15.6 The Spectral Theorem

While we could prove that Hermitian operators are unitarily diagonalizable, this result holds for the more general class of *normal* operators. The proof in the more general case is not harder than the one for Hermitian operators. An operator M is said to be **normal** if it commutes with its adjoint:

$$M \text{ is normal}: \quad [M^\dagger, M] = 0. \tag{15.6.1}$$

Hermitian operators are clearly normal. So are anti-Hermitian operators ($M^\dagger = -M$ means M is anti-Hermitian). Unitary operators U are normal because $U^\dagger U = UU^\dagger = \mathbb{1}$, showing that U and $U^\dagger$ commute. If an operator is normal, a similarity transformation with a unitary operator gives another normal operator:

Exercise 15.3. *If M is normal, show that $V^\dagger MV$, where V is a unitary operator, is also normal.*

It is a useful fact that a normal operator T and its adjoint $T^\dagger$ share the same set of eigenvectors:

Lemma. *Let w be an eigenvector of the normal operator M: $Mw = \lambda w$. Then w is also an eigenvector of $M^\dagger$ with a complex conjugate eigenvalue:*

$$M^\dagger w = \lambda^* w. \tag{15.6.2}$$

Proof. Define $u = (M^\dagger - \lambda^* \mathbb{1})w$. The result holds if u is the zero vector. To show this we compute the norm squared of u:

$$\langle u, u\rangle \;=\; \langle (M^\dagger - \lambda^*\mathbb{1})w, (M^\dagger - \lambda^*\mathbb{1})w\rangle. \tag{15.6.3}$$

Using the adjoint property to move the operator in the first entry to the second entry,

$$\langle u, u\rangle \;=\; \langle w, (M - \lambda\mathbb{1})(M^\dagger - \lambda^*\mathbb{1})w\rangle. \tag{15.6.4}$$

Since M and $M^\dagger$ commute, so do the two factors in parentheses, and therefore,

$$\langle u, u\rangle = \langle w, (M^\dagger - \lambda^* \mathbb{1})(M - \lambda\mathbb{1})w\rangle = 0, \tag{15.6.5}$$

since $(M - \lambda\mathbb{1})$ kills w. It follows that $u = 0$ and therefore (15.6.2) holds.

□

We can now state the main result: the **spectral theorem**. It states that a matrix is unitarily diagonalizable if and only if it is normal. We will prove this result for finite-dimensional matrices.

Theorem 15.6.1. Spectral theorem. *Let M be an operator in a finite-dimensional complex vector space. The vector space has an orthonormal basis of M eigenvectors if and only if M is normal.*

Proof. It is easy to show that if M is unitarily diagonalizable, it is normal. Indeed, from (15.5.8), when M is unitarily diagonalizable, there is a unitary U such that

$$M = UD_M U^\dagger \text{ and therefore } M^\dagger = UD_M^\dagger U^\dagger.$$

We then get

$$M^\dagger M = UD_M^\dagger D_M U^\dagger \quad \text{and} \quad MM^\dagger = UD_M D_M^\dagger U^\dagger,$$

so that

$$[M^\dagger, M] = U(D_M^\dagger D_M - D_M D_M^\dagger)U^\dagger = 0$$

because any two diagonal matrices commute.

We must now prove that for any normal M, viewed as a matrix on an arbitrary orthonormal basis, there is a unitary matrix U such that $U^\dagger MU$ is diagonal. By our general discussion, this implies that the eigenvectors of M are an orthonormal basis. We will prove this by induction in the dimension of the vector space where the result holds.

The result is clearly true for $\dim V = 1$: any 1×1 matrix is normal and automatically diagonal. We now assume that a normal matrix in an $(n-1)$-dimensional vector space is unitarily diagonalizable and try to prove the same is true for a normal matrix in an n-dimensional space.

