

L15-Inner Product: Orthonormality and Completeness

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* Review: last class we did steps a)-c) to end up with a "spectrum of solutions to the TISE [infinite square well]: Today we will learn how to interpret and work with these solutions.

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \quad \psi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n x) \quad E_n = \frac{\hbar^2 k_n^2}{2m} \quad k_n = \frac{n\pi}{a}$$

$A \vec{v} = \lambda \vec{v}$ This looks a lot like an eigenvalue equation!

We also compared the general solution to vector components [twice!]

$$\psi(x) = \sum_n c_n \psi_n(x) = c_1 \psi_1(x) + c_2 \psi_2(x) + c_3 \psi_3(x) + \dots$$

$$\vec{v} = \sum_i v_i \hat{e}_i = v_1 \hat{x} + v_2 \hat{y} + v_3 \hat{z}$$

We compared $\psi_n(x)$ to the unit vector $\hat{e}_n$ and even gave it a vector notation $|\psi_n\rangle$

* The vector analogy is more than an analogy!
 $|\psi_n\rangle \sim \psi_n(x)$ IS a vector!

a) vectors add componentwise: $(\vec{v} + \vec{w})_i = v_i + w_i$

$$|\psi\rangle = |\psi_1\rangle + |\psi_2\rangle \quad \psi(x) = \psi_1(x) + \psi_2(x)$$

b) vector scale with scalars: $(\alpha \vec{v})_i = \alpha v_i$

$$|\alpha\psi\rangle = \alpha|\psi\rangle \quad (\alpha\psi)(x) = \alpha \cdot \psi(x)$$

Vectors and functions are both "Linear" objects in a "Linear" space.
 The space of functions is called a "Hilbert space".
 All operations can be combined into the "Linear combination"

$$\vec{v} = \sum_i \underbrace{v_i}_{\text{components}} \underbrace{\hat{e}_i}_{\text{basis vector}}$$

$$|\psi\rangle = \sum_i \underbrace{c_i}_{\text{components}} \underbrace{|\psi_i\rangle}_{\text{basis function}}$$

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- * The concept of vectors becomes much more powerful, when endowed with an "inner product" [dot product], which both
- a) gives a measure of magnitude [metric], and $\|\vec{v}\|^2 = \vec{v} \cdot \vec{v}$
 - b) gives a sense of orthogonality [perpendicular] $\vec{v}_i \cdot \vec{v}_j = 0$

The metric [inner product] is a "symmetric bilinear form"

$$\vec{v} \cdot \vec{w} = \vec{w} \cdot \vec{v} \quad (a_i \vec{v}_i) \cdot \vec{w} = a_i (\vec{v}_i \cdot \vec{w}) \quad \vec{v} \cdot (b_i \vec{w}_i) = (\vec{v} \cdot \vec{w}_i) b_i$$

Once you have an orthonormal basis: $\hat{e}_i \cdot \hat{e}_j = \delta_{ij} = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$, it is easy to calculate a dot product using these properties:

$$\vec{v} \cdot \vec{w} = (\hat{x} v_x + \hat{y} v_y) \cdot (\hat{x} w_x + \hat{y} w_y) = \hat{x} \cdot \hat{x} v_x w_x + \hat{x} \cdot \hat{y} v_x w_y + \hat{y} \cdot \hat{x} v_y w_x + \hat{y} \cdot \hat{y} v_y w_y = v_x w_x + v_y w_y$$

$$\text{or in general } \vec{v} \cdot \vec{w} = (v_i \hat{e}_i) \cdot (w_j \hat{e}_j) = v_i w_j \hat{e}_i \cdot \hat{e}_j = v_i w_j \delta_{ij} = v_i w_i$$

$$\text{likewise: } \langle a | b \rangle = (a_i^* \langle \psi_i |) (| \psi_j \rangle b_j) = a_i^* \langle \psi_i | \psi_j \rangle b_j = a_i^* \delta_{ij} b_j = a_i^* b_j$$

- * but what is $\langle \psi_i | \psi_j \rangle$? Note that $\psi(x)$ is the x^{th} component of $| \psi \rangle$

$$\vec{v} = \sum_i v_i \hat{e}_i \Rightarrow | \psi \rangle = \int dx \psi(x) | x \rangle \quad | x \rangle \text{ is a delta function } \delta(x-x')$$

$$\text{thus } \vec{v} \cdot \vec{w} = \sum_i v_i w_i \Rightarrow \langle \psi | \phi \rangle = \int dx \psi^*(x) \phi(x) \quad \text{infinite sum!}$$

note the * to guarantee that $\langle \psi | \psi \rangle = \int dx \psi^*(x) \psi(x) = \int |\psi(x)|^2 dx$ is real.

Thus "normalization" is the same for wavefunctions and vectors.

WAVE FUNCTIONS are LINEAR!

- * What does this buy us?

a) The T.I.S.E is simply an eigenvector/value equation

$$A \vec{v}_i = \lambda_i \vec{v}_i \Rightarrow \hat{H} | \psi_n \rangle = E_n | \psi_n \rangle$$

By Sturm Liouville theory, the solutions have the properties:

i) orthonormal $\langle \psi_m | \psi_n \rangle = \delta_{nm}$ $\hat{x} \cdot \hat{y} = 0$

ii) closed $\sum_n |\psi_n\rangle \langle \psi_n| = I$ $[\hat{x} \hat{x} \cdot + \hat{y} \hat{y} \cdot + \hat{z} \hat{z} \cdot] \vec{v} = \vec{v}$

b) the general solution to the TDSE (+ B.C.'s) is a linear combination of eigenfunctions of the TISE with pure time dependence $e^{-i\omega t}$

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-iE_n t / \hbar} \quad \text{where } \psi_n(x) \text{ satisfy TISE + B.C.'s.}$$

c) use the inner product to calculate c_n from the initial condition

$$|\Psi_0\rangle = \left[\sum_n |\psi_n\rangle \underbrace{\langle \psi_n|}_{c_n} \right] |\Psi_0\rangle = \sum_n c_n |\psi_n\rangle \quad \Psi(x,0) = \sum_n c_n \psi_n(x)$$

$$\langle \psi_m | \Psi_0 \rangle = \langle \psi_m | \sum_n c_n |\psi_n\rangle = \sum_n c_n \langle \psi_m | \psi_n \rangle = \sum_n c_n \delta_{mn} = c_m$$

Thus we can get the coefficients $c_n = \int dx \psi_n^*(x) \Psi(x,0)$
from the initial state (wavefunction)