

WE'VE BEEN SOLVING INHOMOGENEOUS ODE'S, NOW
WE BROADEN OUR REPERTOIRE TO INCLUDE...

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CH. 17 — EIGENFUNCTION METHODS

OUTLINE:

| | |
|-----------------------------------|--------|
| EIGENFUNCTIONS AND DIRAC NOTATION | § 17.0 |
| ORTHONORMAL BASES | § 17.1 |
| HERMITIAN OPERATORS | § 17.2 |
| WHY HERMITIAN OPERATORS ARE NICE | § 17.3 |
| → GREEN'S FUNCTIONS | § 17.5 |
| STURM-LIOUVILLE EQUATIONS | § 17.4 |

SEE ALSO CH. 19, QUANTUM OPERATORS

MOTIVATION FOR CH. 17

CONSIDER A SIMPLE PDE, (HELMHOLTZ EQN.):

$$(\nabla^2 + k^2) \psi = 0 \quad \text{OR} \quad \boxed{\nabla^2 \psi = -k^2 \psi} \quad (1), \quad k \in \mathbb{R}$$

SOLUTIONS HAPPEN TO BE PLANE WAVES:

$$\psi = Ae^{i\vec{k} \cdot \vec{r}}, \quad A \in \mathbb{C}, \quad k = |\vec{k}|, \quad \vec{k} \in \mathbb{R}^3$$

WITH SUFFICIENT SYMMETRY, WE CAN REDUCE (1) TO AN ODE. E.G., IF $\partial_y = \partial_z = 0$, WE HAVE

$$\nabla^2 \psi = \boxed{\frac{d^2 \psi}{dx^2} = -k^2 \psi} \quad (2)$$

NOTE THAT (1), (2), (3) ARE HOMOGENEOUS ODE DIFFERENTIAL EQUATIONS. INHOMOGENEOUS WOULD LOOK LIKE $(\nabla^2 + k^2)\psi = f(\vec{r})$.

WITH SOLUTIONS

$$\psi = Ae^{ikx} + B e^{-ikx} \quad (\text{WHY TWO TERMS NOW?})$$

BUT IF INSTEAD WE HAVE SPHERICAL SYMMETRY, $\partial_\phi = \partial_\theta = 0$,

$$\nabla^2 \psi = \boxed{\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) = -k^2 \psi} \quad (3)$$

IN ~~THESE~~ EQ'S (1-3), THE GENERAL FORM IS

$$\mathcal{D} \psi = \lambda \psi$$

↑ LINEAR DIFFERENTIAL OPERATOR ↑ EIGENVALUE

WHICH IS EXACTLY ANALOGOUS TO THE EIGENVALUE PROBLEM IN LINEAR ALGEBRA:

$$M \vec{x} = \lambda \vec{x}.$$

FOR LINEAR ALGEBRA IN HILBERT SPACES, IT IS COMMON TO

USE DIRAC NOTATION, E.G. $\mathcal{D} |\psi\rangle = \lambda |\psi\rangle.$

AN INNER (SCALAR, DOT) PRODUCT:

$$\vec{x} \cdot \vec{y} = \sum_i x_i^* y_i$$

$$\langle \psi | \phi \rangle = \int_a^b \psi^*(x) \phi(x) \rho(x) dx$$

E.G. $\rightarrow = \int_0^\infty \psi^*(r) \phi(r) \underbrace{r^2 dr}_{dV = 4\pi r^2 dr} \text{ (SPHERICAL COORD'S)}$

IDENTITY OPERATOR FROM A COMPLETE, ORTHONORMAL SET OF VECTORS (BASIS) $\hat{e}_i / |e_i\rangle$:

$$\vec{x} = \sum_i (\hat{e}_i \cdot \vec{x}) \hat{e}_i = \mathbb{I} \vec{x}, \quad \mathbb{I} \equiv \sum_i (\hat{e}_i \hat{e}_i \cdot)$$

$$\psi = \underbrace{\sum_i |e_i\rangle \langle \hat{e}_i |}_\mathbb{I} x = \mathbb{I} \vec{x}$$

