10/5/98

Lec. #15 Formalism of QM

So far: Solve

$$\hat{H}\,\psi_n(x) = E_n\,\psi_n(x)$$

where boundary conditions determine allowed energies E_n

Can expand any inital wave function

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

Note, sum over n for bound states and integrate over a cont. variable k for scattering states

Time dependence of ψ_n is simple

$$\Psi_n(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$$

so

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

Calculate expectation values

$$\langle \hat{O} \rangle = \int dx\, \Psi^*(x,t)\, \hat{O}\, \Psi(x,t)$$

We will now generalize this formalism and cast it in elegant language of linear algebra. Start Reading Chap 3

Linear algebra

We will come to think of $|\Psi\rangle$ as the state vector of the system

A vector space consists of a set of vectors $|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \ldots$ and a set of scalars (complex #s) $(a, b, c \ldots)$

Vector addition: Sum of any two vectors is another vector

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle$$

and

Scalar multiplication: The "product" of any scalar with any vector is another vector $a|\alpha\rangle = |\gamma\rangle$

A linear combination of the vectors $|\alpha\rangle, |\beta\rangle, \ldots |\gamma\rangle$ is an expression of the form

$$a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle + \ldots$$

A vector $|\lambda\rangle$ is linearly independent if it cannot be written as a linear combination of them. A collection of vectors **span** s the space if ~~any~~ every vector can be written as a linear combination. A set of linearly independent vectors that spans the space is a **basis**. The number of vectors in any basis is the **dimension** of the space. For now dimension n is assumed finite $\rightarrow$ infinite

With respect to a given basis

$$|e_1\rangle, |e_2\rangle \dots |e_n\rangle$$

any given vector

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \dots a_n|e_n\rangle$$

is uniquely represented by the n-tuple of its **components**

$$|\alpha\rangle \longleftrightarrow (a_1, a_2, \dots, a_n)$$

Inner products

In 3 dim know dot product and cross product. Cross product does not generalize to other dimensions. Generalization of dot product $\rightarrow$ inner product.

<u>Inner product</u> is a complex number

$$\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle^*$$

$$\langle \alpha | \alpha \rangle \geq 0 \qquad \langle \alpha | \alpha \rangle = 0 \Rightarrow | \alpha \rangle = | 0 \rangle$$

$$\langle \alpha | \left(b | \beta \rangle + c | \gamma \rangle \right) = b \langle \alpha | \beta \rangle + c \langle \alpha | \gamma \rangle$$

A vector space with an inner product is called an <u>inner product space</u>

<u>Norm</u> (length) of a vector

$$\| \alpha \| = \sqrt{\langle \alpha | \alpha \rangle}$$

Two vectors with zero inner product are <u>orthogonal</u>

A set of vectors $\langle \alpha_i | \alpha_j \rangle = \delta_{ij}$ is called an <u>orthonormal</u> set.

It is always possible to chose an orthonormal basis. In this case inner product is just

$$\langle \alpha | \beta \rangle = a_1^* b_1 + a_2^* b_2 + \dots a_n^* b_n$$

$$\langle \alpha | \alpha \rangle = |a_1|^2 + |a_2|^2 + \dots |a_n|^2$$

The components themselves are just

$$a_i = \langle e_i | \alpha \rangle$$

<u>Schwarz inequality</u>

Generalization of angle between two vectors $\cos\theta \leq 1$

$$|\langle \alpha | \beta \rangle|^2 \leq \langle \alpha | \alpha \rangle \langle \beta | \beta \rangle$$

Define
$$\cos\theta \equiv \left[\frac{|\langle \alpha | \beta \rangle|^2}{\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle} \right]^{1/2}$$

<u>Linear transformations</u>

$\hat{T}$ transforms each vector $|\alpha\rangle \to |\alpha'\rangle = \hat{T}|\alpha\rangle$

<u>linear</u> $\hat{T}(a|\alpha\rangle + b|\beta\rangle) = a\hat{T}|\alpha\rangle + b\hat{T}|\beta\rangle$

