Lecture 22: 03/11/09

- Formalism II
  - Observables and hermitian operators
  - determinate states
  - Eigenfunctions of a hermitian operator

Recap

III$_1$ Superposition of stationary, bound states:

- potential well with only bound states: $V = V(x)$

$\Rightarrow$ subset of solutions of time-dep. SE: $\Psi_n = \psi_n(x)\, e^{-i\frac{E_n}{\hbar}t}$

stationary states

$\Rightarrow$ solution of eigenvalue equ. $\hat{H}\psi_n = E_n \psi_n$ time-indep. S.E.

$\Rightarrow$ are orthonormal: $\langle \psi_m | \psi_n \rangle = \int_{-\infty}^{+\infty} \psi_m^* \psi_n \, dx = \delta_{nm}$

inner product of two functions ψ_n and ψ_m

$\Rightarrow$ general solution of time dep. SE:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-i\frac{E_n}{\hbar}t}$$

$\Rightarrow$ expansion of Ψ in terms of stationary states!

Recap II:

III_2 Hilbert Space:

set $\{f(x)\}$ functions such that $\int_a^b |f(x)|^2 dx < \infty$

$\boxed{\Rightarrow \text{Wave functions live in Hilbert space}}$

$\Rightarrow$ inner product exists: $\langle f | g \rangle = \int_{-\infty}^{+\infty} f^*(x)\, g(x)\, dx$

$\Rightarrow$ $\boxed{\langle f | g \rangle = \langle g | f \rangle^*}$ $\Rightarrow$ $\langle f | f \rangle$ is real

$\Rightarrow$ function is normalized, if $\langle f | f \rangle = 1$

$\Rightarrow$ set of functions is orthonormal, if $\langle f_m | f_n \rangle = \delta_{nm}$

$\Rightarrow$ set of functions is complete, if $f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$

Projection amplitudes: $c_n = \langle f_n | f \rangle$

III_3 Operators and Observables:

Observable: something one can measure (E, position, p...)

- Expectation value of an observable $Q(x,p)$

$$\langle Q \rangle = \int_{-\infty}^{+\infty} \Psi^* \hat{Q} \Psi \, dx = \langle \Psi | \hat{Q} \Psi \rangle = \langle \Psi | \hat{Q} | \Psi \rangle$$

Operator representing observable Q

- results of a measurement has to be real!

$\Rightarrow \langle Q \rangle = \langle Q \rangle^*$

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

complex conj. reverses order

$\Rightarrow$ must be true for any wave function Ψ

$$\Rightarrow \boxed{\langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle}$$

$\Rightarrow$ for operator representing observables:

$$\langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle \text{ for } \underline{\text{all}} \ f(x)$$

in hilbert space

$\Rightarrow$ such operators are called <u>hermitian</u>

$$\boxed{\text{Observables are represented by hermitian operators!}}$$

<u>Note:</u> If $\langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle$ for all $f(x)$

then also: $\boxed{\langle f | \hat{Q} g \rangle = \langle \hat{Q} f | g \rangle}$

for all $f(x), g(x)$! (see homework...)

Which of these operators is ***not*** hermitian?

A. x

B. $\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$

C. ix

D. **All of the above**

E. **None of the above**

Note: if $a = \text{const}$:

$$\langle f | a g \rangle = a \langle f | g \rangle$$

$$\langle a f | g \rangle = a^* \langle f | g \rangle$$

- $\langle \Psi | x \Psi \rangle = \int_{-\infty}^{+\infty} \Psi^* x \Psi \, dx = \int_{-\infty}^{+\infty} x \Psi^* \Psi \, dx$

$$= \int_{-\infty}^{+\infty} (x\Psi)^* \Psi \, dx = \langle x \Psi | \Psi \rangle$$

- $\dfrac{\hbar}{i}\dfrac{\partial}{\partial x} = \hat{p}$ = momentum operator

$\Rightarrow$ hermitian

- $\langle \Psi | i x \Psi \rangle = i \langle \Psi | x \Psi \rangle$

$$= i \langle x \Psi | \Psi \rangle$$

$$= - \langle i x \Psi | \Psi \rangle$$

$\Rightarrow$ not hermitian

(anti-hermitian)

• <u>general:</u>

indeterminancy in Quantum Theory $\Longleftrightarrow$ measurement of observable Q on ensemble of identically prepared systems does <u>not</u> give same result each time!

• <u>special case:</u>

determinate state for observable Q $\Longleftrightarrow$ measurement of observable Q on ensemble of identically prepared systems does give same result (call it q) each time!

