Lecture 2 (Sep. 11, 2017)

2.1 More Relevant Math

2.1.1 Inner Products

Last time, we discussed the concept of a maximally linearly independent set, which is a set $\{|\alpha_j\rangle\}$ of vectors that are linearly independent, and such that there exists no $|\beta\rangle$ such that $\{|\alpha_j\rangle, |\beta\rangle\}$ is linearly independent. In this case, $\{|\alpha_j\rangle\}$ forms a basis for V. If $|\alpha_1\rangle, \ldots, |\alpha_n\rangle$ form a basis for V, then any vector $|\beta\rangle$ can be decomposed in terms of the basis vectors as

$$|\beta\rangle = \sum_i c_i |\alpha_i\rangle \,. \tag{2.1}$$

Next, we discuss the concept of an inner product (we will assume that V is a vector space $\mathbb{C}$). A (Hermitian) *inner product* is a map $(\cdot,\cdot)\colon V \times V \to \mathbb{C}$ with the following properties:

1. For all $c \in \mathbb{C}$ and $|\alpha\rangle, |\beta\rangle \in V$, we have

$$\begin{aligned}(|\alpha\rangle, c|\beta\rangle) &= c(|\alpha\rangle, |\beta\rangle)\,,\\ (c|\alpha\rangle, |\beta\rangle) &= c^*(|\alpha\rangle, |\beta\rangle)\,,\end{aligned} \tag{2.2}$$

   where c^* is the complex conjugate of c.

2. For all $|\alpha\rangle, |\beta\rangle \in V$,

$$(|\alpha\rangle, |\beta\rangle)^* = (|\beta\rangle, |\alpha\rangle)\,. \tag{2.3}$$

3. For all $|\alpha\rangle, |\beta\rangle, |\beta'\rangle \in V$,

$$(|\alpha\rangle, |\beta\rangle + |\beta'\rangle) = (|\alpha\rangle, |\beta\rangle) + (|\alpha\rangle, |\beta'\rangle)\,. \tag{2.4}$$

4. For all $|\alpha\rangle \in V$,

$$(|\alpha\rangle, |\alpha\rangle) \geq 0\,, \tag{2.5}$$

   and if $(|\alpha\rangle, |\alpha\rangle) = 0$, then $|\alpha\rangle$ is the zero ket, $|\alpha\rangle = 0$.

Let's consider some examples. First, consider $V = \mathbb{C}^n$, whose vectors are of the form

$$|z\rangle = \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix}, \quad z_1, \ldots, z_n \in \mathbb{C}\,. \tag{2.6}$$

One definition of an inner product on this space is

$$(|z\rangle, |w\rangle) = z_1^* w_1 + z_2^* w_2 + \cdots + z_n^* w_n\,, \tag{2.7}$$

which we can check satisfies all of the required properties of an inner product.

A more exciting example is the vector space of square-integrable functions on the interval $[0, 1]$,

$$V = \left\{ f\colon [0,1] \to \mathbb{C} \;\middle|\; \int_0^1 \mathrm{d}x\; f^*(x) f(x) < \infty \right\}, \tag{2.8}$$

as we discussed in the last lecture, which can be endowed with the inner product

$$(f, g) = \int_0^1 \mathrm{d}x \; f^*(x) g(x) \,. \tag{2.9}$$

Now we introduce a bit of terminology. The vectors we have been discussing are referred to as *kets*. Two kets are *orthogonal* if $(|\alpha\rangle, |\beta\rangle) = 0$. The *norm* of a ket is given by

$$N := \sqrt{(|\alpha\rangle, |\alpha\rangle)} := \||\alpha\rangle\| \,. \tag{2.10}$$

