Notes on Selected topics to accompany Sakurai's "Modern Quantum Mechanics"

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Linear vector space and Hilbert space

In quantum mechanics, we encounter kets that represent the state of a system. A ket is an abstract entity denoted by the symbol $|\cdot\rangle$. Inside the symbol, one can include any information that corresponds uniquely to the state of the system. Typically, one mentions the eigenvalue of an observable (as in $|Z+\rangle$, where $Z+$ implies that in this state, the value of the observable S_z is $+\hbar/2$) or a quantum number (as in $|n\rangle$, seen in the particle in a box or harmonic oscillator problem).

Even though the ket is an abstract quantity, one can form a vector space (denoted by $\mathbb{V}$), where each element is a ket. In order to define such a vector space, it should be possible to define the following two *binary operations*:

1. a rule for addition of kets so that for any two kets, $|1\rangle$ and $|2\rangle$

$$|1\rangle + |2\rangle \in \mathbb{V}; \quad \text{if } |1\rangle, |2\rangle \in \mathbb{V}$$

2. a rule for scalar multiplication of a ket by a number c

$$c|1\rangle \in \mathbb{V}; \quad \text{if } |1\rangle \in \mathbb{V}$$

It is important to note that the operations defined above (ket addition and scalar multiplication) do not mean that the corresponding states add up, get multiplied, or anything like that. We could have chosen different symbols for addition and multiplication too. Individually, these two binary operations are not physically relevant, but when they are combined, one can define a linear superposition of kets that can correspond to a physical state of the system. So, properties (1) and (2) are prerequisites to define a superposition of kets.

$$|\alpha\rangle = \sum_{k=1}^{N} c_k |k\rangle.$$

Since a linear combination of basis kets, $|1\rangle \ldots |N\rangle$, is defined in the same space that contains the basis, we will call our vector space, $\mathbb{V}$, as linear vector space. From our knowledge of vector algebra, we already know that for a superposition to be meaningful (*i.e.* devoid of redundancy), the basis kets should be linearly independent.

In vector algebra, our basis kets are the three orthogonal unit vectors in real space. In mathematical terms, the three-dimensional vector space is defined over the real number field, $\mathbb{R}$. For application in quantum mechanics, we need the linear vector space to be of arbitrary dimension, *i.e.* N can be any integer, even much greater than 3. Further, we will also assume that the linear expansion coefficients, c_k, are complex numbers. With these two assumptions we can call the linear vector space as the Hilbert space (or the ket space). So, a Hilbert space is an N-dimensional linear vector space defined over the complex number field, $\mathbb{C}$. In some text books a Hilbert space may be denoted by the symbol $\mathbb{H}$ or $\mathbb{C}^N$.

Hilbert space axioms

For any three kets, $|1\rangle$, $|2\rangle$, and $|3\rangle$, in $\mathbb{H}$, and two complex numbers, c_1 and c_2, the following axioms are defined

1. Both the binary operations defined above are commutative

$$\begin{aligned} |1\rangle + |2\rangle &= |2\rangle + |1\rangle \\ c|k\rangle &= |k\rangle c \end{aligned}$$

2. Addition of kets is associative

$$|1\rangle + (|2\rangle + |3\rangle) = (|1\rangle + |2\rangle) + |3\rangle$$

3. Scalar multiplication is distributive over addition of kets

$$c\left(|1\rangle + |2\rangle\right) = c|1\rangle + c|2\rangle$$

4. Scalar multiplication is distributive over addition of scalars

$$(c_1 + c_2)\,|k\rangle = c_1|k\rangle + c_2|k\rangle$$

5. Scalar multiplication is associative in multiplication of scalars

$$c_1\left(c_2|k\rangle\right) = (c_1 c_2)\,|k\rangle$$

6. There is an identity element (zero ket or null ket, $|\text{null}\rangle$) for addition of kets (which is the first binary operation required to define a vector space).

$$|k\rangle + |\text{null}\rangle \quad = \quad |k\rangle;\, \forall |k\rangle \in \mathbb{H}$$

The symbol $\forall$ stands for *for all* and the symbol $\in$ stands for *in* or *belongs to*.

