vocal onset (from −20 to 20 ms after vocal onset). A 100 ms-long baseline was taken between 200 and 100 ms before vocal onset. The scale used for the topography for correct trials was larger than the one used for incorrect trials as the amplitude of the Ne was smaller in correct trials than in errors.

Brain Scans

Electrodynamics

$$\nabla^2 \phi = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \phi \qquad \left(\phi = \int_{\mathsf{A}}^{\mathsf{B}} \mathbf{E} \cdot d\mathbf{l} \right)$$

Electrodynamics

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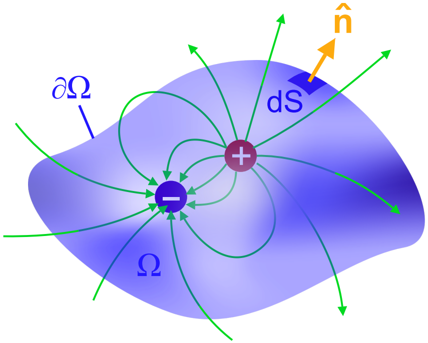
$$= \boldsymbol{\nabla} \cdot \mathbf{E}$$



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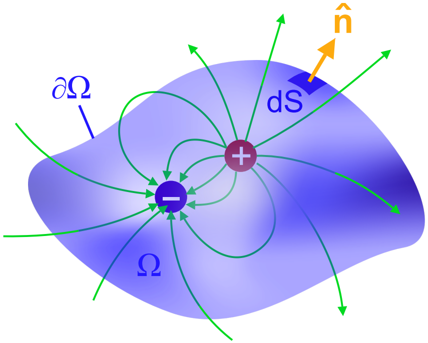
$$= \int_{\Omega} (\boldsymbol{\nabla}\cdot\mathbf{E})\cdot d\mathbf{s} = \oint_{\partial\Omega} \mathbf{E}\cdot d\mathbf{s}$$



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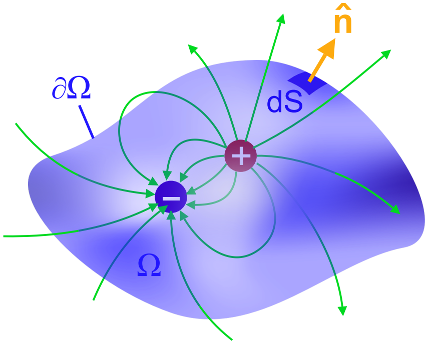
$$= \frac{\rho}{\varepsilon}$$



Brain Scans

Electrodynamics

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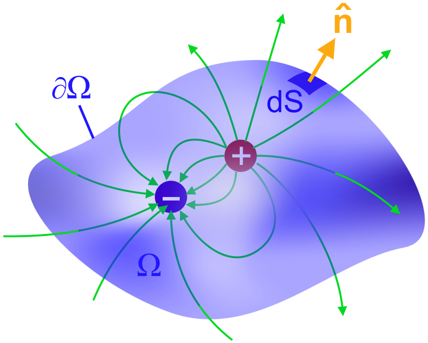

So over the scalp

$$\nabla_s^2\phi = \frac{\rho_s}{\varepsilon} = \text{Current flow in the brain}$$

New Hard Problem

The Problem

$$\nabla_s^2 f(\varphi, \vartheta) = \lambda f(\varphi, \vartheta)$$

New Hard Problem

The Problem

$$\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial f}{\partial\vartheta}\right)+\frac{1}{\sin^2\vartheta}\frac{\partial^2 f}{\partial\varphi^2}=\lambda f(\varphi,\vartheta)$$

New Hard Problem

The Problem

$$\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial f}{\partial\vartheta}\right)+\frac{1}{\sin^2\vartheta}\frac{\partial^2 f}{\partial\varphi^2}=\lambda f(\varphi,\vartheta)$$

Idea

Separation ansatz:

$$f(\varphi,\vartheta)=\Phi(\varphi)\Theta(\vartheta)$$

From the “easy” part:

$$\frac{d^2\Phi}{d\varphi^2}=\kappa\Phi(\varphi)\implies\Phi(\varphi)=e^{im\varphi},\quad m\in\mathbb{Z}$$

Associated Legendre Differential Equation

Separation (cont.)

The hard part is the ODE for $\Theta(\vartheta)$:

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

Definition (Associated Legendre Differential Equation)

$$\left(1 - x^2\right)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx}$$

Associated Legendre Differential Equation

Separation (cont.)

