L14-Inner Product: Orthonormality and Completeness

Friday, September 30, 2016 07:59

* 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.

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

$$A\,\vec{v} = \lambda\,\vec{v}$$ 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: $(\vec{V}+\vec{W})_i = V_i + W_i$

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

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

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

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

$$\vec{V} = \sum_i \underbrace{V_i}_{\text{components}}\,\overbrace{\hat{e}_i}^{\text{basis vector}} \qquad |\psi\rangle = \sum_i \underbrace{c_i}_{\text{components}}\,\overbrace{|\psi_i\rangle}^{\text{basis function}}$$

* The concept of vectors becomes much more powerful, when endowed with an "inner product" [dot product], which both

* 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 $\|V\|^2 = \vec{V}\cdot\vec{V}$
  b) gives a sense of orthogonality [perpendicular] $\vec{V}_i \cdot \vec{V}_j = 0$

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

$$\vec{V}\cdot\vec{W} = \vec{W}\cdot\vec{V} \in \mathbb{R} \quad (a_i\vec{V}_i)\cdot\vec{W} = a_i\,(\vec{V}_i\cdot\vec{W}) \quad \vec{V}\cdot(b_i\vec{W}_i) = (\vec{V}\cdot\vec{W}_i)\,b_i$$

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:

$$\vec{V}\cdot\vec{W} = (\hat{x}V_x + \hat{y}V_y)\cdot(\hat{x}W_x + \hat{y}W_y) = \hat{x}\cdot\hat{x}\,V_xW_x + \hat{x}\cdot\hat{y}\,V_xW_y + \hat{y}\cdot\hat{x}\,V_yW_x + \hat{y}\cdot\hat{y}\,V_yW_y = V_xW_x + V_yW_y$$

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

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

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

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

thus $\vec{V}\cdot\vec{W} = \sum_i V_iW_i \Rightarrow \langle\psi|\phi\rangle = \int dx\ \psi^*(x)\,\phi(x)$ infinite sum!

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

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

WAVEFUNCTIONS are LINEAR!

* What does this buy us?

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

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

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 $e^{-i\omega t}$

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

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

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

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

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