

Lecture 2

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Wave Function

$$|\psi\rangle = \int dx \psi(x) |x\rangle$$

The wave function must not be mistaken for the state vector. The wave function $\psi(x)$ calculates the coefficients for all possible positions x in the x basis. The definition of the wave function is $|\psi\rangle = \langle x|\psi\rangle$

Operators

Definition: Takes a ket and returns a ket. It must be linear and Hermitian. As a consequence of being Hermitian the eigenvalues are real.

$$\begin{aligned}\hat{L} |u\rangle &= |v\rangle \\ \hat{L} (|u\rangle + |v\rangle) &= \hat{L} |u\rangle + \hat{L} |v\rangle \\ \hat{L} &= \hat{L}^\dagger\end{aligned}$$

Continuous Operators

$$|\psi\rangle = \int \langle x|\psi\rangle |x\rangle dx = |x\rangle \underbrace{\langle x|\psi\rangle dx}_{\text{Identity operator } \hat{I}} = \int (|x\rangle \langle x| dx) |\psi\rangle$$

Discrete Operators

$$\begin{aligned}|\psi\rangle &= \sum_i \psi_i |i\rangle = \sum_i \langle i|\psi\rangle |i\rangle = \sum_i \underbrace{|i\rangle \langle i|}_{\hat{I}} |\psi\rangle \\ \langle j|\psi\rangle &= \sum_i \psi_i \underbrace{\langle j|i\rangle}_{\delta_{ji}} = \psi_j\end{aligned}$$

Representation of Operators

The ket $|u\rangle$ and operator \hat{L} can be represented in the following way:

$$\begin{aligned}|u\rangle &\simeq \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \\ \hat{L} &\simeq \begin{bmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{bmatrix} \\ |u\rangle &\simeq u(x) \\ \hat{L} &\simeq c_0(x) + c_1(x) \frac{d}{dx} + c_2(x) \frac{d^2}{dx^2} + \dots\end{aligned}$$

Discrete basis

$$\langle m | \hat{K} | n \rangle = K_{nm} = \text{m,n'th matrix element of } \hat{K}$$

$$|v\rangle = \sum_m V_m |m\rangle$$

$$\hat{K} |v\rangle = \langle n | \hat{K} | v \rangle = \langle n | \hat{K} \sum_m V_m |m\rangle = \sum_m V_m \langle n | \hat{K} | m \rangle = \sum_m V_m K_{nm}$$

Composite Operators

$$\begin{aligned} \hat{K} \hat{L} |v\rangle &= \hat{K} (\hat{L} |v\rangle) = (\hat{K} \hat{L}) |v\rangle \\ \langle n | \hat{K} \hat{L} | m \rangle \end{aligned}$$

Inserting the identity operator:

$$\begin{aligned} \langle n | \hat{K} \underbrace{\sum_r |r\rangle \langle r|}_{\hat{I}} \hat{L} | m \rangle \\ \sum_r \langle n | \hat{K} | r \rangle \langle r | \hat{L} | m \rangle = \underbrace{\sum_r K_{nr} L_{rm}}_{\text{Matrix multiplication}} \end{aligned}$$

Change of Basis

Give to different bases $\{|n\rangle\}$ and $\{|n'\rangle\}$.

$$|\psi\rangle = \sum_n \underbrace{\psi_n}_{\langle n|\psi\rangle} |n\rangle, \quad |\psi\rangle = \sum_{n'} \underbrace{\psi_{n'}}_{\langle n'|\psi\rangle} |n'\rangle$$

$$\langle m' | \psi \rangle = \sum_n \psi_n \underbrace{\langle m' | n \rangle}_{S_{m'n}}$$

We define $S_{m'n}$ to be $\langle m' | n \rangle$ which is a matrix relation between ψ_n to $\psi_{n'}$.

$$\psi_{m'} = \sum_n S_{m'n} \psi_n$$

S is unitary meaning $S^\dagger = S^{-1}$

Proof of unitarity: Set $|\psi\rangle = |n'\rangle$

$$\underbrace{\langle m' | n' \rangle}_{\delta_{m'n'}} = \sum_n S_{m'n'} \underbrace{\langle n | n' \rangle}_{\langle n' | n \rangle^* = S_{n'm}^*}$$

Remember $S_{m'n} = \langle m' | n \rangle$.

$$\begin{aligned} \langle n | n' \rangle &= \langle n' | n \rangle^* = S_{n'm}^* = S_{m'n}^{T*} = S_{m'n}^\dagger \\ SS^\dagger &= 1 \rightarrow S^\dagger = S^{-1} \end{aligned}$$

Operators in different bases

$$K_{m'n'} = \langle m' | \hat{K} | n' \rangle = \langle m' | \hat{I} \hat{K} \hat{I} | n' \rangle$$

$$\sum_{mn} \underbrace{\langle n' | m \rangle}_{S_{m'n'}} \langle m | \hat{K} | n \rangle \underbrace{\langle n | n' \rangle}_{S_{nn'}^\dagger}$$

$$\sum_{mn} S_{m'n} K_{mn} S_{nn'}^\dagger = S^\dagger K S = K'$$

Now we have the operator \hat{K} in a new basis defined as \hat{K}'

Hermitian Conjugate of an Operator

Definition by the inner product:

$$\left(|u\rangle, \hat{K} |v\rangle \right) = \left(\hat{K}^\dagger |u\rangle, |v\rangle \right) \text{ for all } |u\rangle, |v\rangle$$

Is not as simple as "just transposing and taking the complex conjugate". A function could be Hermitian.

Definition in Dirac-Notation:

$$\langle u | \hat{K} | v \rangle = \langle v | \hat{K}^\dagger | u \rangle^* \text{ for all } |u\rangle, |v\rangle$$

It is enough to define:

$$\langle u | \hat{K} | v \rangle = \langle v | \hat{K}^\dagger | u \rangle \text{ problem 2.3(L)}$$

Exercise: Find \hat{K}^\dagger

$$\hat{K} = \alpha |a\rangle \langle b|$$

$$\langle u | \hat{K}^\dagger | v \rangle = \langle v | \hat{K} | u \rangle^* = \langle v | a \rangle^* \langle b | u \rangle^*$$

$$\langle u | (|b\rangle \langle a|) | v \rangle \rightarrow \hat{K}^\dagger = |b\rangle \langle a| \alpha^*$$

Check the following correspondence

$$\hat{K} |v\rangle \leftrightarrow \langle v | \hat{K}^\dagger$$

We set $|w\rangle = \hat{K} |v\rangle$ and act on it with an arbitrary bra $\langle n|$.

$$\langle u | w \rangle = \langle u | \hat{K} | v \rangle = \langle v | \hat{K}^\dagger | u \rangle^* \rightarrow \langle w | u \rangle = \langle v | \hat{K}^\dagger | u \rangle$$

This holds for any $|w\rangle \rightarrow \langle w| = \langle v | \hat{K}^\dagger$

Exercise: Find the Hermitian conjugate of the following operator

$$\hat{K} \simeq \frac{d}{dx}$$

$$|u\rangle = u(x)$$

$$|v\rangle = v(x)$$

$$\langle u | \hat{K}^\dagger | v \rangle = \langle v | \hat{K} | u \rangle^* = \int \left(v^*(x) \frac{d}{dx} u(x) \right)^* dx = \int v(x) \frac{d}{dx} u^*(x) dx$$

$$\underbrace{v(x)u^*(x)}_0 \bigg|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d}{dx} v(x) u^*(x) dx = \int_{-\infty}^{\infty} u^*(x) \left(-\frac{d}{dx} \right) v(x) dx$$