7. Every ket in H has its own inverse ket in H with respect to addition. The sum of a ket and its inverse gives the null ket (the identity element with respect to ket addition).

$$|k\rangle + (-|k\rangle) \quad = \quad |\text{null}\rangle;\, \forall |k\rangle \in \mathbb{H}$$

8. There is an identity element for scalar multiplication (the second binary operation required to define a vector space). This means that the there is a scalar $c = 1$ so that

$$1|k\rangle \quad = \quad |k\rangle;\, \forall |k\rangle \in \mathbb{H}$$

An important point to note is that there is no equivalent of Axiom-2 for the identity element for scalar multiplication. What this means is that for every ket, there is no inverse ket so that the identity element for scalar multiplication 1 can be obtained. To define such an operation, we have to define the Hermitian adjoint of a ket, $|k\rangle$, called a bra, denoted by $\langle k|$. For a Hilbert space, $\mathbb{H}$, one can define its dual, $\mathbb{H}^\dagger$, by considering a dual of every ket, $|k\rangle$, in $\mathbb{H}$ denoted by the symbol bra, $\langle k|$. The dual of the ket $c|k\rangle$ is $(c|k\rangle)^\dagger = (|k\rangle)^\dagger (c)^\dagger = \langle k|c^* = c^*\langle k|$.

Using a ket and its dual, we can define other types of products encountered in quantum mechanics.

Inner product

The field of the Hilbert space is the complex field, there each element is a complex number that can be defined as an inner product of a ket and a dual (of the same ket or a different ket) denoted by the symbol $\langle j|k\rangle$. Some of the properties of an inner product are as follows

1. Inner product is skew-symmetric.

$$\langle j|k\rangle^* = \langle k|j\rangle$$

2. Inner product is positive semi-definite

$$\langle j|k\rangle \geq 0$$

If $\langle j|k\rangle = 0$, then we say that the kets $|j\rangle$ and $|k\rangle$ are orthogonal or linearly indepedent.

3. Inner product is linear

$$\langle i| \left(c_1|j\rangle + c_2|k\rangle\right) = c_1\langle i|j\rangle + c_2\langle i|k\rangle$$

The norm of a ket is a real number defined in terms of its inner product

$$\text{Norm}\left(|k\rangle\right) = \sqrt{\langle k|k\rangle}$$

When the norm of a ket is 1, we call the ket a normalized ket. In general, it is always possible to normalize a ket by dividing it by its norm.

$$\frac{\langle k|}{\sqrt{\langle k|k\rangle}}\frac{|k\rangle}{\sqrt{\langle k|k\rangle}} = 1$$

Outer product and its relation to operators

Suppose we change the order in which the ket and the bra appear in the inner product, we get an outer product, $|j\rangle\langle k|$, which is no longer a scalar.

We can see that an outer product is an *operator* that when acted on a ket changes it to another ket.

$$\left(|j\rangle\langle k|\right)|i\rangle = |j\rangle\langle k|i\rangle = |j\rangle c = c|j\rangle$$

What's going on is that, an outer product acting on a ket scales the ket part of the outer product. While $|j\rangle\langle k|$ acting on $|i\rangle$ has resulted in a multiple of $|j\rangle$, we cannot be sure if all components of $|i\rangle$ along $|j\rangle$ is captured by the scalar $c = \langle k|i\rangle$.

Using this example, we can understand the effect of acting an operator on a ket. An operator acting on a ket gives another ket.

$$\hat{O}|i\rangle = |j\rangle$$

A special class of outer product is when both the bra and the ket parts are dual pairs. Such an outer product is called the projection operator of the ket.

$$\hat{P}_{|j\rangle} = |j\rangle\langle j|$$

When this operator acts on $|i\rangle$, we get $\hat{P}_{|j\rangle}|i\rangle = |j\rangle\langle j|i\rangle = c|j\rangle$, where c is the projection $|i\rangle$ along $|j\rangle$.