Let M be an $n \times n$ normal matrix referred to the orthonormal basis ($|1\rangle$, …, $|n\rangle$) of V so that $M_{ij} = \langle i|M|j\rangle$. We know there is at least one eigenvalue λ_1 of M with a nonzero eigenvector $|x_1\rangle$ of unit norm:

$$M|x_1\rangle = \lambda_1|x_1\rangle \quad \text{and} \quad M^\dagger|x_1\rangle = \lambda_1^*|x_1\rangle, \tag{15.6.6}$$

in view of the lemma. We claim now that there is a unitary matrix U_1 such that

$$|x_1\rangle = U_1|1\rangle \quad \Rightarrow \quad U_1^\dagger|x_1\rangle = |1\rangle. \tag{15.6.7}$$

U_1 is not unique and can be constructed as follows: Take $|x_1\rangle$ and $n - 1$ additional vectors that together span V and use the Gram-Schmidt procedure to construct an orthonormal basis $|x_1\rangle$, …, $|x_n\rangle$. Then write $U_1 = \sum_i |x_i\rangle\langle i|$ that, as required, maps $|1\rangle$ to $|x_1\rangle$.

Now define

$$M_1 \equiv U_1^\dagger M U_1. \tag{15.6.8}$$

M_1 is also normal, and $M_1|1\rangle = U_1^\dagger M U_1|1\rangle = U_1^\dagger M|x_1\rangle = \lambda_1 U_1^\dagger|x_1\rangle = \lambda_1|1\rangle$ so that

$$M_1|1\rangle = \lambda_1|1\rangle, \tag{15.6.9}$$

which says that the first column of M_1 has zeroes in all entries except the first. Indeed,

$$\langle j|M_1|1\rangle = \lambda_1\langle j|1\rangle = \lambda_1\delta_{1,j}. \tag{15.6.10}$$

The normality of M_1 implies that the first row of M_1 is also zero except for the first element. Indeed,

$$\langle 1|M_1|j\rangle = (\langle j|M_1^\dagger|1\rangle)^* = (\lambda_1^*\langle j|1\rangle)^* = \lambda_1\langle 1|j\rangle = \lambda_1\delta_{1,j}, \tag{15.6.11}$$

where we used $M_1^\dagger|1\rangle = \lambda_1^*|1\rangle$, which follows from the lemma. It follows from the last two equations that M_1, in the original basis, takes the form

$$M_1 = \left(\begin{array}{c|ccc} \lambda_1 & 0 & \dots & 0 \\ \hline 0 & & & \\ \vdots & & M' & \\ 0 & & & \end{array}\right),$$

where M' is an $(n-1)$ by $(n-1)$ matrix. Since M_1 is normal and matrices multiply in blocks, one can quickly see that M' is also normal. By the induction hypothesis, M' can be unitarily diagonalized, so there exists an $(n-1)$ by $(n-1)$ unitary matrix U' such that $U'^{\dagger}M'U'$ is diagonal:

$$U'^{\dagger}M'U' = D_{M'}, \quad \text{with } D_{M'} \text{ diagonal.} \tag{15.6.12}$$

The matrix U' can be extended to an n by n unitary matrix $\hat{U}$ as follows:

$$\hat{U} = \left(\begin{array}{c|ccc} 1 & 0 & \dots & 0 \\ \hline 0 & & & \\ \vdots & & U' & \\ 0 & & & \end{array}\right). \tag{15.6.13}$$

We can now confirm that $\hat{U}$ diagonalizes M_1—that is, $\hat{U}^{\dagger}M_1\hat{U}$ is a diagonal matrix D_M:

