Sturm-Liouville Theory

On the Hilbert Space $\mathcal{L}^2$ and it's applications to PDEs

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Directed Reading Program, March 2021

Definition: Let $L : \mathcal{L}^2(a,b) \cap C^2(a,b) \to \mathcal{L}^2(a,b)$ be the second-order differential operator on an interval $I \subset \mathbb{R}$ such that

$$Ly = p(x)y'' + q(x)y' + r(x)y$$

where $p \in C^2(a,b)$, $q \in C^1(a,b)$, and $r \in C(a,b)$ where C is the collection of complex continuous functions.

Function space and operator theory

Definition: $C([a,b])$ equipped with the inner product $\langle f, g\rangle = \int_a^b f(x)\overline{g(x)}dx < \infty$ and norm $||f|| = \sqrt{\langle f, f\rangle} = \sqrt{\int_a^b |f(x)|^2 dx}$ for some $f, g \in C([a,b])$.

For an inner product space X and operator $A : X \to X$,

- Linearity: A has the properties $A(ax + by) = aAx + bAy$ and $A(cx) = cA(x)\, \forall a, b, c \in \mathbb{F}$ and $x, y \in X$.
- Adjoint: We can find an A' satisfying the relation $\langle Ax, y\rangle = \langle x, A'y\rangle$ if A exists. Self-adjoint if $A' = A$.

Sturm-Liouville Problems require that our operator L be self-adjoint...

Self-adjoint operator

Every 2nd-order, self adjoint differential operator has the following form:

$$L = \frac{d}{dx} p(x) \frac{d}{dx} + r(x)$$

Problem Setup

Let $L = \frac{d}{dx}(p(x)\frac{d}{dx}) + r(x)$ be formally self-adjoint.

The Sturm-Liouville Problem

We have an eigenvalue equation

$$Lu + \lambda\rho(x)u = 0, \;\; x \in (a, b)$$

under the separated homogeneous boundary conditions,

$$\begin{aligned} \alpha_1 u(a) + \alpha_2 u'(a) &= 0 \qquad & |\alpha_1| + |\alpha_2| > 0 \\ \beta_1 u(b) + \beta_2 u'(b) &= 0 \qquad & |\beta_1| + |\beta_2| > 0 \end{aligned}$$

where $\alpha_1, \alpha_2, \beta_1, \beta_2$ are real. Assume that $\rho(x) = 1$.

What's the Purpose?

- Solving partial differential equations in conjunction with physical phenomena
- Technique: Separation of Variables
- Solutions: eigenfunctions (measurable quantity) corresponding to eigenvalues

Remark

The eigenfunctions form an orthonormal basis for $\mathcal{L}^2$.

Theorem

For any $f \in \mathcal{L}^2$, an orthogonal set of functions $\{\rho_n\}_n$ as $n \to \infty$ is *complete* iff it satisfies *Parseval's Relation*,

$$||f||^2 = \sum_{n=1}^{\infty} \frac{|\langle f, \rho_n \rangle^2|}{||\rho_n||^2}$$

Moreover, this sum converges to f in the $\mathcal{L}^2$ norm as $n \to \infty$

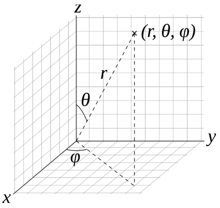
Examples of Sturm-Liouville Forms

- Laplace's Equation

$$\nabla^2 \rho = f$$

- Schrödinger's Equation (Rigid Rotor)

$$-i\hbar\psi_t = -\frac{\hbar}{2m_e}\Delta\psi - k\frac{e^2}{r}\psi$$



Credit: Andeggs, *Wikimedia*

Laplace's Equation on a Sphere

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin(\theta)\frac{\partial u}{\partial\theta}) + \frac{1}{\sin^2(\theta)}\frac{\partial^2 u}{\partial\phi^2} = \hat{M}u = -l(l+1)u$$

Ansatz: $u(\theta, \phi) = \Theta(\theta)\Phi(\phi)$

Applying separation of variables in terms of θ and ϕ, we get

$$\frac{\sin(\theta)(\sin(\theta))\Theta')}{\Theta} - \lambda\sin^2(\theta) = m^2$$

$$\frac{\Phi''}{\Phi} = -m^2$$

Solving for the Variables

General Solution:

$$\Theta(\theta) = P_l^m(\cos\theta)$$
$$\Phi(\phi) = Ae^{im\phi} + Be^{-im\phi}$$

Combining the two equations, we get the following

$$Y_l^m(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{l-m}{l+m}}P_l^m(\cos(\theta))e^{im\phi}$$

Remark

P_l^M denotes the Legendre Polynomials, the sequence of polynomial solutions from Legendre's Equation,

$$(1-x^2)u'' - 2xu' + n(n+1)u = 0$$

such that $x \in (-1,1)$, $p(x) = 1 - x^2$ and $\lambda = n(n+1)$.

