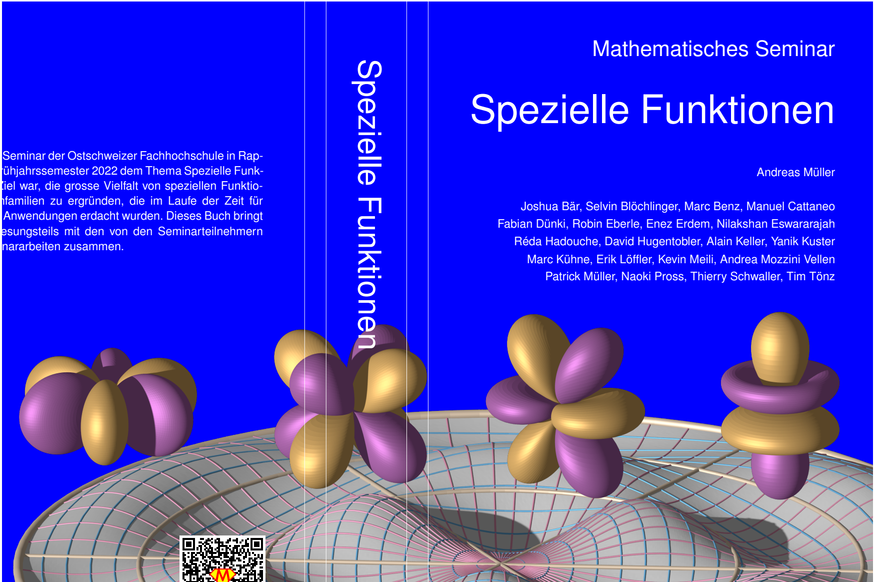
Spherical Harmonics

Naoki Pross, Manuel Cattaneo

OST FHO Campus Rapperswil

Spring Semester 2022

Spherical Harmonics



Goals for Today

Spherical Harmonics *and* **Electron Orbitals**

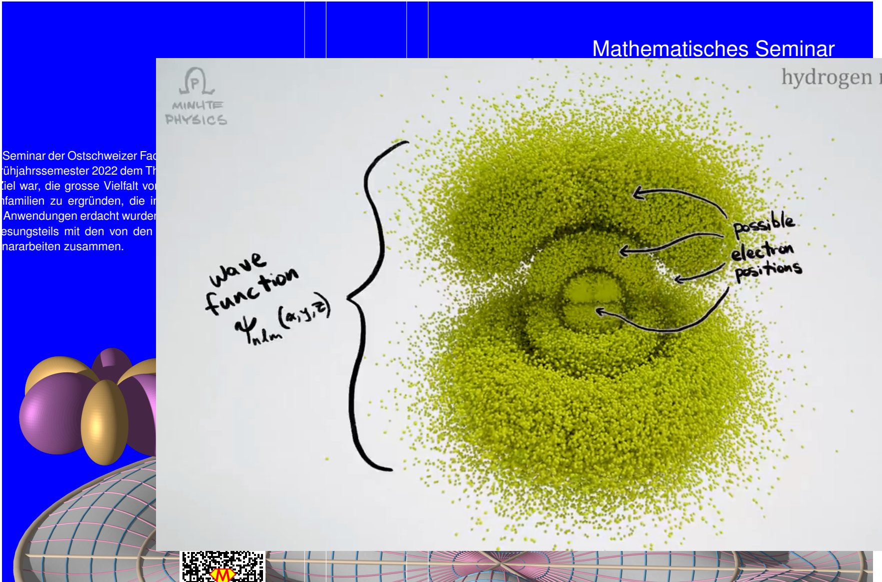


Table of Contents

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.