Using this norm, we can normalize any nonzero ket by defining

$$|\tilde{\alpha}\rangle = \frac{1}{N}|\alpha\rangle \,, \tag{2.11}$$

which has

$$(|\tilde{\alpha}\rangle, |\tilde{\alpha}\rangle) = 1 \,. \tag{2.12}$$

2.1.2 Dual Space

Now we introduce the dual space. The space V that we have described so far is the space of kets $|\alpha\rangle$. The *dual space* V^* is the space of objects called *bras*, which is “dual” to the ket space. To every $|\alpha\rangle \in V$, we associate a bra $\langle\alpha| \in V^*$, and define an operation between bras and kets,

$$\langle\alpha|\beta\rangle := (|\alpha\rangle, |\beta\rangle) \,. \tag{2.13}$$

This shows us the motivation for these names: when we combine a bra and a ket, we get a “bra(c)ket.”

Consider the space of linear functionals $\gamma\colon V \to \mathbb{C}$. We introduce the notation $\gamma \to \langle\gamma|$, such that for any basis $\{|\alpha_j\rangle\}$, the statement

$$\gamma\colon |\alpha_j\rangle \mapsto c_j \tag{2.14}$$

implies that

$$\langle\gamma|\alpha_j\rangle = c_j \,. \tag{2.15}$$

We see that the dual space is just the space of linear functionals on V. The $\{\gamma\}$ form an n-dimensional vector space V^*, where $n = \dim V$. We then have a duality $V \leftrightarrow V^*$, given by $|\alpha\rangle \leftrightarrow \langle\alpha|$. Note that scalars are conjugated under this duality, so that for all $c \in \mathbb{C}$ and $|\alpha\rangle \in V$, $c|\alpha\rangle \leftrightarrow c^*\langle\alpha|$.

2.1.3 Orthonormal Bases

An *orthonormal basis* is a basis $\{|\phi_i\rangle\}$ such that

$$\langle\phi_i|\phi_j\rangle = \delta_{ij} \,, \tag{2.16}$$

where δ_{ij} is the Kronecker delta. We know that we can write any ket in the form

$$|\alpha\rangle = \sum_i c_i |\phi_i\rangle \,. \tag{2.17}$$

If the $|\phi_i\rangle$ form an orthonormal basis, then we find that $c_i = \langle\phi_i|\alpha\rangle$. Thus, if we have an orthonormal basis, then we can write any ket in the form

$$|\alpha\rangle = \sum_i |\phi_i\rangle\langle\phi_i|\alpha\rangle. \tag{2.18}$$

These is an example of a *completeness relation*.

2.1.4 Operators

Recall the second postulate of quantum mechanics: observables are represented in quantum mechanics as Hermitian operators acting on the Hilbert space $\mathcal{H}$ (from here on out, we will consider states in the Hilbert space $\mathcal{H}$ rather than an arbitrary vector space V). In order to understand this statement, we first need to understand what an operator is, and then we must understand what a Hermitian operator is.

An *operator* is an object that acts on a ket and returns another ket. Thus, if X is an operator, then X acts on a ket $|\alpha\rangle \in \mathcal{H}$ as

$$X(|\alpha\rangle) := X|\alpha\rangle \in \mathcal{H}\,, \tag{2.19}$$

where the right-hand side is a naming convention. Two operators A and B are said to be *equal* ($A = B$) if and only if $A|\alpha\rangle = B|\alpha\rangle$ for all $|\alpha\rangle \in \mathcal{H}$.

We introduce an addition operation '+' on the space of operators, which is commutative and associative: for all operators X, Y, Z, we have

$$\begin{aligned} X + Y &= Y + X\,, \\ X + (Y + Z) &= (X + Y) + Z\,. \end{aligned} \tag{2.20}$$

We will primarily be interested in linear operators: a *linear* operator X satisfies the property

$$X(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle) = c_\alpha X|\alpha\rangle + c_\beta X|\beta\rangle \tag{2.21}$$

for all $c_\alpha, c_\beta \in \mathbb{F}$ and $|\alpha\rangle, |\beta\rangle \in \mathcal{H}$. We can also define the notion of an anti-linear operator: an *anti-linear* operator X satisfies

$$X(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle) = c_\alpha^* X|\alpha\rangle + c_\beta^* X|\beta\rangle \tag{2.22}$$

for all $c_\alpha, c_\beta \in \mathbb{F}$ and $|\alpha\rangle, |\beta\rangle \in \mathcal{H}$.

