Formalism of Quantum Mechanics

Phys 460, Fall 2009, JP Hu

Dirac Notation

- Quantum systems: (Hilbert Space)

$$\{\psi_n(x,t), E_n\} \Leftrightarrow \{|n>, E_n\}$$

$$\Psi(x) = \sum_n C_n \Psi_n(x) \Leftrightarrow |\Psi> = \sum_n C_n |n>$$

Completeness!

- Orthornormal condition:

$$\int dx \psi^*_n(x)\psi_n(x) = 1 \Leftrightarrow < n|n> = 1$$

$$\int dx \psi^*_n(x)\psi_m(x) = \delta_{nm} \Leftrightarrow < n|m> = \delta_{nm}$$

|>, ket-space, <| bra-space:

Quantum Operator

Quantum Operators: $\hat{Q}$

$$\Psi(x) \to \Psi_Q(x) = \hat{Q}\Psi(x)$$

$$<\hat{Q}> = \int_{-\infty}^{\infty} dx \Psi^*(x)\hat{Q}\Psi(x)$$

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$$|\Psi> \to \hat{Q}|\Psi>$$

$$<\hat{Q}> = <\Psi|\hat{Q}|\Psi>$$

Matrix representation of quantum operator: $\{|n>, E_n\}$

$$\hat{Q}|n> = \sum_m Q_{nm}|m>$$

$$Q_{nm} = <m|\hat{Q}|n>$$

For given an orthornomal basis, Q matrix is fixed.

Observables: Hermitian Operators

- Observables are Hermitian Operators

The expectation values of observables must be real in any states:

$$\mathrm{Im}(<\Psi|\hat{Q}|\Psi>)=0 \quad \Longleftrightarrow \quad <\Psi|\hat{Q}|\Psi'>=<\Psi|\hat{Q}|\Psi'>^*$$

Proof: $$\mathrm{Im}(<a\Psi+b\Psi'|\hat{Q}|a\Psi+b\Psi'>)=0$$

Take: a=i,b=1

a=b=1

Prove it.

- Hermitian conjugate: $$<\Psi|\hat{Q}|\Psi'>=<\hat{Q}^{+}\Psi|\Psi'>=<\Psi'|\hat{Q}^{+}|\Psi>^*$$

- Hermitian Operator: $$\hat{Q}=\hat{Q}^{+}$$ $$Q_{nm}=<m|\hat{Q}|n>=<\hat{Q}^{+}m|n>=(Q^{+}{}_{mn})^*$$

Example of Hermitian Operators

- Momentum operators:

$$< \Psi | \hat{P} | \Psi' >= \int_{-\infty}^{\infty} dx \Psi^*(x)(-i\hbar \frac{d}{dx})\Psi'(x)$$

$$= -i\hbar | \Psi^2(x) |_{-\infty}^{\infty} + \int_{-\infty}^{\infty} dx((i\hbar \frac{d}{dx})\Psi^*(x))\Psi'(x)$$

$$= \int_{-\infty}^{\infty} dx((-i\hbar \frac{d}{dx})\Psi(x))^* \Psi'(x) =< \hat{P}\Psi | \Psi' >$$

- Position Operator
- $(\hat{Q}_1\hat{Q}_2)^+ = \hat{Q}^+{}_2\hat{Q}^+{}_1$

If A, B are Hermitian operator, AB in general is not Hermitian if [A,B] is not zero. However, AB+BA is Hermitian Operator.

Eigenvalue problems

- Eigenvalues of Hermitian operator is real.

$$\hat{Q} | \Psi >= q | \Psi >$$
$$q =< \Psi | \hat{Q} | \Psi >$$

- Eigenfunctions belonging to distinct eigenvalues are orthogonal

$$< \Psi' | \hat{Q} \Psi >= q < \Psi' | \Psi >$$
$$=< \hat{Q}^{+} \Psi' | \Psi >=< \hat{Q} \Psi' | \Psi >$$
$$= q' < \Psi' | \Psi >$$

- Handle Degeneracy: Gram-Schmidt Orthogonalization Procedure

Continuous Spectra

- Position: $\hat{X}$

$$\hat{X}|x> = x|x>$$
$$<x'|x> = \delta(x-x')$$

$$\Psi(x) = <x|\Psi>$$

- Momentum: $\hat{P} = -i\hbar\frac{\partial}{\partial x}$

$$\hat{P}|k> = \hbar k|k>$$
$$<k'|k> = \delta(k-k')$$

$$\Psi_k(x) = <x|k> = \frac{1}{\sqrt{2\pi}}e^{ikx}$$

- Identical Operator:

$$\int dk\,|k><k| = \hat{I}$$
$$\int dx\,|x><x| = \hat{I}$$

Unitary transformation

- Unitary Matrix: $U^{+}U = I$ $\quad U^{+}{}_{mn} = U_{nm}{}^{*}$
- Unitary Operator: $\hat{U}^{+}\hat{U} = \hat{I}$
- Quantum Systems: (Hilbert Space) $\psi_n(x) \Leftrightarrow |n>$

$$\int dx\psi^{*}{}_{n}(x)\psi_{n}(x) = 1 \Leftrightarrow <n|n>=1$$
$$\int dx\psi^{*}{}_{n}(x)\psi_{m}(x) = \delta_{nm} \Leftrightarrow <n|m>=\delta_{nm}$$

- Form Another Basis $\{|n'>=\hat{U}|n>\}$

$$<n'|m'>=\delta_{n'm'}$$

All completed bases can by connected by a unitary transformation.

Operators and representations

- Position base: $\hat{X}$

$$\hat{P} = -i\hbar \frac{\partial}{\partial x}$$

$$\Psi_k(x) = < x \mid k >= \frac{1}{\sqrt{2\pi}} e^{ikx}$$

$$\hat{X} \mid x >= x \mid x >$$
$$< x' \mid x >= \delta(x - x')$$

$$\hat{P}\Psi(x) = < x \mid \hat{P}\Psi >= -i\hbar \frac{\partial}{\partial x} \Psi(x)$$

- Momentum base:

$$\hat{P} \mid k >= \hbar k \mid k >$$
$$< k' \mid k >= \delta(k - k')$$

$$\Psi(k) = < k \mid \Psi >$$

$$\hat{X} = i\hbar \frac{\partial}{\partial p}$$

$$\hat{X}\Psi(k) = < k \mid \hat{X}\Psi >= \int dxx \frac{1}{\sqrt{2\pi}} e^{-ikx} \Psi(x)$$
$$= i \frac{\partial}{\partial k} \int dx < k \mid x >< x \mid \Psi >= i \frac{\partial}{\partial k} \Psi(k)$$

$$\Rightarrow \quad \hat{X} = i\hbar \frac{\partial}{\partial p}$$