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Substituting $x = \cos\vartheta$ and $y = \Theta$:

Definition (Associated Legendre Differential Equation)

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

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Legendre Polynomials

Definition (Legendre Polynomials)

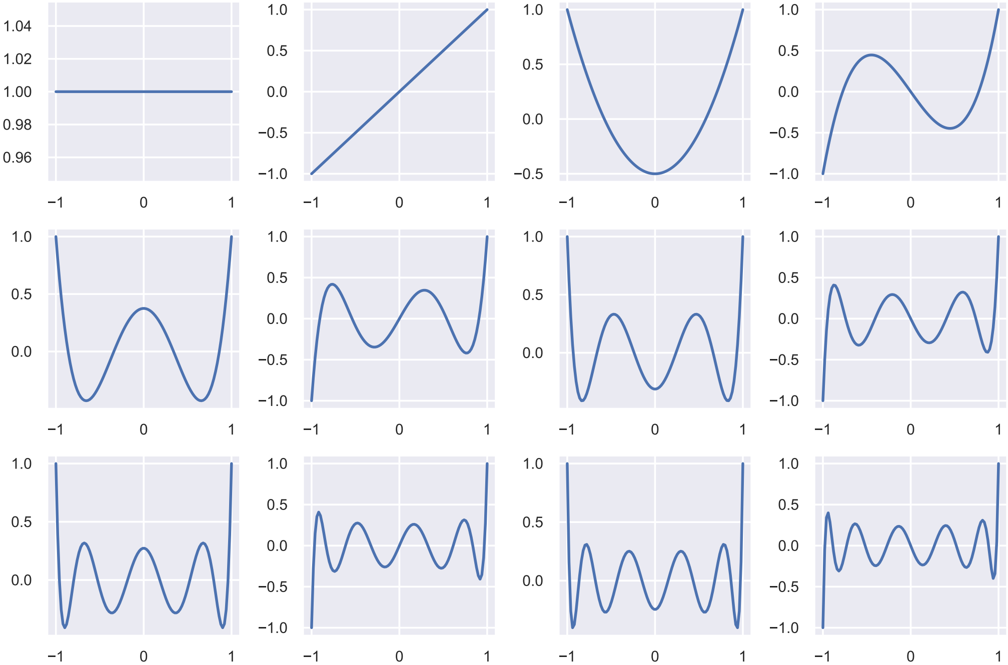
The polynomials

$$P_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k (2n-2k)!}{2^n k!(n-k)!(n-2k)!} x^{n-2k}$$

$$= {}_2F_1 \left(\begin{matrix} n+1, & -n \\ & 1 \end{matrix} ; \frac{1-x}{2} \right)$$

$$= \frac{1}{n! 2^n} \frac{d^n}{dx^n} (x^2 - 1)^n$$

are a solution to the associated Legendre differential equation when $m = 0$.


1.04
1.02
1.00
0.98
0.96
1.0
0.5
0.0
−0.5
−1.0
−1
0
1

Associated Legendre Polynomials

Lemma

For $x \in [-1, 1]$ *the polynomials*

$$P_{m,n}(x) = \left(1 - x^2\right)^{m/2} \frac{d^m}{dx^m} P_n(x)$$

solve the associated Legendre differential equation.

