QM
Phys 651

Lecture #4

Examples of Bra-ket algebra

Consider the states $|\Psi\rangle = 3i|\varphi_1\rangle - 7i|\varphi_2\rangle$ and $|\chi\rangle = -|\varphi_1\rangle + 2i|\varphi_2\rangle$, where $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are orthonormal.

1) Calculate $|\Psi+\chi\rangle$ and $\langle\Psi+\chi|$
Calculate the scalar products $\langle\Psi|\chi\rangle$ and $\langle\chi|\Psi\rangle$

Solution:

1) $|\Psi+\chi\rangle = |\Psi\rangle + |\chi\rangle = 3i|\varphi_1\rangle - 7i|\varphi_2\rangle - |\varphi_1\rangle + 2i|\varphi_2\rangle = (3i-1)|\varphi_1\rangle - 5i|\varphi_2\rangle$

$\langle\Psi+\chi| = (|\Psi+\chi\rangle)^* = (-3i-1)\langle\varphi_1| + 5i\langle\varphi_2|$

) $\langle\Psi|\chi\rangle = (-3i\langle\varphi_1| + 7i\langle\varphi_2|)(-|\varphi_1\rangle + 2i|\varphi_2\rangle)$

$= 3i\underbrace{\langle\varphi_1|\varphi_1\rangle} - 7i\underbrace{\langle\varphi_2|\varphi_1\rangle} + 6\underbrace{\langle\varphi_1|\varphi_2\rangle} - 14\underbrace{\langle\varphi_2|\varphi_2\rangle}$

$= 3i - 14$

$$\langle \chi | \Psi \rangle = \langle \Psi | \chi \rangle^* = -3i - 14$$

Operators

An operator A is the mathematical rule that when applied to a ket $|\Psi\rangle$ transforms it into another ket $|\Psi'\rangle$ of the same space (same is valid for a bra)

$$A|\Psi\rangle = |\Psi'\rangle \quad ; \quad \langle \Psi | A = \langle \Psi' |$$

An operator is linear if for any vectors $|\Psi_1\rangle$, $|\Psi_2\rangle$ and any complex numbers a_1, a_2 $\Rightarrow$

$$A\left(a_1|\Psi_1\rangle + a_2|\Psi_2\rangle\right) = a_1 A|\Psi_1\rangle + a_2 A|\Psi_2\rangle;$$

$$\left(\langle \Psi_1 | a_1 + \langle \Psi_2 | a_2\right) A = a_1 \langle \Psi_1 | A + a_2 \langle \Psi_2 | A$$

- The expectation or mean value of an operator A with respect to a state $|\Psi\rangle$ is defined as

$$\bar{A} = \langle \Psi | A | \Psi \rangle$$

- Products of the type $|\Psi\rangle A$ and $A\langle\Psi|$ are forbidden (no physical meaning!)
- The quantity $|\varphi\rangle\langle\Psi|$ is a linear operator when $|\varphi\rangle\langle\Psi|$ is applied to a ket $|\Psi'\rangle \Rightarrow$ get another ket: $\big(\underbrace{|\varphi\rangle\langle\Psi|}_{\text{so-called "outer product"}}\big)|\Psi'\rangle =$

$$= \underbrace{\langle\Psi|\Psi'\rangle}_{\text{complex number}} \, |\varphi\rangle$$

- Hermitian adjoint (or conjugate) of a complex number α is the complex conjugate of this number: $\alpha^{+} = \alpha^{*}$

  Hermitian adjoint of an operator A is defined as: $\langle\Psi|A^{+}|\varphi\rangle = \langle\varphi|A|\Psi\rangle^{*}$

  Note that in general case $A^{+} \neq A^{*}$!!

- An operator A is Hermitian if $A = A^{+}$

  (or $\langle\Psi|A|\varphi\rangle = \langle\varphi|A|\Psi\rangle^{*}$)

  An operator B is anti-Hermitian if $B^{+} = -B$

  (or $\langle\Psi|B|\varphi\rangle = -\langle\varphi|B|\Psi\rangle^{*}$)

Examples of finding Hermitian conjugates and bra-ket algebra

- $(\alpha A)^{+} = \alpha^{*} A^{+}$
- $(A^{+})^{+} = A$
- $(A+B+C+D)^{+} = A^{+} + B^{+} + C^{+} + D^{+}$
- $(ABCD)^{+} = D^{+} C^{+} B^{+} A^{+}$
- $(A^{n})^{+} = (A^{+})^{n}$
- $(ABCD|\psi\rangle)^{+} = \langle\psi|D^{+}C^{+}B^{+}A^{+}$
- $(|\psi\rangle\langle\varphi|)^{+} = |\varphi\rangle\langle\psi|$
- $|\alpha A \psi\rangle = \alpha A|\psi\rangle$
- $\langle\alpha A\psi| = \alpha^{*}\langle\psi|A^{+}$
- $\langle\alpha A^{+}\psi| = \alpha^{*}\langle\psi|(A^{+})^{+} = \alpha^{*}\langle\psi|A$

Note: all operators that correspond to physical observables are Hermitian (e.g. Hamiltonian, operators of position, momentum, angular momentum, etc.)

Example Consider the following operators:

$$X\ ,\quad \frac{d}{dx}\ ,\quad \underbrace{-i\hbar\frac{d}{dx}}_{=\,P_x}$$

X ← position operator

P_x ← momentum operator

Are they Hermitian?