$$\begin{aligned} \hat{U}^{\dagger}M_1\hat{U} &= \left(\begin{array}{c|ccc} 1 & 0 & \dots & 0 \\ \hline 0 & & & \\ \vdots & & U'^{\dagger} & \\ 0 & & & \end{array}\right)\left(\begin{array}{c|ccc} \lambda_1 & 0 & \dots & 0 \\ \hline 0 & & & \\ \vdots & & M' & \\ 0 & & & \end{array}\right)\left(\begin{array}{c|ccc} 1 & 0 & \dots & 0 \\ \hline 0 & & & \\ \vdots & & U' & \\ 0 & & & \end{array}\right) \\ &= \left(\begin{array}{c|ccc} \lambda_1 & 0 & \dots & 0 \\ \hline 0 & & & \\ \vdots & & U'^{\dagger}M'U' & \\ 0 & & & \end{array}\right) = \left(\begin{array}{c|ccc} \lambda_1 & 0 & \dots & 0 \\ \hline 0 & & & \\ \vdots & & D_{M'} & \\ 0 & & & \end{array}\right) = D_M. \end{aligned} \tag{15.6.14}$$

But then, using the definition of M_1,

$$D_M = \hat{U}^{\dagger}M_1\hat{U} \;=\; \hat{U}^{\dagger}U_1^{\dagger}M\,U_1\hat{U} \;=\; (U_1\hat{U})^{\dagger}M\,(U_1\hat{U}). \tag{15.6.15}$$

Since the product of unitary matrices is unitary, $\tilde{U} \equiv U_1\hat{U}$ is unitary, and we have shown that $\tilde{U}^{\dagger}M\tilde{U}$ is diagonal. This is the desired result. We have used the induction hypothesis to prove that an n by n normal matrix M is unitarily diagonalizable. This completes the induction argument and thus the proof.

□

This theorem implies that Hermitian and unitary operators are unitarily diagonalizable: their eigenvectors can be chosen to form an orthonormal basis. The proof did not require a separate discussion of degeneracies. If an eigenvalue of M is degenerate and appears k times, then k orthonormal eigenvectors are associated with the corresponding k-dimensional, M-invariant subspace of the vector space.

Let us now describe the general situation we encounter when diagonalizing a normal operator T on a vector space V. In general, we expect degeneracies in the eigenvalues so that each eigenvalue λ_k is repeated $d_k \geq 1$ times. An eigenvalue λ_k is degenerate if $d_k > 1$. It follows that V has T-invariant subspaces of different dimensionalities. Let U_k denote the T-invariant subspace of dimension $d_k \geq 1$ spanned by eigenvectors with eigenvalue λ_k:

$$U_k \equiv \{v \in V \mid Tv = \lambda_k v\}, \quad \dim U_k = d_k. \tag{15.6.16}$$

By the spectral theorem, U_k has a basis comprised by d_k orthonormal eigenvectors:

$$(u_1^{(k)}, \ldots, u_{d_k}^{(k)}).$$

The full space V is decomposed as the direct sum of the invariant subspaces of T:

$$V = U_1 \oplus \cdots \oplus U_m, \quad \dim V = \sum_{i=1}^{m} d_i, \ m \geq 1. \tag{15.6.17}$$

All U_i subspaces are guaranteed to be orthogonal to each other. In fact, the full list of eigenvectors is a list of orthonormal vectors that form a basis for V and is conveniently ordered as follows:

$$(u_1^{(1)}, \ldots, u_{d_1}^{(1)}, \ldots, u_1^{(m)}, \ldots, u_{d_m}^{(m)}). \tag{15.6.18}$$

The matrix T is manifestly diagonal in this basis because each vector above is an eigenvector of T. The matrix representation of T reads

$$T = \operatorname{diag}\,(\underbrace{\lambda_1, \ldots, \lambda_1}_{d_1 \text{ times}}, \ldots, \underbrace{\lambda_m, \ldots, \lambda_m}_{d_m \text{ times}}). \tag{15.6.19}$$

This is clear because the first d_1 vectors in the list are in U_1, the second d_2 vectors are in U_2, and so on until the last d_m vectors are in U_m.