Associated Legendre Polynomials

Lemma

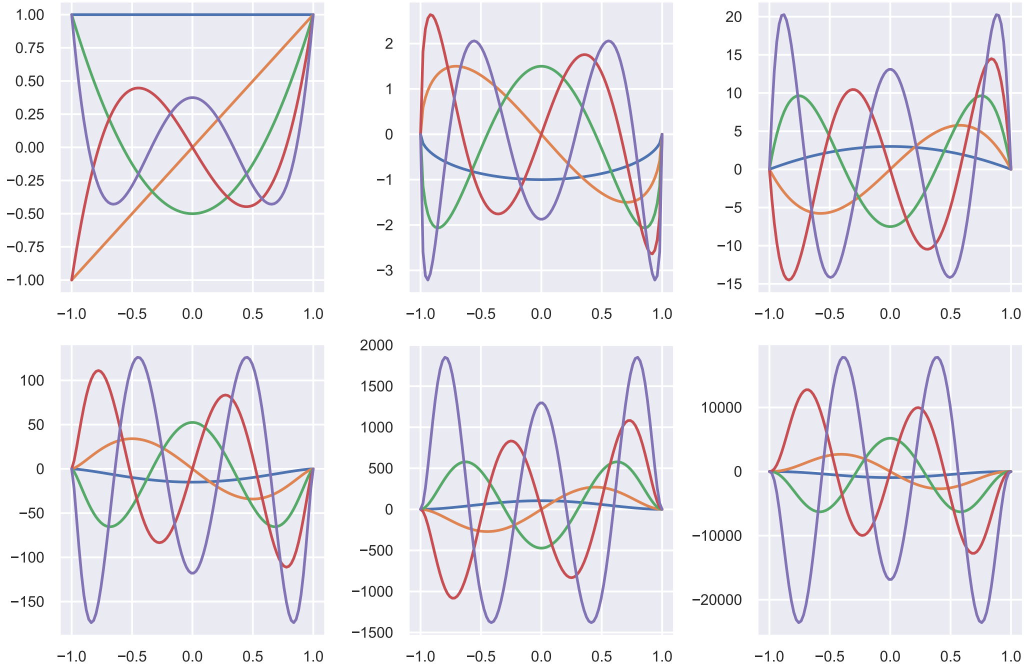
For $x \in [-1, 1]$ *the polynomials*

$$P_{m,n}(x) = \left(1 - x^2\right)^{m/2} \frac{d^m}{dx^m} P_n(x)$$

solve the associated Legendre differential equation.

Observation

If $m > n$ then $P_{m,n}(x) = 0$ for all x.


1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−1.0
−0.5
0.0
0.5
1.0
2
1
0
−1
−2
−3
20
15
10
5
0
−5
−10
−15
100
50
0
−50
−100
−150
2000
1500
1000
500
0
−500
−1000
−1500
10000
0
−10000
−20000

Putting it back together

The Problem

$$\nabla_s^2 f(\varphi, \vartheta) = \lambda f(\varphi, \vartheta)$$

Current solution

$$\tilde{Y}_{m,n}(\varphi, \vartheta) = \Phi(\varphi)\Theta(\vartheta) = e^{im\varphi} P_{m,n}(\cos\vartheta)$$

Putting it back together

The Problem

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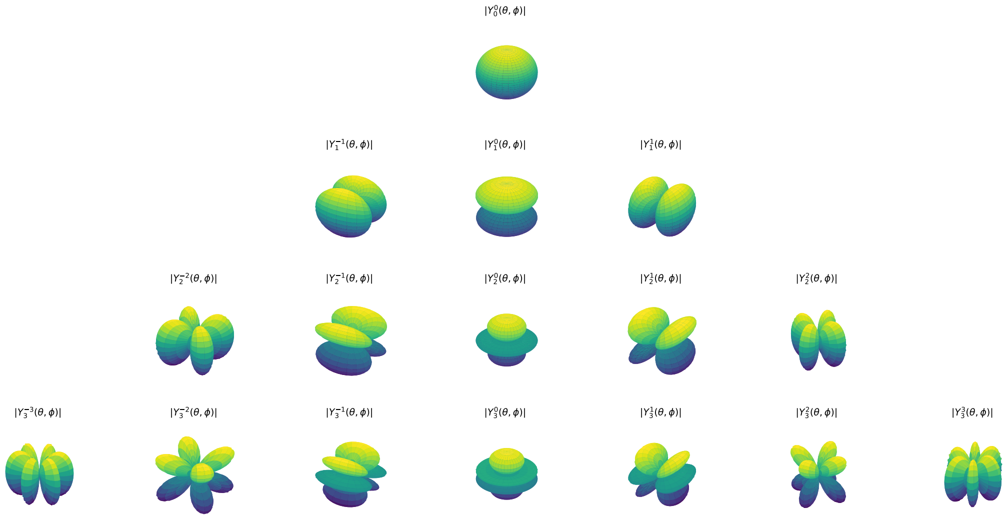
Conditions

$m, n \in \mathbb{Z}$ and $m < n$

Intuition for why m and n are Integers


$|Y_0^0(\theta, \phi)|$
$|Y_1^{-1}(\theta, \phi)|$
$|Y_1^0(\theta, \phi)|$
$|Y_1^1(\theta, \phi)|$
$|Y_2^{-2}(\theta, \phi)|$
$|Y_2^{-1}(\theta, \phi)|$
$|Y_2^0(\theta, \phi)|$
$|Y_2^1(\theta, \phi)|$
$|Y_2^2(\theta, \phi)|$
$|Y_3^{-3}(\theta, \phi)|$
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$|Y_3^{-1}(\theta, \phi)|$
$|Y_3^0(\theta, \phi)|$
$|Y_3^1(\theta, \phi)|$
$|Y_3^2(\theta, \phi)|$
$|Y_3^3(\theta, \phi)|$