A MATRIX ELEMENT OF AN OPERATOR \mathcal{D} IS

$$\begin{aligned} \mathcal{D}_{ij} &= \langle e_i | \mathcal{D} | e_j \rangle \\ &= \int_a^b e_i(x) (\mathcal{D} e_j(x)) \rho(x) dx. \end{aligned}$$

E.G. THE IDENTITY:

$$\begin{aligned} \mathbb{I}_{ij} &= \langle e_i | \mathbb{I} | e_j \rangle = \langle e_i | \left[\sum_k |e_k\rangle \langle e_k| \right] | e_j \rangle \\ &= \langle e_i | e_j \rangle = \delta_{ij} \checkmark \end{aligned}$$

★ YOU'LL FIND MORE ON DIRAC NOTATION IN ANY GOOD Q.M. TEXT, E.G. SHANKAR OR COHEN-TANNOUDJI.

MOTIVATION'S DONE, ON TO CH. 17.

I HAVE TO BEGIN BY POINTING OUT A PROBLEM WITH OUR BOOK'S APPROACH.

RHB DOES EIGENFUNCTIONS THIS WAY:

EIGENFUNCTION \swarrow

$$\mathcal{L} y_i(x) = \lambda_i \rho(x) y_i(x)$$

\nwarrow DIFFERENTIAL OPERATOR ON DOMAIN $a < x < b$ WITH GIVEN B.C.'S

\nearrow EIGENVALUE

\nwarrow WEIGHTING FUNCTION (E.G. r^2 FOR SPHERICAL COORD'S)

Q: HOW WOULD THE RADIAL HELMHOLTZ EQUATION LOOK IN THIS FORM?

$$\frac{d}{dr} \left(r^2 \frac{d}{dr} \right) \psi = r^2 (-k^2) \psi$$

\uparrow $\rho(r)$ \uparrow λ

IN DIRAC NOTATION:

$$\mathcal{L} |y_i\rangle = \lambda_i \rho(x) |y_i\rangle$$

THEY DEFINE INNER PRODUCTS THIS WAY:

$$\langle y_i | y_j \rangle = \int_a^b y_i^*(x) y_j(x) \underbrace{\rho(x) dx}_{\text{VOLUME ELEMENT}} \underbrace{\rho(x)}_{\text{WEIGHTING FACTOR}}$$

NOW TRY WRITING THE MATRIX ELEMENT:

$$\langle y_i | \mathcal{L} | y_j \rangle = \langle y_i | \rho(x) \lambda_j | y_j \rangle$$

$$= \int_a^b y_i^*(x) \rho(x) \lambda_j y_j(x) \rho(x) dx$$

OH NO, 2 FACTORS OF $\rho(x)$!!

THIS SCREWS UP THE DEFINITION OF HERMITIAN OPERATORS!

RHB FIX THIS BY DEFINING

$$\langle Y_i | \mathcal{L} | Y_j \rangle \equiv \int_a^b Y_i^*(x) [\mathcal{L} Y_j(x)] dx$$

↑
NO $\rho(x)$

ARFKEN DOES THE SAME, THIS IS PERVERSE:

- BREAKS THE DIRAC NOTATION
(RHB QUILTS USING DIRAC NOTATION FROM §17.3 TO AVOID THE OBVIOUS CONTRADICTIONS!)
- BREAKS THE DEFINITION OF AN EIGENVECTOR, WHICH SHOULD ALWAYS BE

$$\mathcal{L} | Y_i \rangle = \lambda_i | Y_i \rangle$$

- CALLS THEIR \mathcal{L} HERMITIAN, WHEN IT CLEARLY IS NOT.