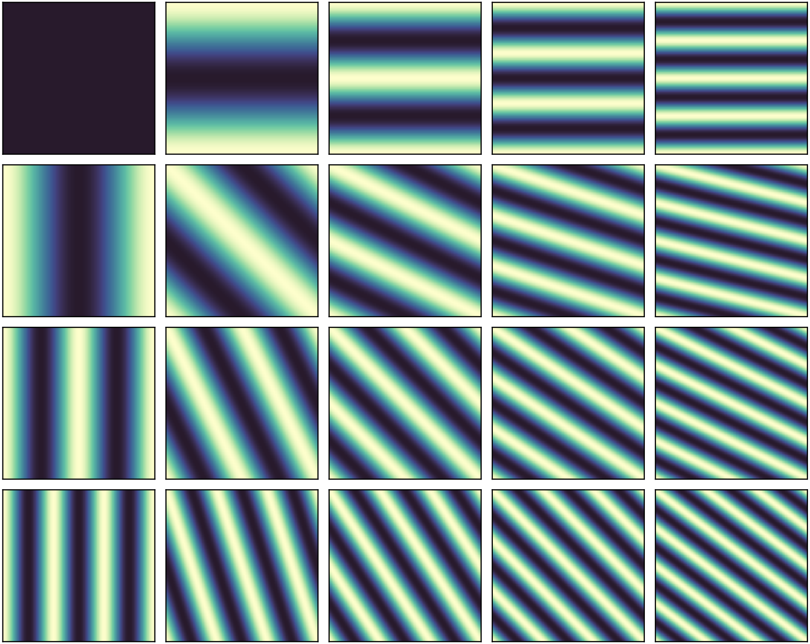
$$f(\mu, \nu) = f(\mu + 1, \nu) = f(\mu, \nu + 1).$$

Function Space

Basis Functions

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

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



Inner Product

Definition

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

$$\langle f, g \rangle = \iint_{[0,1]^2} f g^* \, d\mu d\nu.$$

Inner Product

Definition

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

$$\langle f, g \rangle = \iint_{[0,1]^2} f g^* \, d\mu d\nu.$$

Definition

For a nice periodic function $f(\mu, \nu)$: 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:

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

where

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

Why exponentials?

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

Because ∇^2

The Problem

Fourier's Problem

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

The Problem

Fourier's Problem

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

Solution

Separation ansatz:

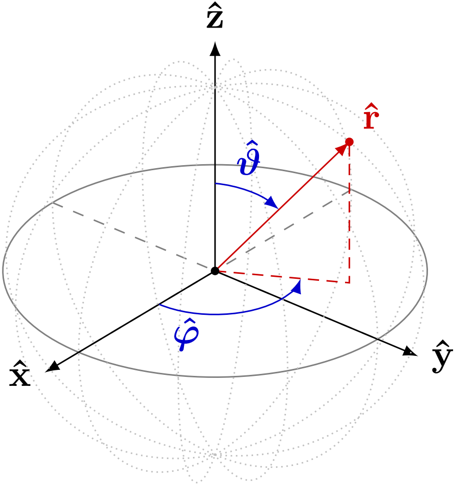
$$f(\mu, \nu) = M(\mu) N(\nu)$$

Resulting ODEs:

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

Table of Contents

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

$$\nabla^2 \equiv \frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2}$$

Spherical Laplacian

Cartesian Laplacian

$$\nabla^2 \equiv \frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2}$$

Spherical Laplacian

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

Spherical Laplacian

Cartesian Laplacian

$$\nabla^2 \equiv \frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2}$$

Spherical Laplacian

$$\nabla^2 \equiv \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2} \underbrace{\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial \vartheta}\left(\sin\vartheta \frac{\partial}{\partial \vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial \varphi^2}\right]}_{\text{Surface Spherical Laplacian } \nabla_s^2}$$

Spherical Laplacian

Cartesian Laplacian

$$\nabla^2 \equiv \frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2}$$

Spherical Laplacian

$$\nabla^2 \equiv \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2}\underbrace{\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial \vartheta}\left(\sin\vartheta \frac{\partial}{\partial \vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial \varphi^2}\right]}_{\text{Surface Spherical Laplacian } \nabla_s^2}$$

Surface Spherical Laplacian

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

Geometrical Intuition

Where is ∇_s^2 useful?