We can also define an action of these same operators on the dual space, which will be a right action of the form $\langle\beta|X$ for $\langle\beta| \in \mathcal{H}^*$. We define this object via its inner product with kets, by requiring that it satisfy the property

$$(\langle\beta|X)|\alpha\rangle = \langle\beta|(X|\alpha\rangle) \tag{2.23}$$

for all $|\alpha\rangle \in \mathcal{H}$. Using an orthonormal basis $\{|\phi_j\rangle\}$, we can then express this bra as

$$\langle\beta|X = \sum_j \langle\beta|X|\phi_j\rangle\langle\phi_j|\,. \tag{2.24}$$

We also define multiplication of operators, such that for all operators X, Y and $|\alpha\rangle \in \mathcal{H}$,

$$(XY)|\alpha\rangle = X(Y|\alpha\rangle)\,. \tag{2.25}$$

This multiplication is not necessarily commutative, $XY \neq YX$, but it is associative,

$$X(YZ) = (XY)Z = XYZ\,. \tag{2.26}$$

2.1.5 Operators as Matrices in a Given Basis

In a given basis, the action of an operator can be expressed by a matrix. To see this, we first define the identity operator $\mathbb{1}$, which satisfies

$$\mathbb{1}|\alpha\rangle = |\alpha\rangle \tag{2.27}$$

for all $|\alpha\rangle \in \mathcal{H}$. Given an orthonormal basis $|\{a'\}\rangle$ (notation from Sakurai), the identity operator can be expressed in the form

$$\mathbb{1} = \sum_{a'} \big|a'\big\rangle\big\langle a'\big| \,. \tag{2.28}$$

We can use Eq. (2.28) to write any operator X in the form

$$\begin{aligned} X &= \mathbb{1}X\mathbb{1} \\ &= \left(\sum_{a'} \big|a'\big\rangle\big\langle a'\big|\right) X \left(\sum_{a''} |{*a''}\rangle\langle a''|\right) \\ &= \sum_{a',a''} \big|a'\big\rangle\big\langle a'\big|X\big|a''\big\rangle\big\langle a''\big| \,. \end{aligned} \tag{2.29}$$

Note that $\langle a'|X|a''\rangle \in \mathbb{C}$ is simply a number. Thus, all information about X is equivalently contained in the complex numbers $\langle a'|X|a''\rangle$, given any orthonormal basis $|\{a'\}\rangle$. This defines an $n \times n$ matrix with complex entries corresponding to each operator X. For this reason, we will often use the words "operator" and "matrix" interchangeably if the chosen basis is clear, even though the concept of an operator is more fundamental.

2.1.6 Adjoint Operators

For each operator X, we define its *adjoint operator* (also called the *Hermitian conjugate*) $X^\dagger$ to be the operator satisfying

$$X^\dagger|\alpha\rangle \leftrightarrow \langle\alpha|X \tag{2.30}$$

under the duality $\mathcal{H} \leftrightarrow \mathcal{H}^*$. If $X^\dagger = X$, then the operator X is called *self-adjoint* or *Hermitian*. (Note that in infinite-dimensional spaces, the concepts of self-adjointness and Hermiticity are technically distinct. We may discuss this later in the course.) Note that $(XY)^\dagger = Y^\dagger X^\dagger$. The proof of this fact is straightforward: For arbitrary $|\alpha\rangle \in \mathcal{H}$, consider the kets defined by

$$|\beta\rangle = Y|\alpha\rangle \,, \quad |\gamma\rangle = X|\beta\rangle \,. \tag{2.31}$$