Research Question

Recurrence Relation(s)?

$$\tilde{Y}_{m+1,n} \stackrel{?}{=} f(\tilde{Y}_{m,n}, \tilde{Y}_{m-1,n}, \tilde{Y}_{m,n-1}, \ldots)$$
$$\tilde{Y}_{m,n+1} \stackrel{?}{=} f(\tilde{Y}_{m,n}, \tilde{Y}_{m-1,n}, \tilde{Y}_{m,n-1}, \ldots)$$
$$\tilde{Y}_{m+1,n+1} \stackrel{?}{=} f(\tilde{Y}_{m,n}, \tilde{Y}_{m-1,n}, \tilde{Y}_{m,n-1}, \ldots)$$

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The functions $\tilde{Y}_{m,n}$ span the space of nice functions $S^2 \to \mathbb{C}$.

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The inner product of nice functions $f(\varphi, \vartheta)$ and $g(\varphi, \vartheta)$ from S^2 to $\mathbb{C}$ is

$$\langle f, g \rangle = \iint_{S^2} f(\varphi, \vartheta)\overline{g}(\varphi, \vartheta)\, d\Omega$$

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$$\langle f, g \rangle = \iint_{S^2} f(\varphi, \vartheta)\overline{g}(\varphi, \vartheta)\, d\Omega = \int_0^{2\pi} \int_0^{\pi} f(\varphi, \vartheta)\overline{g}(\varphi, \vartheta) \sin\vartheta \, d\vartheta d\varphi$$

Orthonormality

Definition

A set of basis functions are *orthonormal* if

$$\langle B_{m,n}, B_{m',n'} \rangle = \begin{cases} 1 & m = m' \wedge n = n' \\ 0 & \text{otherwise} \end{cases}$$

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Problem

$$\langle \tilde{Y}_{m,n}, \tilde{Y}_{m',n'} \rangle = \begin{cases} \dfrac{4\pi}{2n+1} \dfrac{(n+m)!}{(n-m)!} & m = m' \wedge n = n' \\ 0 & \text{otherwise} \end{cases}$$

Spherical Harmonics

Definition

The orthonormal spherical harmonics are

$$Y_{m,n}(\varphi, \vartheta) = N_{m,n} e^{im\varphi} P_{m,n}(\cos \vartheta)$$

where the normalisation constant

$$N_{m,n} = \sqrt{\frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!}}$$

Fixed

$$\langle Y_{m,n}, Y_{m',n'} \rangle = \begin{cases} 1 & m = m' \wedge n = n' \\ 0 & \text{otherwise} \end{cases}$$

Fourier Series

Theorem

For nice periodic functions on S^2:

$$f(\varphi, \vartheta) = \sum_{m \in \mathbb{Z}} \sum_{n \in \mathbb{Z}} c_{m,n} Y_{m,n}(\varphi, \vartheta)$$

where

$$c_{m,n} = \langle f, Y_{m,n} \rangle.$$

Python Script

(glorified pseudocode)

$$f(\varphi, \vartheta) = \sum_m \sum_n c_{m,n} Y_{m,n}(\varphi, \vartheta)$$

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Linear and Rotational Kinetic Energy

Momentum and KE

$$\mathbf{p} = m\mathbf{v}, \quad E_k = \frac{\mathbf{p}^2}{2m}$$

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Angular Momentum and KE

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \quad E_{k,a} = \frac{\mathbf{L}^2}{2mr^2}$$

Linear and Rotational Kinetic Energy

Momentum and KE

$$\mathbf{p} = m\mathbf{v}, \quad E_k = \frac{\mathbf{p}^2}{2m}$$

QM Formulation

$$\hat{\mathbf{p}} = -i\hbar\boldsymbol{\nabla}, \quad \hat{E}_k = -\frac{\hbar^2}{2m}\nabla^2$$