Schrödinger's Equation for Hydrogen Atom

$$-i\hbar\psi_t = -\frac{\hbar}{2m_e}\Delta\psi - k\frac{e^2}{r}\psi$$

$$-i\hbar\psi_t = -\frac{\hbar^2}{2m_e}\left[\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r} + \frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}(\sin(\theta)\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right]\psi - k\frac{e^2}{r}\psi$$

Ansatz: $\Psi(r,\theta,\phi,t) = R(r)u(\theta,\phi)e^{(-iEt)/\hbar}$, but set $t = 0$.

$$\frac{\hbar^2}{R(r)}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R(r) + \frac{2m_e}{R(r)}[E - V]R(r) = \lambda$$

$$\frac{1}{u(\theta,\phi)}\hat{M}^2 u(\theta,\phi) = \lambda$$

note: $\hat{M}$ is the operator for $u(\theta,\phi)$

Solving for the Variables

This system is exactly solvable!

$$\Psi_{n,l,m} = R_l^n Y_l^m e^{(-iEt)/\hbar}$$

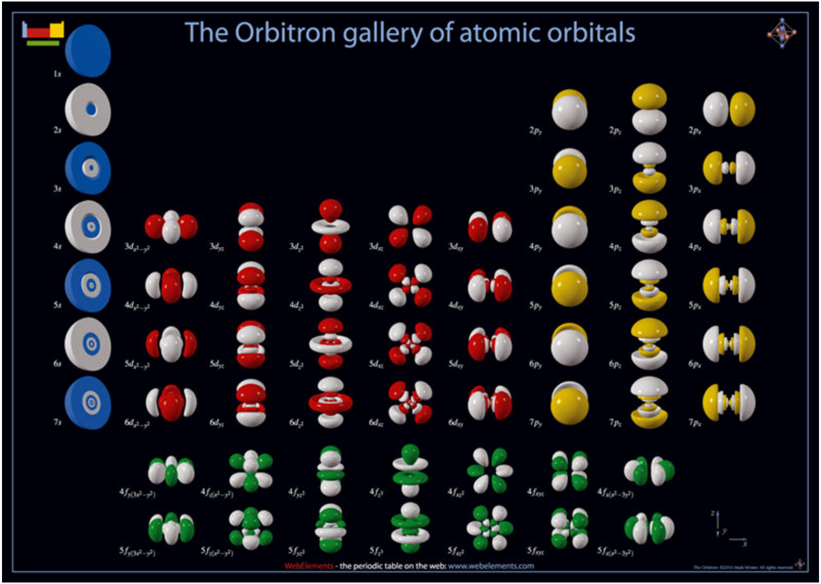
- Wavefunctions for the Spherical Harmonics
- Structure of atomic orbitals

Remark

R_l^n represents the Laguerre polynomials, the sequence of solutions from Laguerre's equation,

$$e^{-x^2}(xu''(1-x)u' + nu) = 0$$

for $x \in \mathbb{R}$ where $p(x) = xe^{-x^2}$ vanishes at $x = 0$.



Credit: Mark Warner, University of Sheffield

In sum

Astounding result

Both the Legendre and Laguerre polynomials form an orthonormal basis with respect to the $\mathcal{L}^2$ inner product!!

Statement

We can construct solutions to Schrödinger's equation from a linear combination of these orthonormal basis functions, particularly those from the wavefunctions $\Psi_{n,l,m}$.

References

- "6.1: The Schrodinger Equation for the Hydrogen Atom Can Be Solved Exactly." *Chemistry LibreTexts*.
- Al-Gwaiz, M. A. *Sturm-Liouville Theory*. Springer-Verlag London Limited, 2008.
- "Schrödinger Equation." *Wikipedia*.