Properties of operators

Just like a ket spaces, it is possible to define operator spaces. However, for this course, it is not important to go to that level of mathematical abstraction. It is worthwhile to note down a few essential properties of operators.

1. If an operator acting on a ket results in zero times another ket, we call the operator a null operator

$$\hat{O}|k\rangle = 0|j\rangle = 0 \Rightarrow \hat{O} = \text{null operator}$$

2. In general, sequential actions of two operators (*i.e.* their multiplication) on a ket is not commutative

$$\hat{A}\hat{B}|k\rangle \neq \hat{B}\hat{A}|k\rangle$$

   In short, we say that operator multiplication is not commutative $\hat{A}\hat{B} \neq \hat{B}\hat{A}$.

3. In general, sequential actions of three operators on a ket is associative

$$\hat{A}\hat{B}\hat{C}|k\rangle = \hat{A}\left(\hat{B}\hat{C}\right)|k\rangle = \left(\hat{A}\hat{B}\right)\hat{C}|k\rangle$$

   In short, we say that operator multiplication is associative.

4. There is an interesting property of operators that arises because of the duality between the ket space and the bra space.

$$|i\rangle = \hat{A}\hat{B}|k\rangle \Rightarrow \langle i| = \left(\hat{A}\hat{B}|k\rangle\right)^{\dagger} = \langle k|\hat{B}^{\dagger}\hat{A}^{\dagger}$$

   In short, we say $\left(\hat{A}\hat{B}\right)^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger}$.

Completeness relationship

Completeness relationship is a very useful relationship that enables transformation of expressions from one representation to another. Suppose, $|1\rangle, \ldots, |N\rangle$ form a complete set of linearly independent kets, then the sum of all their projection operators corresponds to the identity operator.

$$\sum_{k=1}^{N} |k\rangle\langle k| = \sum_{k=1}^{N} \hat{P}_k = \hat{I}$$

As an example of the application of the completeness relation, let see how we can use it to derive $\left(\hat{A}\hat{B}\right)^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger}$.

$$
\begin{aligned}
\langle\alpha|\left(\hat{A}\hat{B}\right)^{\dagger}|\beta\rangle &= \langle\beta|\hat{A}\hat{B}|\alpha\rangle^{\dagger} \\
&= \langle\beta|\hat{A}\hat{I}\hat{B}|\alpha\rangle^{\dagger} \\
&= \left(\langle\beta|\hat{A}\sum_{k=1}^{N}|k\rangle\langle k|\hat{B}|\alpha\rangle\right)^{\dagger} \\
&= \left(\sum_{k=1}^{N}\langle\beta|\hat{A}|k\rangle\langle k|\hat{B}|\alpha\rangle\right)^{\dagger} \\
&= \sum_{k=1}^{N}\langle\beta|\hat{A}|k\rangle^{\dagger}\langle k|\hat{B}|\alpha\rangle^{\dagger} \\
&= \sum_{k=1}^{N}\langle k|\hat{A}^{\dagger}|\beta\rangle\langle\alpha|\hat{B}^{\dagger}|k\rangle \\
&= \sum_{k=1}^{N}\langle\alpha|\hat{B}^{\dagger}|k\rangle\langle k|\hat{A}^{\dagger}|\beta\rangle \\
&= \langle\alpha|\hat{B}^{\dagger}\sum_{k=1}^{N}|k\rangle\langle k|\hat{A}^{\dagger}|\beta\rangle \\
&= \langle\alpha|\hat{B}^{\dagger}\hat{I}\hat{A}^{\dagger}|\beta\rangle \\
&= \langle\alpha|\hat{B}^{\dagger}\hat{A}^{\dagger}|\beta\rangle
\end{aligned}
$$