Let us now consider the uniqueness of the basis (15.6.18). In other words, we ask how much we can change the basis vectors without changing the matrix representation of T. If we have no degeneracies in the spectrum of T ($d_i = 1$, for all i), each basis vector can at most be multiplied by a phase. On the other hand, with degeneracies the list can be changed considerably without changing the matrix representation of T. Let V_k be a unitary operator on U_k—namely, V_k: $U_k \to U_k$ for each $k = 1, \ldots, m$. We claim that the following basis of eigenvectors leads to the same matrix T:

$$\big(V_1 u_1^{(1)}, \ldots, V_1 u_{d_1}^{(1)}, \ldots\ldots, V_m u_1^{(m)}, \ldots, V_m u_{d_m}^{(m)} \big). \tag{15.6.20}$$

This is still a collection of orthonormal T eigenvectors because the first d_1 vectors are still orthonormal eigenvectors in U_1, the second d_2 vectors are still orthonormal eigenvectors in U_2, and so on. More explicitly, we can calculate the matrix elements of T within U_k in the new basis:

$$\langle\, V_k u_i^{(k)},\, T(V_k u_j^{(k)})\,\rangle \;=\; \lambda_k \,\langle\, V_k u_i^{(k)},\, V_k u_j^{(k)} \rangle \;=\; \lambda_k \langle\, u_i^{(k)},\, u_j^{(k)} \rangle \;=\; \lambda_k \delta_{ij}. \tag{15.6.21}$$

In the first step, we noted that any vector in U_k has T eigenvalue λ_k. In the second step, we used the unitarity of V_k. This shows that in the U_k subspace the matrix for T is still diagonal with all entries equal to λ_k.

The spectral theorem affords us a simple way to write a normal operator. For this, consider the basis of orthonormal eigenvectors for the T-invariant subspace U_k of dimension d_k. Let P_k denote the orthogonal projector to this subspace. The projector P_k has rank d_k, and its action on an arbitrary vector v can be written as

$$P_k\, v = \sum_{i=1}^{d_k} u_i^{(k)}\, \langle u_i^{(k)}, v \rangle, \tag{15.6.22}$$

following the prescription in (14.3.6). In bra-ket notation we have

$$P_k = \sum_{i=1}^{d_k} |u_i^{(k)}\rangle \langle u_i^{(k)}|. \tag{15.6.23}$$

By construction, the basis vectors of U_k are left invariant by P_k, and the basis vectors of any U_q, with $q \neq k$, are killed by P_k:

$$P_k u_i^{(q)} = u_i^{(q)} \delta_{kq}. \tag{15.6.24}$$

The various P_k satisfy the following properties:

$$\boxed{P_k^\dagger = P_k, \quad P_k P_l = \delta_{kl} P_l, \quad \sum_k P_k = \mathbb{1}.} \tag{15.6.25}$$

The first relation is manifest from (15.6.23). The second follows because each P_k is a projector, and U_k and U_l are orthogonal subspaces when $k \neq l$. The third expression is also clear from (15.6.23) because by the time we sum over the allowed values of $k = 1, \ldots, m$, we are summing the ket-bra combinations for all the basis vectors of the state space. This last property is the counterpart of $V = U_1 \oplus \cdots \oplus U_m$. A set of projectors P_k satisfying (15.6.25) is called a **complete set of orthonormal projectors.** We have thus seen that any normal operator gives rise to one such complete set. Finally, we now claim that the operator T itself can be written as follows:

$$\boxed{T = \sum_k \lambda_k P_k.} \tag{15.6.26}$$

This equation, in the form of a sum of terms that are each an eigenvalue times its associated projector, is called the **spectral decomposition** of T. The proof of this formula is simple; we just need to check that the right-hand side acts on the vectors of the orthonormal basis exactly as T does. Acting on $u_i^{(q)}$ and using (15.6.24), we see that

$$\sum_k \lambda_k P_k u_i^{(q)} = \sum_k \lambda_k \, u_i^{(q)} \delta_{kq} = \lambda_q u_i^{(q)}, \tag{15.6.27}$$

consistent with $T u_i^{(q)} = \lambda_q u_i^{(q)}$. This proves the decomposition (15.6.26).