Notes for Quantum Mechanics

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Lecture 6

Before we dive into QM, we want to learn some math associated with bra's ket's and operators. This is the mathematics of complex vector spaces - a particular kind of Hilbert space. The first thing we will need to remember is that these spaces are complex, so remember that a number or variable has 2 components now, a real piece and an imaginary piece i.e. a number $c = (c_1 + i\, c_2)$ where c_1 and c_2 are real. c^* is the complex conjugate of c. $c^*\, c$ is written as c^2 and is always real.So the numbers inside the kets and the eigenvalues are often complex.. (real eigenvalues are special since they will correspond to stuff we can see and touch called observables - like momentum, energy, position etc)

So first we start with the space that our kets live in - ket space (Juice-space in our previous example). We will however assume that we are in a continuous space so its more like the wavelength.

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Bra's and Ket's  - the things that specify states
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So lets list some rules. These are known, because mathematicians have been studying complex vector spaces for a long time. We physicists are borrowing the math. Its not so different than when we borrow arithmetic, algebra and geometry from the mathematicians.

$|\alpha\rangle+|\beta\rangle=|\gamma\rangle$ kets can be added and you get another ket (1)

$c|\alpha\rangle=|\alpha\rangle c=|\gamma\rangle$ you can multiply by a number (complex) and get another ket
Note that for we physicists, we normalize everything so $|\alpha\rangle$ and $c|\alpha\rangle$ describe the same state as long as $c\neq 0$ (2)
if c is zero, then $|\gamma\rangle$ is a null ket

Observables such as momentum., energy etc, are represented by operators which act on kets from the left and give another ket (3)
$\hat{A}|\alpha\rangle=|\gamma\rangle$

In general $\hat{A}|\alpha\rangle$ is not a constant times $|\alpha\rangle$. However there are special and very important kets, known as **eigenkets** of an operator $\hat{A}$ which we will denote as $|a'\rangle$, $|a''\rangle$, $|a'''\rangle$, $|a''''\rangle$,... with the property that (4)
$\hat{A}|a'\rangle=a'|a'\rangle$ $\hat{A}|a''\rangle==a''|a''\rangle$ etc so that $|a'\rangle$, $|a''\rangle$, $|a'''\rangle$ are the eigenkets and {a', a'', a''',...} are the eigenvalues

An arbitrary ket can be written as
$|\alpha\rangle = \Sigma c_{a'}|a'\rangle$ It will turn out that eigenkets of observables can be used as a basis and will span the space - but we will get to that later. I also note that if there is a continuous set of eigenkets then the sum turns into an integral. (5)

So if $\hat{A}$ is an observable and $|a'\rangle$ are the eigenkets then an arbitrary ket $|\alpha\rangle = \Sigma c_{a'}|a'\rangle$ (6)

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There exists a dual to $|\alpha\rangle$ which we denote as $\langle\alpha|$ We will say $|\alpha\rangle \overset{DC}{\longleftrightarrow} \langle\alpha|$ (7)

The dual to $c|\alpha\rangle$ is $c^* \langle\alpha|$ NOT $c\langle\alpha|$ (8)

The combination $\langle\beta|\alpha\rangle$ is called an inner product or a braket "bra""ket" which is a c-number [A c-number is a number or a function like you have always known. It is NOT a ket or a bra. i.e. the inner product will "kill" the bra and ketness just like the dot product of two vectors makes a scalar. (9)

POSTULATE $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$
this of course means that $\langle\alpha|\alpha\rangle = \langle\alpha|\alpha\rangle^*$ hence it is real (10)

POSTULATE $\langle\alpha|\alpha\rangle \geq 0$ that is, it is positive definite and $\langle\alpha|\alpha\rangle = 0$ only if $|\alpha\rangle = 0$ (11)

$|\alpha\rangle$ and $|\beta\rangle$ are orthogonal if $\langle\alpha|\beta\rangle = 0$ (12)

we can normalize our ket $|\alpha\rangle$ by setting $|\alpha_{new}\rangle = \frac{1}{\sqrt{\langle\alpha|\alpha}}|\alpha\rangle$ so that $\langle\alpha_{new}|\alpha_{new}\rangle = 1$ (13)