$\Rightarrow$ standard deviation of Q is zero for determinate state!

$$\Rightarrow \sigma_Q^2 = 0 = \langle Q^2 \rangle - \langle Q \rangle^2 = \langle (\hat{Q} - \langle Q \rangle)^2 \rangle$$

$$= \langle \Psi | (\hat{Q} - \langle Q \rangle)^2 \Psi \rangle = \langle \Psi | (\hat{Q} - q)^2 \Psi \rangle \quad \langle Q \rangle \overset{!}{=} q$$

$$= \langle \Psi | (\hat{Q} - q)(\hat{Q} - q) \Psi \rangle = \langle (\hat{Q} - q) \Psi | (\hat{Q} - q) \Psi \rangle \overset{!}{=} 0$$

$(\hat{Q} - q)$ is a hermitian operator

$\Rightarrow (\hat{Q} - q)\Psi = 0$ (inner product of non-zero function with itself is $\neq 0$)

eigenvalue (number)

$$\Rightarrow \quad \left\| \quad \hat{Q}\Psi = q\Psi \quad \right\|$$

eigenvalue equation for the operator $\hat{Q}$

eigenfunction : determinate states of $\hat{Q}$

Determinate states of an observable Q are eigenfunctions of the hermitian operator $\hat{Q}$!

Note:

- Zero is not an eigenfunction
- Zero can be an eigenvalue
- Collection of all eigenvalues of an operator is called its spectrum
- sometimes two (or more) linear independent eigenfunctions share the same eigenvalue q

$\Rightarrow$ "degenerate spectrum"

Example:

energy = eigenvalues

$$\hat{H}\psi = E\psi$$

Hamiltonian operator for given $V(x)$
= Energy operator

eigenfunctions
= stationary states
= determinate energy states

III_4 Eigenfunctions of a hermitian operator:

$$\boxed{\hat{Q}\Psi = q\Psi}$$

Two categories:

I Spectrum of eigenvalues is discrete:

example: $\hat{H}$ for SHO

$\Rightarrow$ eigenvalues are separated from one another

$\Rightarrow$ eigenfunctions are physical realizable states

II Spectrum is continuous:

examples: $\hat{H}$ for free particle; position op. $\hat{x}$, momentum operator $\hat{p}$...

$\Rightarrow$ turns out that eigenfunctions are not normalizable

$\Rightarrow$ recall: "free particle": $e^{-i(kx-\omega t)}$ is eigenfunction of $\hat{H}\Psi = E\Psi$

$\Rightarrow$ only linear combination of eigenfunctions may be normalizable in this case

$\Rightarrow$ wave packets

[also: partly discrete, partly continuous (example: finite square well)

Case I Discrete Spectra:

a) The eigenvalues are real!

Proof: suppose $\hat{Q}\Psi = q\Psi$

and $\langle \Psi | \hat{Q}\Psi \rangle = \langle \hat{Q}\Psi | \Psi \rangle$

hermitian operator

$\Rightarrow \langle \Psi | q\Psi \rangle = \langle q\Psi | \Psi \rangle$

$\Rightarrow q \langle \Psi | \Psi \rangle = q^* \langle \Psi | \Psi \rangle$

$\Rightarrow q = q^* \Rightarrow q$ is real   Q.E.D.

Note: This proof (and the one on the next page) only works if the inner product exists! This is the case for discrete spectra, where the eigenfunctions are normalizable, but may not be true for the case for continuous spectra!

b) Eigenfunctions belonging to distinct eigenvalues are orthogonal.

Proof: suppose:

$$\hat{Q}\Psi = q\Psi \quad \hat{Q}\Theta = q'\Theta$$

two eigenf., each with its own eigenvalue

start with: $\langle \Psi | \hat{Q}\Theta \rangle = \langle \hat{Q}\Psi | \Theta \rangle$: $\hat{Q}$ is hermitian

$\Rightarrow \langle \Psi | q'\Theta \rangle = \langle q\Psi | \Theta \rangle$

$\Rightarrow q' \langle \Psi | \Theta \rangle = q^* \langle \Psi | \Theta \rangle$

$\Rightarrow q' \langle \Psi | \Theta \rangle = q \langle \Psi | \Theta \rangle$: eigenvalues are real

$\Rightarrow$ if $q' \neq q$, then $\langle \Psi | \Theta \rangle = 0$ Q.E.D.

$\Rightarrow$ orthogonal!