Class 5 Completeness of Eigenfunctions of hermitian Operators

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Completeness of Eigenfunctions of a Hermitian Operator

Recall in Linear algebra if $\hat{e}_1$, $\hat{e}_2$ & $\hat{e}_3$ are basis vectors in the 3-d vector space, then any vector $\vec{V}$ can be written as,

$$\vec{V} = V_1 \hat{e}_1 + V_2 \hat{e}_2 + V_3 \hat{e}_3 \qquad \hat{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

for an n-dimensional space you would need n-independent basis vectors $\hat{e}_i$ $\quad i = 1, 2, \dots, n$

$$\text{Independent} \Rightarrow \sum_i c_i \hat{e}_i = 0 \Rightarrow \hat{c}_i = 0 \quad \forall_{i=1,\dots,n}$$

The basis vectors need not be orthogonal, but they can be made orthogonal

$$\hat{e}_1' = c_1 \hat{e}_1 + c_2 \hat{e}_2 \qquad \forall \ \hat{e}_1' \cdot \hat{e}_2' = 0$$

$$\hat{e}_2' = d_1 \hat{e}_1 + d_2 \hat{e}_2$$

Given a set of basis vectors $\hat{e}_i$ then any vectors in this space can be expressed as linear combination of the $\hat{e}_i$

$$\vec{V} = \sum c_i \hat{e}_i$$

If not the $\vec{V}$ would be another vector independent of the set $\hat{e}_i$ and the dimension of the vector space would be $d+1$.

Also there cannot exist a small set of vectors $\hat{d}_i$ $\quad i = 1, \dots, n'$ w/ $n' = n-1$ which can span the vector space.

$$\hat{e}_l = \sum_{i=1}^{n-1} u_{l i} \hat{d}_i$$

one can always find a set ω_l $\ni$ $\displaystyle\sum_{l=1}^{n} \omega_l \underbrace{u_{l i}}_{n \times n'} = 0$

$$\Rightarrow \sum_{l=1}^{n} \omega_l \hat{e}_l = 0 \quad \text{Contradiction!}$$

Thm: The eigenfunctions of Hermitian Operator form a complete basis.

If $\quad \hat{A} \phi_n = a_n \phi_n(\vec{x})$ & $\hat{A}$ is Hermitian

then, $\quad \displaystyle\int \phi_n^*(\vec{x}) \phi_m(\vec{x}) d^3x = \delta_{nm}$ $\quad$ "for eigenvalues labeled by a discrete index."

We want to show that the set ϕ_n spans the vector space.

i.e. for any function $\psi(\vec{x})$ we can find a set $\{c_1, c_2, \ldots, c_d\}$ $\ni$:

$$\psi(\vec{x}) = \sum_{n=1}^{d} c_n \phi_n(\vec{x})$$

If the dimension of the vector space is d, then there are d basis vectors $\hat{e}_i$ $\ni$

$$\phi_n(\vec{x}) = \sum_i c_i^{(n)} \hat{e}_i \qquad \hat{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\hat{A}\phi_n(x) = \sum_i c_i^{(n)} \hat{A}\hat{e}_i = a_n \sum_j c_j^{(n)} \hat{e}_j$$

$$\hat{e}_l \cdot \sum_i c_i^{(n)} \hat{A}\hat{e}_i = a_n \sum_j c_j^{(n)} \hat{e}_l \cdot \hat{e}_j$$

(Assuming basis is orthogonalized)

$$\sum_i c_i^{(n)} \left(\hat{e}_l \cdot \hat{A}\hat{e}_i\right) = a_n c_l^{(n)}$$

$$\sum_i c_i^{(n)} \hat{A}_{li} = a_n c_l^{(n)} \qquad \hat{A}_{li} \equiv \hat{e}_l \cdot \hat{A}\hat{e}_i$$

$$\sum_i c_i^{(n)} \hat{A}_{li} - a_n c_l^{(n)} = 0$$

$$\sum_i \left(\hat{A}_{li} - \delta_{li} a_n\right) c_l^{(n)} = 0$$

$$\left(\underbrace{\tilde{A}}_{d\times d \text{ matrix}} - a_n \mathbb{1}\right) \underset{\sim}{c}^{(n)} = 0$$

For non-trivial solution $\det\left(\tilde{A} - a_n \mathbb{1}\right) = 0$

$$= (a - a_1)(a - a_2)\cdots(a - a_d) = 0$$

$\Rightarrow$ d solutions i.e. <u>eigenvalues</u>

$\Rightarrow$ d possible values $\underset{\sim}{c}^{(n)}$

$\Rightarrow$ there are d eigenfunctions $\phi_n(\vec{x})$

$\Rightarrow$ that the set $\{\phi_1(\vec{x}), \phi_2(\vec{x}), \ldots, \phi_d(\vec{x})\}$ also spans the vector space.

