

0.1 Lecture II

0.2 Bra-ket notation

In the previous lecture we used the symbols ϕ , or ϕ_a , or Ψ to represent a vector, or quantum state, in Hilbert space. We will now introduce a new notation, called the Dirac bra-ket notation. The Dirac bra-ket notation is a concise and convenient way to describe quantum states. We introduce and define the symbol

$$|\alpha\rangle \tag{1}$$

to represent a quantum state. This is called a ket, or a ket vector. We use it to denote a vector in Hilbert space. We say that a physical system is in quantum state $|\alpha\rangle$, where α is the eigenvalue corresponding to operator \hat{A} that represents a physical measurement.

If we have two distinct quantum states $|\alpha_1\rangle$ and $|\alpha_2\rangle$, then the following ket

$$|\psi\rangle = c_1|\alpha_1\rangle + c_2|\alpha_2\rangle, \tag{2}$$

where c_i is a complex number, is also a possible state for the system.

Dirac defined something called a bra vector, designated by $\langle\alpha|$. This is not a ket, and does not belong in ket space e.g. $|\alpha\rangle + \langle\beta|$ has no meaning. However, we assume for every ket $|\beta\rangle$, there exists a bra labeled $\langle\beta|$. The bra $\langle\gamma|$ is said to be the dual of the ket $|\gamma\rangle$. We can ask the question: since $c_1|\alpha_1\rangle + c_2|\alpha_2\rangle$ is a ket, what is the dual (or bra vector) associated with that vector?

The answer is,

$$c_1|\alpha_1\rangle + c_2|\alpha_2\rangle \iff c_1^* \langle\alpha_1| + c_2^* \langle\alpha_2| \tag{3}$$

where \iff signifies a dual correspondence. This is an anti-linear relation.

Dirac allowed the the bra's and ket's to line up back to back, i.e.

$$\langle\alpha|\beta\rangle \equiv (\langle\alpha|, |\beta\rangle). \tag{4}$$

The symbol $\langle \alpha | \beta \rangle$ represents a complex number that is equal to the value of the inner product of the ket $|\alpha\rangle$ with $|\beta\rangle$. We note, according to the above definition, that

$$\langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle^* . \quad (5)$$

Dirac also defined something called an outer product,

$$|\alpha\rangle\langle\beta|. \quad (6)$$

An outer product is allowed to stand next to a ket on its left, or next to a bra on the bra's right. Lets define $X = |\alpha\rangle\langle\beta|$, then if $|\Psi\rangle$ is an arbitrary ket, one is allowed to construct

$$X|\Psi\rangle = |\alpha\rangle\langle\beta||\Psi\rangle \quad (7)$$

It looks like we have something like an inner product on the r.h.s of this equation. Indeed, according to *Dirac's associative axiom of multiplication*, we are allowed to put parenthesis around the quantity $\langle\beta||\Psi\rangle$ and equate it to the value of the inner product $\langle\beta|\Psi\rangle$. Or

$$X|\Psi\rangle = |\alpha\rangle\langle\beta||\Psi\rangle = c|\alpha\rangle; \quad c = (\langle\beta|\Psi\rangle). \quad (8)$$

The outer product X is an operator in Hilbert space. It acts on ket $|\Psi\rangle$ from the left and turns it into another ket $c|\alpha\rangle$. Be careful! for $|\Psi\rangle X$ has no meaning, however $\langle\Psi|X$ does.

$$\langle\Psi|X = \langle\Psi||\alpha\rangle\langle\beta| = (\langle\Psi|\alpha\rangle)\langle\beta| = d^*\langle\beta|; \quad d = \langle\alpha|\Psi\rangle \quad (9)$$

If we take operator A and operate on a ket $A|\alpha\rangle$, is $\langle\alpha|A$ dual to it? In general it is not, however the dual of $A|\alpha\rangle$ is

$$\langle\alpha|A^\dagger \iff A|\alpha\rangle \quad (10)$$

where A^\dagger is called the *hermitian conjugate* of operator A . Sometimes $A = A^\dagger$, then A is called an hermitian operator. Hermitian operators play a central role in quantum theory.

- Show that $X = \sum_i \epsilon_i |\alpha_i\rangle\langle\alpha_i|$, where ϵ_i is a real number, is hermitian.
- If $Y = aX$ is an operator and a is a complex number, show $Y^\dagger = X^\dagger a^*$

- Find the hermitian conjugate to $X = |\alpha\rangle\langle\beta|$.
- Show that the eigenvalues of a hermitian operator are real numbers.
- Assume there is a unique eigenstate for every eigenvalue of an hermitian operator X . Show that the eigenvectors are orthogonal and linearly independent. Consider the case where the restriction of non-degenerate eigenstates is removed.

