

conjugation which does not affect the question of orthonormality), the result we already have for the columns of a unitary matrix tells us the rows of U are orthonormal.

Proof 2. Since $U^\dagger U = I$,

$$\begin{aligned}\delta_{ij} &= \langle i|I|j\rangle = \langle i|U^\dagger U|j\rangle \\ &= \sum_k \langle i|U^\dagger|k\rangle \langle k|U|j\rangle \\ &= \sum_k U_{ik}^* U_{kj} = \sum_k U_{ki}^* U_{kj}\end{aligned}\quad (1.6.22)$$

which proves the theorem for the columns. A similar result for the rows follows if we start with the equation $UU^\dagger = I$. Q.E.D.

Note that $U^\dagger U = I$ and $UU^\dagger = I$ are not independent conditions.

*Exercise 1.6.4.** It is assumed that you know (1) what a *determinant* is, (2) that $\det \Omega^T = \det \Omega$ (T denotes transpose), (3) that the determinant of a product of matrices is the product of the determinants. [If you do not, verify these properties for a two-dimensional case

$$\Omega = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

with $\det \Omega = (\alpha\delta - \beta\gamma)$.] Prove that the determinant of a unitary matrix is a complex number of unit modulus.

*Exercise 1.6.5.** Verify that $R(\frac{1}{2}\pi i)$ is unitary (orthogonal) by examining its matrix.

Exercise 1.6.6. Verify that the following matrices are unitary:

$$\frac{1}{2^{1/2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}, \quad \frac{1}{2} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix}$$

Verify that the determinant is of the form $e^{i\theta}$ in each case. Are any of the above matrices Hermitian?

1.7. Active and Passive Transformations

Suppose we subject all the vectors $|V\rangle$ in a space to a unitary transformation

$$|V\rangle \rightarrow U|V\rangle \quad (1.7.1)$$

Under this transformation, the matrix elements of any operator Ω are modified as follows:

$$\langle V'|\Omega|V\rangle \rightarrow \langle UV'| \Omega |UV\rangle = \langle V'|U^\dagger \Omega U|V\rangle \quad (1.7.2)$$

It is clear that the same change would be effected if we left the vectors alone subjected all operators to the change

$$\Omega \rightarrow U^\dagger \Omega U \quad (1.7)$$

The first case is called an *active transformation* and the second a *passive transformation*. The present nomenclature is in reference to the vectors: they are affected in active transformation and left alone in the passive case. The situation is exactly opposite from the point of view of the operators.

Later we will see that the physics in quantum theory lies in the matrix elements of operators, and that active and passive transformations provide us with two equivalent ways of describing the same physical transformation.

*Exercise 1.7.1.** The *trace* of a matrix is defined to be the sum of its diagonal matrix elements

$$\text{Tr } \Omega = \sum_i \Omega_{ii}$$

Show that

- (1) $\text{Tr}(\Omega\Lambda) = \text{Tr}(\Lambda\Omega)$
- (2) $\text{Tr}(\Omega\Lambda\theta) = \text{Tr}(\Lambda\theta\Omega) = \text{Tr}(\theta\Omega\Lambda)$ (The permutations are *cyclic*).
- (3) The trace of an operator is unaffected by a unitary change of basis $|i\rangle \rightarrow U|i\rangle$. [Equivalently, show $\text{Tr } \Omega = \text{Tr}(U^\dagger \Omega U)$.]

Exercise 1.7.2. Show that the determinant of a matrix is unaffected by a unitary change of basis. [Equivalently show $\det \Omega = \det(U^\dagger \Omega U)$.]

1.8. The Eigenvalue Problem

Consider some linear operator Ω acting on an arbitrary *nonzero* ket $|V\rangle$:

$$\Omega|V\rangle = |V'\rangle \quad (1.8.1)$$

Unless the operator happens to be a trivial one, such as the identity or its multiple, the ket will suffer a nontrivial change, i.e., $|V'\rangle$ will not be simply related to $|V\rangle$. So much for an arbitrary ket. Each operator, however, has certain kets of its own, called its *eigenkets*, on which its action is simply that of rescaling:

$$\Omega|V\rangle = \omega|V\rangle \quad (1.8.2)$$

Equation (1.8.2) is an eigenvalue equation: $|V\rangle$ is an *eigenket* of Ω with *eigenvalue* ω . In this chapter we will see how, given an operator Ω , one can systematically determine all its eigenvalues and eigenvectors. How such an equation enters physics will be illustrated by a few examples from mechanics at the end of this section, and once we get to quantum mechanics proper, it will be eigen, eigen, eigen all the way.

