1.2: Operators in Hilbert Space

The objects $|\psi\rangle$ are vectors in a Hilbert space. We can imagine applying rotations of the vectors, rescaling, permutations of vectors in a basis, and so on. These are described mathematically as operators, and we denote them by capital letters A, B, C, etc. In general we write

$$A|\phi\rangle = |\psi\rangle \tag{1.6}$$

for some $|\phi\rangle, |\psi\rangle \in \mathcal{V}$. It is important to remember that operators act on all the vectors in Hilbert space. Let $\{|\phi_j\rangle\}_j$ be an orthonormal basis. We can calculate the inner product between the vectors $|\phi_j\rangle$ and A $|\phi_k\rangle$:

$$\langle\phi_j|\left(A\,|\phi_k\rangle\right) = \langle\phi_j|A|\phi_k\rangle \equiv A_{jk} \tag{1.7}$$

The two indices indicate that operators are matrices.

As an example, consider two vectors, written as two-dimensional column vectors

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.8}$$

and suppose that

$$A = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} \tag{1.9}$$

We calculate

$$A_{11} = \langle\phi_1|A|\phi_1\rangle = (1,0)\cdot\begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = (1,0)\cdot\begin{pmatrix} 2 \\ 0 \end{pmatrix} = 2 \tag{1.10}$$

Similarly, we can calculate that $A_{22} = 3$, and $A_{12} = A_{21} = 0$ (check this). We therefore have that $A\,|\phi_1\rangle = 2\,|\phi_1\rangle$ and $A\,|\phi_2\rangle = 3\,|\phi_2\rangle$.

Complex numbers a have complex conjugates a^* and vectors $|\psi\rangle$ have dual vectors $\langle\phi|$. Is there an equivalent for operators? The answer is yes, and it is called the adjoint, or Hermitian conjugate, and is denoted by a dagger †. The natural way to define it is according to the rule

$$\langle\psi|A|\phi\rangle^* = \left\langle\phi\left|A^\dagger\right|\psi\right\rangle \tag{1.11}$$

for any $|\phi\rangle$ and $|\psi\rangle$. In matrix notation, and given an orthonormal basis $\{|\phi_j\rangle\}_j$, this becomes

$$\langle\phi_j|A|\phi_k\rangle^* = A^*_{jk} = \left\langle\phi_k\left|A^\dagger\right|\phi_j\right\rangle = A^\dagger_{kj} \tag{1.12}$$

So the matrix representation of the adjoint $A^\dagger$ is the transpose and the complex conjugate of the matrix A, as given by $\left(A^\dagger\right)_{jk} = A^*_{kj}$. The adjoint has the following properties:

1. $(cA)^\dagger = c^* A^\dagger$,
2. $(AB)^\dagger = B^\dagger A^\dagger$,
3. $(|\phi\rangle)^\dagger = \langle\phi|$.

Note the order of the operators in 2: AB is generally not the same as BA. The difference between the two is called the commutator, denoted by

$$[A,B] = AB - BA \tag{1.13}$$

For example, we can choose

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.14}$$

which leads to

$$\begin{aligned}[A,B] &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} \neq 0. \end{aligned} \tag{1.15}$$

Many, but not all, operators have an inverse. Let $A|\phi\rangle = |\psi\rangle$ and $B|\psi\rangle = |\phi\rangle$. Then we have

$$BA|\phi\rangle = |\phi\rangle \quad \text{and} \quad AB|\psi\rangle = |\psi\rangle \tag{1.16}$$

If Eq. (1.16) holds true for all $|\phi\rangle$ and $|\psi\rangle$, then B is the inverse of A, and we write $B = A^{-1}$. An operator that has an inverse is called invertible. Another important property that an operator may possess is positivity. An operator is positive if

$$\langle\phi|A|\phi\rangle \geq 0 \quad \text{for all } |\phi\rangle \tag{1.17}$$

We also write this as $A \geq 0$.