Using the tools provided by the Dirac bra-ket notation we reconsider Postulate III. Consider a hermitian operator X , whose eigenstates $|a\rangle$ obey the eigenvalue equation

$$X|a\rangle = a|a\rangle \quad (11)$$

where a is an eigenvalue. Suppose these eigenvalues are distinct, then the set $\{|a_1\rangle, |a_2\rangle, \dots, |a_n\rangle\}$ are mutually orthonormal (why?). Suppose a measurement of observable X yields the value a_n , with probability $|c_n|^2$ where

$$|\Psi\rangle = \sum_n c_n |a_n\rangle. \quad (12)$$

Taking the inner product of $|\Psi\rangle$ with state $|a_m\rangle$ we get

$$\langle a_m | \Psi \rangle = \sum_n c_n \langle a_m | a_n \rangle \quad (13)$$

but $\langle a_m | a_n \rangle = \delta_{mn}$ and so

$$\langle a_m | \Psi \rangle = \sum_n c_n \delta_{mn} = c_m. \quad (14)$$

Therefore the probability for a measurement to yield eigenvalue a_n is given by the square of the inner product $\langle a_n | \Psi \rangle$, also called the *probability amplitude*. Furthermore, since $c_n = \langle a_n | \Psi \rangle$ and inserting this into the equation above, we get

$$|\Psi\rangle = \sum_n \langle a_n | \Psi \rangle |a_n\rangle = \sum_n |a_n\rangle \langle a_n | \Psi \rangle \quad (15)$$

Using Dirac's associative axiom we can re-write this

$$|\Psi\rangle = \sum_n (|a_n\rangle \langle a_n|) |\Psi\rangle \quad (16)$$

where the brackets contain the operator $\sum_n |a_n\rangle\langle a_n|$. Since the left hand side is the ket $|\Psi\rangle$ this operator must be the identity operator, i.e. its action to the ket $|\Psi\rangle$ on its right reproduces $|\Psi\rangle$ i.e.,

$$\sum_n |a_n\rangle\langle a_n| = I. \quad (17)$$

If the above relation holds, we say that the set of kets $|a_n\rangle$ are complete and constitute a basis for the Hilbert space. We accept the assumption that the set of eigenstates of an hermitian operator form a Hilbert space basis.

The set of postulates given above say nothing about time dependence (dynamics). We assume that the physical system can change in time, in the sense that the state vector $|\Psi(t)\rangle$ is a function of time. Time plays a special role in quantum mechanics, it is not considered a physical observable (operator) but instead is treated as a classical variable, or parameter.

If the state vector $|\Psi(t)\rangle$ changes in time so do the probability amplitudes $\langle a_n|\Psi(t)\rangle$. The time evolution of the state $|\Psi(t)\rangle$ is not arbitrary but must satisfy the Schrodinger equation

Postulate V The state vector for a quantum system undergoes temporal evolution according to the relation

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = H|\Psi(t)\rangle \quad (18)$$

where the operator H is called the Hamiltonian operator. In many important cases the Hamiltonian operator is hermitian, and represents the conserved total energy.

For a hermitian Hamiltonian, find the time evolution equation for the state $\langle \Psi(t)|$ that is dual to $|\Psi(t)\rangle$.

Expectation value and variance

According to the above discussion the state vector $|\Psi(t)\rangle$ obeys the Schrodinger equation and provides a deterministic description for the state vector. However, according to postulate III we can only obtain probabilities for a measurement to yield a given allowed value (eigenvalue). In general this probability is time-dependent, since the inner product, for the amplitude

$$c_n(t) \equiv \langle n|\Psi(t)\rangle \quad (19)$$

is an explicit function of time. It is a central goal of the physicist making observations on the quantum system to predict these amplitudes. It is useful to introduce the notion of an ensemble when measuring outcomes that are probabilistic. An ensemble is a collection of identical systems. By identical we mean, at given time t , each measurement is on a system with the identical state vector $|\Psi(t)\rangle$. We can then define an average, or mean, value for the ensemble outcomes,

$$\langle \hat{O} \rangle \equiv \sum_i p_i O_i \quad (20)$$

In this notation O_i represents the value of possible outcomes, for operator \hat{O} , and p_i is the probability for the i 'th outcome to occur. The experimenter can estimate p_i by using the central limit theorem for frequency of occurrences. If, out of all N members of the ensemble, a small subset n_i yield the value O_i , probability p_i is approximated by the ratio n_i/N . The value obtained becomes more accurate as $N \rightarrow \infty$. Note, this prescription requires that $\sum_i p_i = 1$. Quantum mechanics tells us that

$$p_i(t) = |\langle O_i | \Psi(t) \rangle|^2 = \langle O_i | \Psi(t) \rangle \langle \Psi(t) | O_i \rangle \quad (21)$$

where we have allowed explicit time dependence. We then get,

$$\langle \hat{O} \rangle = \sum_i \langle O_i | \Psi(t) \rangle \langle \Psi(t) | O_i \rangle O_i \quad (22)$$

but this is the same as,

$$\langle \hat{O} \rangle = \sum_i \langle O_i | \hat{O} | \Psi(t) \rangle \langle \Psi(t) | O_i \rangle = \langle \Psi(t) | O_i \rangle \langle O_i | \hat{O} | \Psi(t) \rangle$$

using Dirac's associative multiplication axiom and assuming closure $\sum_i |O_i\rangle \langle O_i| = \hat{I}$ we obtain

$$\langle \hat{O}(t) \rangle = \langle \Psi(t) | \hat{O} | \Psi(t) \rangle \quad (23)$$

It is also useful to measure how far one is away, on the average, from the average value $\langle \hat{O} \rangle$. This measure is called the variance and is related to the mean standard deviation. We define

$$\begin{aligned} \sigma^2 &\equiv \langle (\langle \hat{O} \rangle - \hat{O})^2 \rangle = \langle \langle \hat{O} \rangle^2 - \langle \hat{O} \rangle \hat{O} - \hat{O} \langle \hat{O} \rangle + \hat{O}^2 \rangle \\ &= \langle \hat{O}(t)^2 \rangle - \langle \hat{O}(t) \rangle^2 \end{aligned} \quad (24)$$