Example 1.8.1. To illustrate how easy the eigenvalue problem really is, we will begin with a case that will be completely solved: the case $\Omega = I$. Since

$$I|V\rangle = |V\rangle$$

for all $|V\rangle$, we conclude that

- (1) the only eigenvalue of I is 1;
- (2) all vectors are its eigenvectors with this eigenvalue. □

Example 1.8.2. After this unqualified success, we are encouraged to take on a slightly more difficult case: $\Omega = \mathbb{P}_V$, the projection operator associated with a *normalized* ket $|V\rangle$. Clearly

- (1) any ket $\alpha|V\rangle = |\alpha V\rangle$, parallel to $|V\rangle$ is an eigenket with eigenvalue 1:

$$\mathbb{P}_V|\alpha V\rangle = |V\rangle\langle V|\alpha V\rangle = \alpha|V\rangle|V|^2 = 1 \cdot |\alpha V\rangle$$

- (2) any ket $|V_\perp\rangle$, perpendicular to $|V\rangle$, is an eigenket with eigenvalue 0:

$$\mathbb{P}_V|V_\perp\rangle = |V\rangle\langle V|V_\perp\rangle = 0 = 0|V_\perp\rangle$$

- (3) kets that are neither, i.e., kets of the form $\alpha|V\rangle + \beta|V_\perp\rangle$, are simply not eigenkets:

$$\mathbb{P}_V(\alpha|V\rangle + \beta|V_\perp\rangle) = |\alpha V\rangle \neq \gamma(\alpha|V\rangle + \beta|V_\perp\rangle)$$

Since every ket in the space falls into one of the above classes, we have found all the eigenvalues and eigenvectors. □

Example 1.8.3. Consider now the operator $R(\frac{1}{2}\pi i)$. We already know that it has one eigenket, the basis vector $|1\rangle$ along the x axis:

$$R(\frac{1}{2}\pi i)|1\rangle = |1\rangle$$

Are there others? Of course, any vector $\alpha|1\rangle$ along the x axis is also unaffected by the x rotation. This is a general feature of the eigenvalue equation and reflects the linearity of the operator:

if

$$\Omega|V\rangle = \omega|V\rangle$$

then

$$\Omega\alpha|V\rangle = \alpha\Omega|V\rangle = \alpha\omega|V\rangle = \omega\alpha|V\rangle$$

for any multiple α . Since the eigenvalue equation fixes the eigenvector only up to an overall scale factor, we will not treat the multiples of an eigenvector as distinct eigenvectors. With this understanding in mind, let us ask if $R(\frac{1}{2}\pi\mathbf{i})$ has any eigenvectors besides $|1\rangle$. Our intuition says no, for any vector not along the x axis necessarily gets rotated by $R(\frac{1}{2}\pi\mathbf{i})$ and cannot possibly transform into a multiple of itself. Since every vector is either parallel to $|1\rangle$ or isn't, we have fully solved the eigenvalue problem.

The trouble with this conclusion is that it is wrong! $R(\frac{1}{2}\pi\mathbf{i})$ has two other eigenvectors besides $|1\rangle$. But our intuition is not to be blamed, for these vectors are in $\mathbb{V}^3(C)$ and not $\mathbb{V}^3(R)$. It is clear from this example that we need a reliable and systematic method for solving the eigenvalue problem in $\mathbb{V}^n(C)$. We now turn our attention to this very question. \square