From the matrix representation of operators you can easily see that the operators themselves form a linear vector space:

1. $A + B = B + A$,
2. $A + (B + C) = (A + B) + C$,
3. $a(A + B) = aA + aB$,
4. $(a + b)A = aA + bA$,
5. $a(bA) = (ab)A$.

We can also define the operator norm $\|A\|$ according to

$$\|A\| = \sqrt{\mathrm{Tr}\left(A^\dagger A\right)} \equiv \sqrt{\sum_{ij} A^*_{ij} A_{ji}}, \tag{1.18}$$

which means that the linear vector space of operators is again a Hilbert space. The symbol Tr(.) denotes the trace of an operator, and we will return to this special operator property later in this section.

Every operator has a set of vectors for which

$$A\left|a_j\right\rangle = a_j\left|a_j\right\rangle, \quad \text{with } a_j \in \mathbb{C} \tag{1.19}$$

This is called the eigenvalue equation (or eigenequation) for A, and the vectors $|a_j\rangle$ are the eigenvectors. The complex numbers a_j are eigenvalues. In the basis of eigenvectors, the matrix representation of A becomes

$$A = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_N \end{pmatrix} \tag{1.20}$$

When some of the a_js are the same, we speak of degenerate eigenvalues. When there are n identical eigenvalues, we have n-fold degeneracy. The eigenvectors corresponding to this eigenvalue then span an n-dimensional subspace of the vector space. We will return to subspaces shortly, when we introduce projection operators.

For any orthonormal basis $\{|\phi_j\rangle\}_j$ we have

$$\langle\phi_j|A|\phi_k\rangle = A_{jk} \tag{1.21}$$

which can be written in the form

$$A = \sum_{jk} A_{jk}\left|\phi_j\right\rangle\left\langle\phi_k\right| \tag{1.22}$$

For the special case where $|\phi_j\rangle = |a_j\rangle$ this reduces to

$$A = \sum_j a_j\left|a_j\right\rangle\left\langle a_j\right| \tag{1.23}$$

This is the spectral decomposition of A. When all a_j are equal, we have complete degeneracy over the full vector space, and the operator becomes proportional (up to a factor a_j) to the identity $\mathbb{I}$.

Note that this is independent of the basis $\{|a_j\rangle\}$. As a consequence, for any orthonormal basis $\{|\phi_j\rangle\}$ we have

$$\mathbb{I}=\sum_j |\phi_j\rangle\langle\phi_j| \tag{1.24}$$

This is the completeness relation, and we will use this many times in our calculations.

Lemma

If two non-degenerate operators commute ($[A,B]=0$), then they have a common set of eigenvectors.

Proof

Let $A=\sum_k a_k|a_k\rangle\langle a_k|$ and $B=\sum_{jk} B_{jk}|a_j\rangle\langle a_k|$. We can choose this without loss of generality: we write both operators in the eigenbasis of A. Furthermore, $[A,B]=0$ implies that $AB=BA$.

$$\begin{aligned} AB&=\sum_{klm} a_k B_{lm}|a_k\rangle\langle a_k \mid a_l\rangle\langle a_m|=\sum_{lm} a_l B_{lm}|a_l\rangle\langle a_m| \\ BA&=\sum_{klm} a_k B_{lm}|a_l\rangle\langle a_m \mid a_k\rangle\langle a_k|=\sum_{lm} a_m B_{lm}|a_l\rangle\langle a_m| \end{aligned} \tag{1.25}$$

Therefore

$$[A,B]=\sum_{lm}\left(a_l-a_m\right)B_{lm}|a_l\rangle\langle a_m|=0 \tag{1.26}$$

If $a_l\neq a_m$ for $l\neq m$, then $B_{lm}=0$, and $B_{lm}\propto\delta_{lm}$. Therefore $\{|a_j\rangle\}$ is an eigenbasis for B.

The proof of the converse is left as an exercise. It turns out that this is also true when A and/or B are degenerate.