Their dual bras are then defined by

$$\langle\alpha|Y^\dagger = \langle\beta| \,, \quad \langle\beta|X^\dagger = \langle\gamma| \,. \tag{2.32}$$

From these definitions, we have

$$XY|\alpha\rangle = |\gamma\rangle \,, \quad \langle\alpha|Y^\dagger X^\dagger = \langle\gamma| \,. \tag{2.33}$$

Taking the dual of the first equation in (2.33) yields

$$\langle\alpha|(XY)^\dagger = \langle\gamma| \,, \tag{2.34}$$

which we can compare with the second equation in (2.33) to yield $(XY)^\dagger = Y^\dagger X^\dagger$.

This same concept has a well-defined meaning for matrices. As we have seen, any operator has the same information content as an $n \times n$ matrix, where $n = \dim \mathcal{H}$. If M is a matrix corresponding to the operator X, then $X^\dagger$ corresponds to the matrix found by conjugating the entries of the transpose M^{T}. This matrix is denoted as $M^\dagger$, and is also called the *Hermitian conjugate*. A matrix satisfying $M^\dagger = M$ is called a *Hermitian* matrix.

2.1.7 Operator Examples

As a first example of an operator, we define the outer product. Given a ket $|\alpha\rangle \in \mathcal{H}$ and a bra $\langle\beta| \in \mathcal{H}^*$, we define the operator

$$\mathcal{O} = |\alpha\rangle\langle\beta| \tag{2.35}$$

to be their *outer product*. This is an operator: for all $|\gamma\rangle \in \mathcal{H}$, we have

$$\mathcal{O}|\gamma\rangle = |\alpha\rangle\langle\beta|\gamma\rangle\,. \tag{2.36}$$

Taking the dual of this equation, we find

$$\begin{aligned}\langle\gamma|\mathcal{O}^\dagger &= \langle\beta|\gamma\rangle^*\langle\alpha| \\ &= \langle\gamma|\beta\rangle\langle\alpha|\,,\end{aligned} \tag{2.37}$$

and so we conclude that

$$\mathcal{O}^\dagger = |\beta\rangle\langle\alpha|\,. \tag{2.38}$$

As a second example, consider the Hilbert space $\mathcal{H}$ of square-integrable functions on $(-\infty, \infty)$, with inner product

$$\langle f_1|f_2\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\; f_1^*(x) f_2(x) \tag{2.39}$$

for $|f_1\rangle, |f_2\rangle \in \mathcal{H}$. Now consider the operator $A = \frac{\mathrm{d}}{\mathrm{d}x}$. Using integration by parts, we see that

$$\int_{-\infty}^{\infty} \mathrm{d}x\; f_1^*(x)\frac{\mathrm{d}}{\mathrm{d}x} f_2(x) = \int_{-\infty}^{\infty} \mathrm{d}x \left(-\frac{\mathrm{d}}{\mathrm{d}x} f_1^*(x)\right) f_2(x)\,, \tag{2.40}$$

telling us that

$$\left\langle f_1 \middle| \frac{\mathrm{d}}{\mathrm{d}x} \middle| f_2 \right\rangle = -\left\langle f_2 \middle| \frac{\mathrm{d}}{\mathrm{d}x} \middle| f_1 \right\rangle^*. \tag{2.41}$$

Thus,

$$\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^\dagger = -\frac{\mathrm{d}}{\mathrm{d}x}\,. \tag{2.42}$$

Operators satisfying $A^\dagger = -A$ are called *anti-Hermitian*. We can make this into a Hermitian operator by multiplying it by the imaginary unit (or its negative):

$$\left(-i\frac{\mathrm{d}}{\mathrm{d}x}\right)^\dagger = -i\frac{\mathrm{d}}{\mathrm{d}x}\,. \tag{2.43}$$

You may recognize this as the momentum operator in one-dimensional quantum mechanics.

A third example is the identity operator $\mathbb{1}$, which we have already seen.