Solution

- Consider $\langle\psi|X|\varphi\rangle = \int_{-\infty}^{+\infty}\psi^*(x)\,X\,\varphi(x)\,dx =$

$$= \int_{-\infty}^{+\infty} x\,\psi^*(x)\,\varphi(x)\,dx = \left[\int_{-\infty}^{+\infty} x^*\psi(x)\,\varphi^*(x)\,dx\right]^* =$$

$$= \left[\int_{-\infty}^{+\infty}\varphi^*(x)\,\underset{\uparrow\ \text{real!}}{x}\,\psi(x)\,dx\right]^* = \langle\varphi|X|\psi\rangle^* \Rightarrow$$

$X^\dagger = X \Rightarrow$ Hermitian

- $\langle\psi|\frac{d}{dx}|\varphi\rangle = \int_{-\infty}^{+\infty}\psi^*(x)\,\frac{d\varphi}{dx}\,dx = \underbrace{\psi^*(x)\,\varphi(x)\Big|_{-\infty}^{+\infty}}_{=\,0} -$

$$-\int_{-\infty}^{+\infty}\varphi(x)\,\frac{d\psi^*}{dx}\,dx =$$

for well-behaved functions

$$= -\left[\int_{-\infty}^{+\infty}\varphi^*(x)\,\frac{d\psi}{dx}\,dx\right]^* = -\langle\varphi|\frac{d}{dx}|\psi\rangle^* \Rightarrow$$

$$\left(\frac{d}{dx}\right)^\dagger = -\frac{d}{dx} \Rightarrow \text{anti-Hermitian}$$

(6)

$$\langle \Psi | -i\hbar \frac{d}{dx} | \varphi \rangle = \int_{-\infty}^{+\infty} \Psi^*(x) \left[-i\hbar \frac{d\varphi}{dx} \right] dx =$$

$$= \underbrace{\Psi^*(x)(-i\hbar)\varphi(x) \Big[_{-\infty}^{+\infty}}_{=0 \text{ for well-behaved functions}} + i\hbar \int_{-\infty}^{+\infty} \varphi(x) \frac{d\Psi^*(x)}{dx} dx =$$

$$= \left[\int_{-\infty}^{+\infty} \varphi^*(x) \left(-i\hbar \frac{d\Psi(x)}{dx} \right) dx \right]^* = \langle \varphi | -i\hbar \frac{d}{dx} | \Psi \rangle^*$$

$$\Downarrow$$

$$\left(-i\hbar \frac{d}{dx} \right)^\dagger = -i\hbar \frac{d}{dx}$$

$$(p^\dagger = p) \Rightarrow \text{Hermitian}$$

Eigenvalues and eigenvectors of an operator

A state vector $|\Psi\rangle$ is an eigenvector (also called an eigenket or eigenstate) of an operator A if $A|\Psi\rangle = a|\Psi\rangle$, where a is a complex number called an eigenvalue of A. This equation is called an eigenvalue equation (or eigenvalue problem)

<u>Theorem</u> : The eigenvalues of a Hermitian operator A are real ; the eigenkets of A corresponding to different eigenvalues are orthogonal.

<u>Proof</u> : $A|\varphi_n\rangle = a_n|\varphi_n\rangle$; $\langle\varphi_m|\varphi_n\rangle = \delta_{mn}$

Hermitian Operator $\Rightarrow$ real number show show

$$\langle\varphi_m|A|\varphi_n\rangle = a_n\langle\varphi_m|\varphi_n\rangle \quad (1)$$

Hermitian conjugate of $A|\varphi_n\rangle \Rightarrow$

$\langle\varphi_n|A^+ \Rightarrow$ let's consider another eigenket $\Rightarrow$

$$\langle\varphi_m|A^+ \Rightarrow \underbrace{\langle\varphi_m|A^+}_{=\,a_m^*\langle\varphi_m|}|\varphi_n\rangle = a_m^*\langle\varphi_m|\varphi_n\rangle \quad (2)$$

Subtract (2) from (1) $\Rightarrow$

$$\langle\varphi_m|A|\varphi_n\rangle - \langle\varphi_m|A^+|\varphi_n\rangle = a_n\langle\varphi_m|\varphi_n\rangle - a_m^*\langle\varphi_m|\varphi_n\rangle;$$

$$n=m \Rightarrow \langle\varphi_n|\underbrace{(A-A^+)}_{=\,0}|\varphi_n\rangle = (a_n - a_n^*)\langle\varphi_n|\varphi_n\rangle$$

0 since A is H[illegible]

$a_n = a_n^* \Rightarrow a_n$ is real!

- $n \neq m \Rightarrow 0 = (a_n - a_m^*) \langle \varphi_m | \varphi_n \rangle$

$\Downarrow$

either $a_n = a_m^* = a_m$
or $\langle \varphi_m | \varphi_n \rangle = 0$

Since we assumed that a_n, a_m are different eigenvalues $\Rightarrow a_n \neq a_m \Rightarrow \langle \varphi_m | \varphi_n \rangle = 0$, i.e. $|\varphi_n\rangle$ and $|\varphi_m\rangle$ are orthogonal

It is conventional to normalize $|\varphi_n\rangle$, so that $\{ |\varphi_n\rangle \}$ form an orthonormal set $\Rightarrow$

$$\langle \varphi_m | \varphi_n \rangle = \delta_{mn}$$