If you know what $\hat{T}$ does to each basis vector

$$\hat{T}|e_1\rangle = T_{11}|e_1\rangle + T_{21}|e_2\rangle + \ldots T_{n1}|e_n\rangle$$

or
$$\hat{T}|e_j\rangle = \sum_{i=1}^{n} T_{ij}|e_i\rangle \quad (j = 1, \ldots n)$$

10/15

For an arbitrary vector

$$|\alpha\rangle = \sum_i a_i |e_i\rangle$$

$$\hat{T}|\alpha\rangle = \sum_j a_j \hat{T}|e_j\rangle = \sum_{j=1}^{n} \sum_{i=1}^{n} a_j T_{ij} |e_i\rangle$$

$$= \sum_i \sum_j T_{ij} a_j |e_i\rangle$$

$\hat{T}$ takes a vector with components a_j and gives a vector with components

$$a'_i = \sum_j T_{ij} a_j$$

Think of $\hat{T}$ as a matrix

$$\hat{T} = \begin{pmatrix} T_{11} & T_{12} & \cdots & T_{1n} \\ T_{21} & T_{22} & \cdots & T_{2n} \\ \vdots & & & \\ T_{n1} & T_{n2} & \cdots & T_{nn} \end{pmatrix}$$

n×1 column matrix   n×n square matrix   n×1 column matrix

$$\begin{pmatrix} a'_1 \\ \vdots \\ a'_n \end{pmatrix} = \begin{pmatrix} & & \\ & \hat{T} & \\ & & \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}$$

Problem Set #4 average $\lesssim 20$

Example 2.10

$$\Psi(x,t) = \sum_i c_i \psi_i(x) e^{-iE_i t/\hbar}$$

assume $\int dx\, \psi_i^* \psi_j = \delta_{ij}$

and $\hat{H}\psi_i(x) = E_i \psi_i(x)$

(a) What is the condition on the c_i so $\Psi(x,t)$ is normalized?

$$\int_{-\infty}^{\infty} dx\, \Psi^*(x,t)\Psi(x,t) = 1 = \sum_k c_k^* e^{iE_k t/\hbar} \int_{-\infty}^{\infty} dx\, \psi_k^*(x) \sum_i c_i \psi_i(x) e^{-iE_i t/\hbar}$$

$$= \sum_{k=1}^{\infty} c_k^* e^{iE_k t/\hbar} \sum_{i=1}^{\infty} c_i e^{-iE_i t/\hbar} \underbrace{\int_{-\infty}^{\infty} dx\, \psi_k^*(x)\psi_i(x)}_{\delta_{ki}}$$

$$\delta_{ki} = \begin{cases} 1 & k = i \\ 0 & k \neq i \end{cases}$$

$$= \sum_i c_i^* e^{iE_i t/\hbar} c_i e^{-iE_i t/\hbar}$$

$$= \boxed{\sum_i c_i^* c_i = 1}$$

Prob. of being in state i is $P_i = c_i^* c_i$

$$\sum_i P_i = 1$$

Now calculate $\langle H \rangle$

$$\langle H \rangle = \int_{-\infty}^{\infty} dx\, \Psi^*(x,t)\, \hat{H}\, \Psi(x,t)$$

$$\langle H \rangle = \sum_k c_k^* e^{+iE_k t/\hbar} \int_{-\infty}^{\infty} dx\, \psi_k^*(x)\, \hat{H} \sum_i c_i \psi_i(x) e^{-iE_i t/\hbar}$$

$$\hat{H}\psi_i = E_i \psi_i$$

$$\int dx\, \psi_k^* \psi_i = \delta_{ik}$$

$$\langle H \rangle = \sum_k c_k^* e^{iE_k t/\hbar} \sum_i c_i e^{-iE_i t/\hbar} \underbrace{\int_{-\infty}^{\infty} dx\, \psi_k^*(x)\, \hat{H}\, \psi_i(x)}_{\delta_{ik} E_i}$$

$$\langle H \rangle = \sum_i c_i^* c_i E_i = \sum_i P_i E_i$$