For some operators, we can define an inverse operator: for an operator A, its inverse operator A^{-1} (if it exists) satisfies

$$A^{-1}A = AA^{-1} = \mathbb{1}\,. \tag{2.44}$$

Inverse operators are not guaranteed to exist.

Of special interest to us are unitary operators: a *unitary* operator U is one that satisfies $U^{-1} = U^\dagger$. These are useful because they preserve the inner product:

$$\Big(\langle\beta|U^\dagger\Big)(U|\alpha\rangle) = \langle\beta|U^{-1}U|\alpha\rangle = \langle\beta|\alpha\rangle\,. \tag{2.45}$$

We are also interested in *projection* operators, which are operators A satisfying $A^2 = A$. An example of a projection operator is $A = |\alpha\rangle\langle\alpha|$, for some $|\alpha\rangle \in \mathcal{H}$.

2.1.8 Eigenstates and Eigenvalues

If, for some operator A and ket $|\alpha\rangle \in \mathcal{H}$, we have

$$A|\alpha\rangle = a|\alpha\rangle\,, \tag{2.46}$$

with $a \in \mathbb{C}$, then $|\alpha\rangle$ is an *eigenket* or *eigenstate* of the operator A, with *eigenvalue* a. The *spectrum* of an operator A is the set of its eigenvalues $\{a\}$.

We now prove an important theorem regarding the eigenkets and eigenvalues of Hermitian operators.

Theorem 1 (Spectral Theorem)**.** *If A is a Hermitian operator, $A = A^\dagger$, then*

1. *all eigenvalues a_i of A are real, and*
2. *eigenkets of A with distinct eigenvalues are orthogonal.*

Proof. Suppose that for some Hermitian operator A and kets $|a'\rangle, |a''\rangle \in \mathcal{H}$ we have

$$A\big|a'\big\rangle = a'\big|a'\big\rangle\,, \tag{2.47a}$$
$$\big\langle a''\big|A = \big\langle a''\big|(a'')^*\,. \tag{2.47b}$$

Multiplying Eq. (2.47a) by $\langle a''|$ on the left and multiplying Eq. (2.47b) by $|a'\rangle$ on the right yields

$$\big\langle a''\big|A\big|a'\big\rangle = a'\big\langle a''\big|a'\big\rangle\,, \tag{2.48a}$$
$$\big\langle a''\big|A\big|a'\big\rangle = \big(a''\big)^*\big\langle a''\big|a'\big\rangle\,. \tag{2.48b}$$

Comparing Eqs. (2.48a) and (2.48b), we see that

$$\big[\big(a''\big)^* - a'\big]\big\langle a''\big|a'\big\rangle = 0\,. \tag{2.49}$$

If $|a'\rangle = |a''\rangle$, then this proves that $(a')^* = a'$, which means that $a' \in \mathbb{R}$. If $|a'\rangle \neq |a''\rangle$ and we have $a' \neq a''$, then this proves that $\langle a''|a'\rangle = 0$, i.e., $|a'\rangle$ and $|a''\rangle$ are orthogonal. This completes the proof. □

If we normalize each eigenket $|a_i\rangle$ of a Hermitian operator, so that $\langle a_i|a_i\rangle = 1$, and have chosen the eigenkets so that distinct eigenkets with the same eigenvalue are orthogonal, then Thm. 1 tells us that we have

$$\langle a_i|a_j\rangle = \delta_{ij}\,, \tag{2.50}$$

i.e., the normalized eigenkets are orthonormal. We can then decompose

$$A = \sum_a a|a\rangle\langle a|\,. \tag{2.51}$$

We can check that for some eigenket $|b\rangle$, we have

$$A|b\rangle = \sum_a a|a\rangle\langle a|b\rangle = \sum_a a|a\rangle\delta_{ab} = b|b\rangle\,. \tag{2.52}$$

Note that the equation

$$\mathbb{1} = \sum_a |a\rangle\langle a| \tag{2.53}$$

is simply a special case of Eq. (2.51).