MY APPROACH:

DEFINE $\mathcal{D} = \frac{\mathcal{L}}{\rho(x)}$

↙ COMPARE RADIAL HELMHOLTZ EQN.
VOLUME ELEMENT

$$\langle Y_i | Y_j \rangle = \int_a^b Y_i^*(x) Y_j(x) \rho(x) dx$$

$$\begin{aligned} \langle Y_i | \mathcal{D} | Y_j \rangle &= \int_a^b Y_i^*(x) \mathcal{D} Y_j(x) \rho(x) dx \\ &= \lambda_j \langle Y_i | Y_j \rangle \text{ AS IT SHOULD BE.} \end{aligned}$$

AN IMPORTANT CLASS OF ODEs TAKE THE FORM

$$\mathcal{L} u(x) = \lambda u(x) \quad \star$$

NOTE THAT THIS ODE IS HOMOGENEOUS. WE WILL ULTIMATELY BE CONCERNED WITH

$$\mathcal{L} u(x) = f(x) \quad (\text{INHOMOGENEOUS}).$$

\mathcal{L} IS CALLED HERMITIAN IF $\mathcal{L} = \mathcal{L}^\dagger$, I.E.

$$\langle f | \mathcal{L} g \rangle = \langle \mathcal{L} f | g \rangle, \text{ OR}$$

$$\int_a^b f^*(x) [\mathcal{L} g(x)] p(x) dx = \int_a^b [\mathcal{L} f(x)]^* g(x) p(x) dx$$

(CF. EQ. 17.16)

THIS DEFINITION DEPENDS NOT ONLY ON THE FORM OF \mathcal{L} , BUT ALSO ON THE BOUNDARY CONDITIONS AT a AND b .

IF \mathcal{L} IS HERMITIAN, THEN SOLN'S TO \star CAN FORM AN ORTHONORMAL BASIS WITH REAL λ_i :

$$\mathcal{L} y_i = \lambda_i y_i, \quad \langle y_i | y_j \rangle = \delta_{ij}$$

WHAT DO I MEAN BY CAN? \rightarrow DISCUSS DEGENERACY.

PROOFS: SUPPOSE \mathcal{D} IS HERMITIAN, AND

$$\mathcal{D} |y_i\rangle = \lambda_i |y_i\rangle, \quad \left(\Leftrightarrow \langle y_i | \mathcal{D} = \langle \mathcal{D} y_i | \right. \\ \left. = \langle y_i | \lambda_i^* \right)$$

THEN

$$\langle y_i | (\mathcal{D} y_j) \rangle = \langle \mathcal{D} y_i | y_j \rangle$$

$$\lambda_j \langle y_i | y_j \rangle = \lambda_i^* \langle y_i | y_j \rangle$$

$$(\lambda_j - \lambda_i^*) \langle y_i | y_j \rangle = 0$$

IF $i = j$ THEN $\lambda_i = \lambda_i^* \Rightarrow \lambda_i \in \mathbb{R} \checkmark$

EVIDENTLY, $\langle y_i | y_j \rangle = 0$ IF $\lambda_i \neq \lambda_j$
 \Rightarrow ORTHOGONAL \checkmark

WE ARE FREE TO NORMALIZE y_i SO THAT

$$\langle y_i | y_i \rangle = 1. \checkmark$$

IF $\lambda_i = \lambda_j$ FOR SOME $i \neq j$, AND $|y_i\rangle \neq k |y_j\rangle$,

THEN WE CAN CONSTRUCT AN ORTHONORMAL SET BY THE GRAM-SCHMIDT PROCEDURE, SO THAT

$$\langle y_i | y_j \rangle = \delta_{ij} \quad \forall i, j \quad (\text{ORTHONORMAL}). \checkmark$$

EXERCISE (DO IN CLASS)

USING THE LINEARLY INDEPENDENT FUNCTIONS

$$Y_0 = 1$$

$$Y_1 = x$$

$$Y_2 = x^2$$

CREATE AN ORTHONORMAL SET OF THE INTERVAL $[-1, 1]$.