Angular Momentum and KE

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Angular Momentum and KE

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QM Formulation

Pretty long derivation yields:

$$\hat{E}_{k,a} = -\frac{\hbar^2}{2mr^2}\nabla_s^2$$

Intuition for the Operators

Schrödinger Equation

Time independent SE

$$\hat{\mathcal{H}}|\Psi\rangle = E|\Psi\rangle$$

Schrödinger Equation

Time independent SE

$$\left(\hat{E}_k + U\right)|\Psi\rangle = E|\Psi\rangle$$

Schrödinger Equation

Time independent SE

$$\left(\frac{\hat{\mathbf{p}}^2}{2m} + U\right)|\Psi\rangle = E|\Psi\rangle$$

Schrödinger Equation

Time independent SE

Meili $$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]\Psi(x) = E\Psi(x)$$

Schrödinger Equation

Time independent SE

3D $$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{x})\right]\Psi(\mathbf{x}) = E\Psi(\mathbf{x})$$

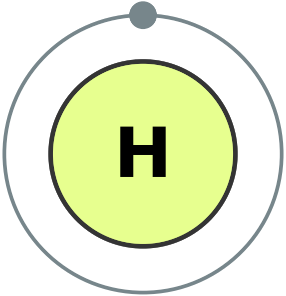
Schrödinger Equation

Time independent SE

$$\left\{-\frac{\hbar^2}{2m}\frac{1}{r^2}\left[\nabla_s^2-\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right]+U(\mathbf{r})\right\}\Psi(\mathbf{r})=E\Psi(\mathbf{r})$$

But why?

Hydrogen atom has radial symmetry!



Schrödinger Equation

Time independent SE

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Schrödinger Equation

Time independent SE

$$\left[\frac{\hat{\mathbf{L}}^2}{2mr^2} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + U(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Schrödinger Equation

Time independent SE

$$\left[\hat{E}_{k,a} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + U(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Schrödinger Equation

Time independent SE

$$\left[\underbrace{\hat{E}_{k,a} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)}_{\text{Kinetic Energy}} + U(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Schrödinger Equation

Time independent SE

$$\left[\hat{E}_{k,a} + \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)}_{\text{Radial KE } \hat{E}_{k,r}} + U(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Schrödinger Equation

Time independent SE

$$\left\{ \hat{E}_{k,a} + \hat{E}_{k,r} + U(\mathbf{r}) \right\} \Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Schrödinger Equation

Time independent SE

$$\left\{\hat{E}_{k,a} + \hat{E}_{k,r} + U(\mathbf{r})\right\}\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Eigenvalue Problem

$$\hat{E}_{k,a}\Psi(\varphi,\vartheta) = E\Psi(\varphi,\vartheta)$$

Electron Orbitals[1]

Eigenvalue Problem

$$\hat{E}_{k,a}\Psi(\varphi, \vartheta) = E\Psi(\varphi, \vartheta)$$

[1] Only the angular component

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Eigenvalue Problem

$$-\frac{\hbar^2}{2m}\nabla_s^2\Psi(\varphi,\vartheta) = E\Psi(\varphi,\vartheta)$$

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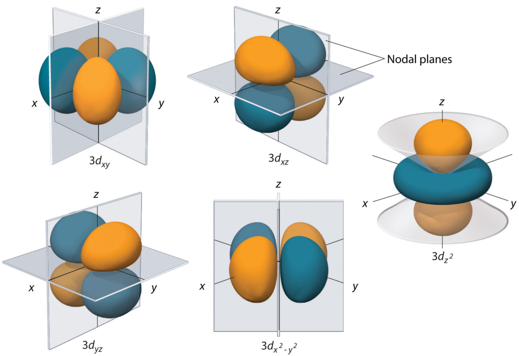
Solutions

$$\Psi(\varphi,\vartheta) = Y_{m,n}(\varphi,\vartheta)$$



[1] Only the angular component

Electron Orbitals[1]

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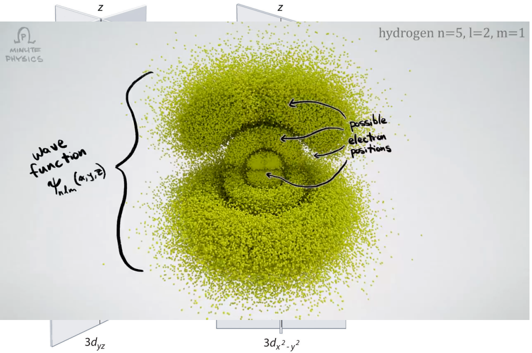

Radial component

We can leave that for another day.

[1] Only the angular component

It was a lot, but I'm sure you got all of that.

Questions?

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