OPERATORS – the things that specify obervables

we will denote as general operators $\hat{X}$, $\hat{Y}$, ... and
operators which are observables (Hermitian Operators) as $\hat{A}, \hat{B}, \ldots$ (14)

$\hat{X} = \hat{Y}$ if $\hat{X}|\alpha\rangle = \hat{Y}|\alpha\rangle$ for any $|\alpha\rangle$ (15)

if $\hat{X}|\alpha\rangle = 0$ $\hat{X}$ is a null operator (16)

Operators are associative and commutative under addition (17)

The operators we will deal with in this class will be linear [Except the time reversal operator if we get to it]
This means (18)
$\hat{X}[c|\alpha\rangle + b|\beta\rangle] = c\hat{X}|\alpha\rangle + b\hat{X}|\beta\rangle$

The dual conjugate of $\hat{X}|\alpha\rangle$ is $\langle\alpha|\hat{X}^\dagger$ (19)

$\hat{X}^\dagger$ is called the hermitian adjoint of $\hat{X}$ (20)

$\hat{X}$ is Hermitian if $\hat{X}^\dagger = \hat{X}$ a very important one (21)

Observables are represented by Hermitian Operators

In general $\hat{X}$ and $\hat{Y}$ do not commute under multiplication - that is
$\hat{X}\hat{Y} \neq \hat{Y}\hat{X}$ another important one! (22)

the associative law is ok under multiplication i.e.
$\hat{X}(\hat{Y}\hat{Z}) = (\hat{X}\hat{Y})\hat{Z} = \hat{X}\hat{Y}\hat{Z}$ and $\hat{X}(\hat{Y}|\alpha\rangle) = (\hat{X}\hat{Y})|\alpha\rangle = \hat{X}\hat{Y}|\alpha\rangle$ (23)

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$(\hat{X}\,\hat{Y})^\dagger = \hat{Y}^\dagger\,\hat{X}^\dagger$

proof

first recall that $\hat{Y}|\alpha\rangle \overset{DC}{\longleftrightarrow} \langle\alpha|\hat{Y}^\dagger$

$\langle\alpha|(\hat{X}\,\hat{Y})^\dagger \overset{DC}{\longleftrightarrow} \hat{X}\,\hat{Y}|\alpha\rangle = \hat{X}(\hat{Y}|\alpha\rangle) \overset{DC}{\longleftrightarrow} (\langle\alpha|\hat{Y}^\dagger)\hat{X}^\dagger = \langle\alpha|\hat{Y}^\dagger\hat{X}^\dagger$ hence $(\hat{X}\,\hat{Y})^\dagger = \hat{Y}^\dagger\,\hat{X}^\dagger$

We will define a new thing called an outer product which will act as a operator
$|\beta\rangle\langle\alpha|$ outer product (25)

Note that $|\alpha\rangle|\beta\rangle$ is illegal unless they are in different spaces - e.g. for an electron if $|\alpha\rangle$ is the space part of the eigenfunction and $|\beta\rangle$ is the spin part. this may be confusing now, but I hope it will become clear to you. (26)

$(|\beta\rangle\langle\alpha|)\,|\gamma\rangle = |\beta\rangle\,(\langle\alpha|\gamma\rangle)$ Dirac's associative axiom of multiplication - An outer product acting on a ket is another ket (27)

this is sort of like a rotation i.e. $(|\beta\rangle\langle\alpha|)$ "rotates" $|\gamma\rangle$ into $|\beta\rangle$

if $\hat{X}=|\beta\rangle\langle\alpha|$ then $\hat{X}^\dagger = |\alpha\rangle\langle\beta|$ (28)

Proof:
$\langle\gamma|\hat{X}^\dagger \overset{DC}{\longleftrightarrow} \hat{X}\,|\gamma\rangle = |\beta\rangle\,\langle\alpha|\,\gamma\,\rangle \overset{DC}{\longleftrightarrow} \langle\alpha\,|\gamma\rangle^*\langle\beta| = \langle\gamma|\alpha\rangle\langle\beta| = \langle\gamma|(|\alpha\rangle\langle\beta|)$ hence $\hat{X}^\dagger = |\alpha\rangle\langle\beta|$ (29)