To do brain scans, apparently [2]

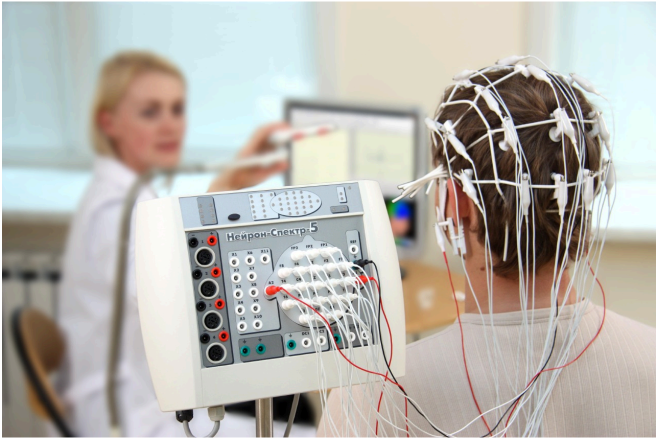


Figure 1: Electroencephalogram (EEG). Image from Wikimedia [3].

Where is ∇_s^2 useful?

To do brain scans, apparently [2]

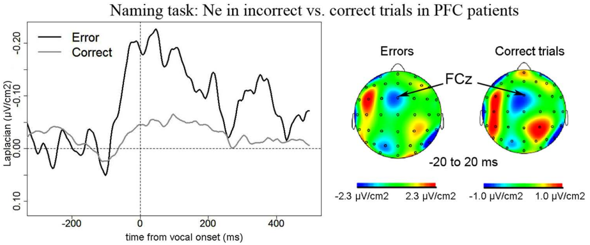


FIGURE 2 | EEG activity in PFC patients in the Naming task after surface Laplacian transformation, recorded at FCz for errors (black line) and correct trials (gray line). Zero of time represents vocal onset. The cartographies were made on a 40-ms time-window centered on vocal onset (from −20 to 20 ms 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.

Figure 1: Surface Laplacian in EEG. Taken from [4].

Brain Scans

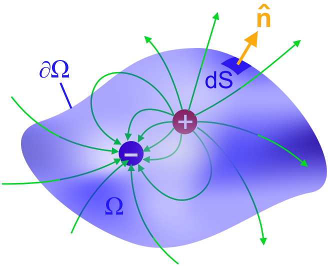
Electrodynamics

$$\nabla^2\phi = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\phi \qquad \left(\phi = \int_A^B \mathbf{E}\cdot d\mathbf{s}\right)$$

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

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

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



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 $\Theta(\vartheta)$:

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

Associated Legendre Differential Equation

Separation (cont.)

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

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

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

Definition (Associated Legendre Differential Equation)

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

Legendre Polynomials

Definition (Legendre Polynomials)