The Hamiltonian Operator is a Hermitian Operator

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(\vec{x}) \qquad \int \Psi^*(\vec{x},t)\, \hat{Q}\, \Psi(\vec{x},t)\, d^3x$$

$$= \int \left(\hat{Q}^\dagger \Psi(\vec{x},t)\right)^* \Psi(\vec{x},t)\, d^3x$$

$$\hat{H}^\dagger = \hat{H} \qquad \Rightarrow \langle \hat{Q} \rangle^* = \langle \hat{Q} \rangle$$

$$\left(\hat{Q}^\dagger = \hat{Q}\right)$$

If ... "stationary state solutions"

$H = H$ "Stationary state solutions"

$\Rightarrow \langle \hat{Q} \rangle^* = \langle \hat{Q} \rangle$

$(\hat{Q}^\dagger = \hat{Q})$

$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger = \hat{B}\hat{A} \neq \hat{A}\hat{B}$

If

$$\hat{H}\psi_n(\vec{x}) = E_n \psi_n(\vec{x}) \longrightarrow \text{Time Indep. Sch. Eqn.}$$

$n = 1, 2, \dots, d$

Dimension of the space is d.

$\Rightarrow$ for any wave function $\psi(\vec{x})$:

$$\psi(\vec{x}) = \sum_n c_n \psi_n(\vec{x}) \qquad i = 1, \dots, d$$

$$\Psi(\vec{x}, t) = e^{-i/\hbar \hat{H} t} \psi(\vec{x})$$

only for $\hat{H} \neq \hat{H}(t)$

$$e^{-i/\hbar \hat{H} t} \neq e^{-i/\hbar \frac{\hat{P}^2}{2m}} e^{-\frac{i}{\hbar} V(\vec{x})}$$

$$= e^{-i/\hbar \hat{H} t} \sum_n c_n \psi_n(\vec{x})$$

$$\Psi(\vec{x}, t) = \sum_n c_n e^{-i/\hbar E_n t} \psi_n(\vec{x})$$

"Superposition Principle"

$t = 0$

$$\Psi(\vec{x}, 0) = \sum_n c_n \psi_n(\vec{x})$$

"Initial Conditions"

$$\int \psi_m^*(\vec{x}) \Psi(\vec{x}, 0)\, d^3x = \sum_n c_n \int \psi_m^*(\vec{x}) \psi_n(\vec{x})\, d^3x$$

$$c_m = \int \psi_m^*(\vec{x}) \Psi(\vec{x}, 0)\, d^3x$$

$$\langle \hat{H} \rangle = \int \Psi^*(\vec{x}, t) \hat{H} \Psi(\vec{x}, t)\, d^3x$$

$$= \int \left(\sum_m c_m^* e^{+i/\hbar E_m t} \psi_m^*(\vec{x}) \right) \hat{H} \left(\sum_n c_n e^{-i/\hbar E_n t} \psi_n(\vec{x}) \right) d^3x$$

$$= \sum_{m,n} c_m^* c_n e^{i/\hbar (E_m - E_n) t} E_n \underbrace{\int \psi_m^*(\vec{x}) \psi_n(\vec{x})\, d^3x}_{\delta_{mn}}$$

$$\langle \hat{H} \rangle = \sum_n |c_n|^2 E_n$$

Independent of Time!

$\Rightarrow$ Conservation of Energy

Normalization:

$$\int \Psi^*(\vec{x}, t) \Psi(\vec{x}, t)\, d^3x = 1$$

$$\int \sum_m c_m^* e^{+i/\hbar E_m t} \psi_m^*(\vec{x}) \sum_n c_n e^{-i/\hbar E_n t} \psi_n(\vec{x})\, d^3x = 1$$

$$\sum_{m,n} c_m^* c_n e^{i/\hbar (E_m - E_n) t} \int \psi_m^*(\vec{x}) \psi_n(\vec{x})\, d^3x = 1$$

$$\sum_n |c_n|^2 = 1$$

" $|c_n|^2$ = prob. of measuring E_n "