$\langle\beta|\hat{X}|\alpha\rangle = \langle\alpha\,|\,\hat{X}^\dagger\,|\beta\rangle^*$ CORRECTED EQN (30)

Proof: first recall $\langle\beta\,|\alpha\rangle = \langle\alpha\,|\beta\rangle^*$
$\langle\beta|\hat{X}|\alpha\rangle = \langle\beta|\,(\hat{X}|\alpha\rangle) = [\,(\langle\alpha\,|\,\hat{X}^\dagger)\,|\beta\rangle]^* = \langle\alpha\,|\,\hat{X}^\dagger\,|\beta\rangle^*$ (31)

So if $\hat{X}$ is Hermitian, i.e. $\hat{X}=\hat{X}^\dagger$ then $\langle\beta|\hat{X}|\alpha\rangle = \langle\alpha\,|\,\hat{X}\,|\beta\rangle^*$ CORRECTED EQN (32)

It turns out that observables will be represented by Hermitian Operators
Theorem
The eigenvalues of Hermitian operator $\hat{A}$ are real
The eigenkets of $\hat{A}$ are orthogonal (33)

Proof::

$\hat{A}|a'\rangle \equiv a'|a'\rangle$

Since $\hat{A}$ is Hermitian ($\hat{A}=\hat{A}^\dagger$) the DC of this eqn is

$\langle a''|\hat{A} = a''^*\langle a''|$ hence [here if you have a problem with $\langle a''|\hat{A}$, think of it as the DC of $|\gamma\rangle = \hat{A}\,|a'\rangle$]

$\langle a''\,|\,\hat{A}\,|\,a'\rangle = a'\langle a''|a'\rangle$ also

$\langle a''\,|\,\hat{A}\,|\,a'\rangle = a''^*\langle a''|a'\rangle$ subtract these two

$0=(a'-a''^*)\langle a''|a'\rangle$ so one of the two terms here must be zero

Now if $a'=a''$ Then $a'=a'^*$ and a' is real [proof of first statement]

if $a'\neq a''$ then $\langle a''|a'\rangle = 0$

so summarizing if $a'=a''$ then $\langle a''|a'\rangle = \langle a'|a'\rangle$=some number - lets normalize it so that the number is 1 and we get

$\langle a''|a'\rangle = \delta_{a''a'}$ [proof of 2nd statement]

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this means that the eigenkets $|a\rangle$ are a set of basis eigenkets.! (We will see later that they span the space)

So now we can write any arbitrary ket $|\alpha\rangle$ as $|\alpha\rangle = \sum_a c_a |a\rangle$ Now if we want to find the c_a's

$$\langle a'|\alpha\rangle = \sum_a c_a \langle a'|a\rangle \implies \langle a'|\alpha\rangle = \sum_a c_a \delta_{aa'} \implies c_a = \langle a|\alpha\rangle \implies |\alpha\rangle = \sum_a |a\rangle\langle a|\alpha\rangle \tag{34}$$

From here we get something which is called the completeness relation (note that this is not a proof- we used this to write (5)

$$\hat{1} = \sum_a |a\rangle\langle a| \tag{35}$$

As before we see the normalization condition- we assume $|\alpha\rangle$ is normalized

$$1 = \langle\alpha|\alpha\rangle = \langle\alpha|(\sum_a |a\rangle\langle a|)|\alpha\rangle = \sum_a |\langle a|\alpha\rangle|^2 = \sum_a |c_a|^2 \tag{36}$$

Now we can define something called a projection operator
We shall consider
$\hat{\Lambda}_a \equiv |a\rangle\langle a|$ which behaves as an operator

$\hat{\Lambda}_a|\alpha\rangle = |a\rangle\langle a|\alpha\rangle = c_a|a\rangle$ so it "projects out a pice of $|\alpha\rangle$ which is parallel to $|a\rangle$ and the length is $c_a = \langle a|\alpha\rangle$

$$\hat{1} = \sum_a |a\rangle\langle a| = \sum_a \hat{\Lambda}_a \tag{38}$$

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