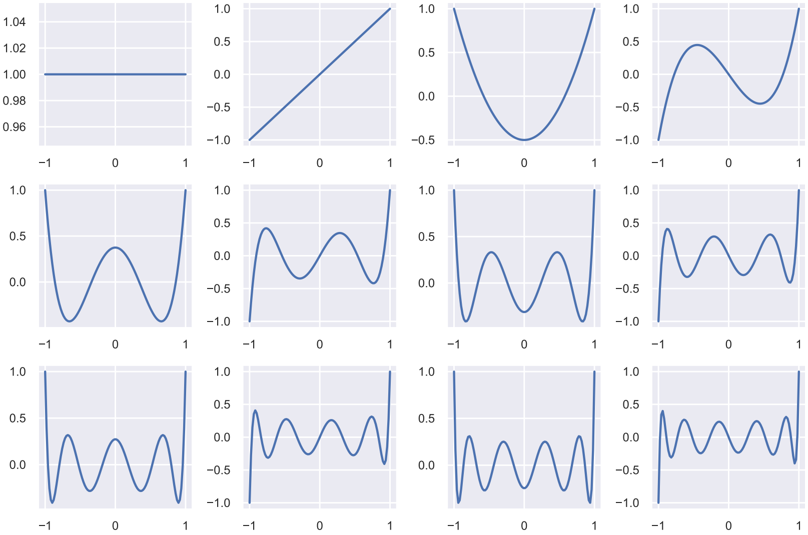
The polynomials

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

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

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

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

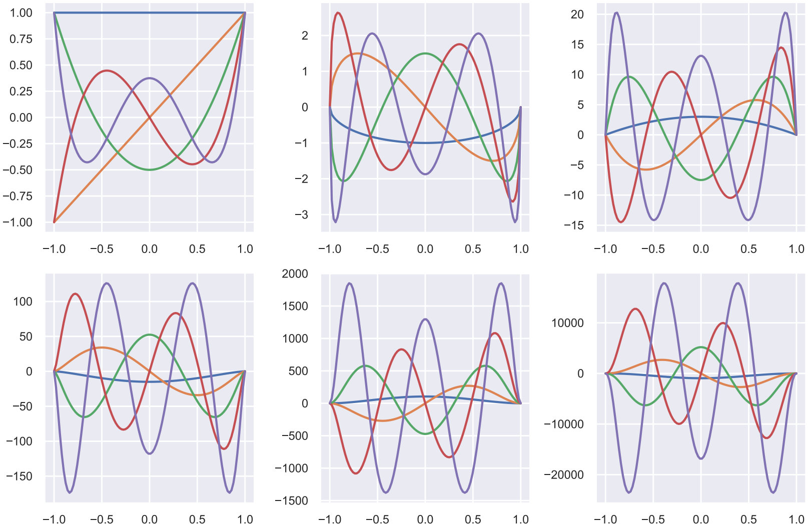
For $x \in [-1, 1]$ *the polynomials*

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

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

For $m \in \mathbb{Z}$ and $m < n$:

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

Intuition of conditions for m and n

Table of Contents

Basis functions?

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

Basis functions?

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

Definition

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

$$\langle f, g \rangle = \iint_{S^2} f g^* \, d\Omega$$

Basis functions?

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

Definition

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

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

Orthonormality

Definition

A set of basis functions are *orthonormal* if

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

Orthonormality

Definition

A set of basis functions are *orthonormal* if

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

Problem

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

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

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

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

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

Table of Contents

Linear and Rotational Kinetic Energy

Momentum and KE

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

Linear and Rotational Kinetic Energy

Momentum and KE

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

Angular M. 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 M. 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 M. and KE

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

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

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

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

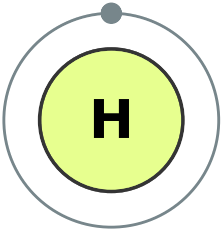
$$\left[\hat{E}_{k,a} + \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)}_{\text{Radial KE } \hat{E}_{k,r}} + U(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Schrödinger Equation

Time independent SE

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

But why?



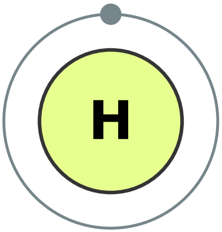
Schrödinger Equation

Time independent SE

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

But why?

Hydrogen atom has radial symmetry!



Electron Orbitals

Bibliography

[1] minutephysics, *A better way to picture atoms*, May 19, 2021. [Online]. Available: https://www.youtube.com/watch?v=W2Xb2GFK2yc (visited on 05/19/2022).

[2] C. Carvalhaes and J. A. de Barros, "The surface laplacian technique in EEG: Theory and methods," *International Journal of Psychophysiology*, vol. 97, no. 3, pp. 174–188, Sep. 2015, ISSN: 01678760. DOI: 10.1016/j.ijpsycho.2015.04.023. [Online]. Available: https://linkinghub.elsevier.com/retrieve/pii/S0167876015001749 (visited on 05/16/2022).

[3] Baburov, *Русский: Процесс регистрации электроэнцефалографии*, Aug. 21, 2009. [Online]. Available: https://commons.wikimedia.org/wiki/File:Eeg_registration.jpg (visited on 05/19/2022).

[4] S. K. Riès, K. Xie, K. Y. Haaland, N. F. Dronkers, and R. T. Knight, "Role of the lateral prefrontal cortex in speech monitoring," *Frontiers in Human Neuroscience*, vol. 7, 2013, ISSN: 1662-5161. DOI: 10.3389/fnhum.2013.00703. [Online]. Available: http://journal.frontiersin.org/article/10.3389/fnhum.2013.00703/abstract (visited on 05/16/2022).

[5] Maschen, *Divergence theorem in EM*, May 12, 2013. [Online]. Available: https://commons.wikimedia.org/wiki/File:Divergence_theorem_in_EM.svg (visited on 05/19/2022).

[6] DePiep, *Electron shell 001 hydrogen (diatomic nonmetal)*, Aug. 14, 2013. [Online]. Available: https://commons.wikimedia.org/wiki/File:Electron_shell_001_Hydrogen_(diatomic_nonmetal)_-_no_label.svg (visited on 05/18/2022).