The Characteristic Equation and the Solution to the Eigenvalue Problem

We begin by rewriting Eq. (1.8.2) as

$$(\Omega - \omega I)|V\rangle = |0\rangle \quad (1.8.3)$$

Operating both sides with $(\Omega - \omega I)^{-1}$, assuming it exists, we get

$$|V\rangle = (\Omega - \omega I)^{-1}|0\rangle \quad (1.8.4)$$

Now, any finite operator (an operator with finite matrix elements) acting on the null vector can only give us a null vector. It therefore seems that in asking for a nonzero eigenvector $|V\rangle$, we are trying to get something for nothing out of Eq. (1.8.4). This is impossible. It follows that our assumption that the operator $(\Omega - \omega I)^{-1}$ exists (as a finite operator) is false. So we ask when this situation will obtain. Basic matrix theory tells us (see Appendix A.1) that the inverse of any matrix M is given by

$$M^{-1} = \frac{\text{cofactor } M^T}{\det M} \quad (1.8.5)$$

Now the cofactor of M is finite if M is. Thus what we need is the vanishing of the determinant. The condition for nonzero eigenvectors is therefore

$$\det(\Omega - \omega I) = 0 \quad (1.8.6)$$

This equation will determine the eigenvalues ω . To find them, we project Eq. (1.8.3) onto a basis. Doting both sides with a basis bra $\langle i|$, we get

$$\langle i|\Omega - \omega I|V\rangle = 0$$

and upon introducing the representation of the identity [Eq. (1.6.7)], to the left of $|V\rangle$, we get the following image of Eq. (1.8.3):

$$\sum_j (\Omega_{ij} - \omega \delta_{ij}) v_j = 0 \quad (1.8.7)$$

Setting the determinant to zero will give us an expression of the form

$$\sum_{m=0}^n c_m \omega^m = 0 \quad (1.8.8)$$

Equation (1.8.8) is called the *characteristic equation* and

$$P^n(\omega) = \sum_{m=0}^n c_m \omega^m \quad (1.8.9)$$

is called the *characteristic polynomial*. Although the polynomial is being determined in a particular basis, the eigenvalues, which are its roots, are basis independent, for they are defined by the abstract Eq. (1.8.3), which makes no reference to any basis.

Now, a fundamental result in analysis is that every n th-order polynomial has n roots, not necessarily distinct and not necessarily real. Thus every operator in $\mathbb{V}^n(C)$ has n eigenvalues. Once the eigenvalues are known, the eigenvectors may be found, at least for Hermitian and unitary operators, using a procedure illustrated by the following example. [Operators on $\mathbb{V}^n(C)$ that are not of the above variety may not have n eigenvectors—see Exercise 1.8.4. Theorems 10 and 12 establish that Hermitian and unitary operators on $\mathbb{V}^n(C)$ will have n eigenvectors.]

Example 1.8.4. Let us use the general techniques developed above to find all the eigenvectors and eigenvalues of $R(\frac{1}{2}\pi\mathbf{i})$. Recall that the matrix representing it is

$$R(\tfrac{1}{2}\pi\mathbf{i}) \leftrightarrow \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

Therefore the characteristic equation is

$$\det(R - \omega I) = \begin{vmatrix} 1 - \omega & 0 & 0 \\ 0 & -\omega & -1 \\ 0 & 1 & -\omega \end{vmatrix} = 0$$

i.e.,

$$(1 - \omega)(\omega^2 + 1) = 0 \quad (1.8.10)$$

with roots $\omega = 1, \pm i$. We know that $\omega = 1$ corresponds to $|1\rangle$. Let us see this come out of the formalism. Feeding $\omega = 1$ into Eq. (1.8.7) we find that the components x_1, x_2 , and x_3 of the corresponding eigenvector must obey the equations

$$\begin{bmatrix} 1-1 & 0 & 0 \\ 0 & 0-1 & -1 \\ 0 & 1 & 0-1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \rightarrow \begin{cases} 0=0 \\ -x_2-x_3=0 \\ x_2-x_3=0 \end{cases} \rightarrow x_2=x_3=0$$

Thus any vector of the form

$$x_1|1\rangle \leftrightarrow \begin{bmatrix} x_1 \\ 0 \\ 0 \end{bmatrix}$$

is acceptable, as expected. It is conventional to use the freedom in scale to normalize the eigenvectors. Thus in this case a choice is

$$|\omega = 1\rangle = |1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

I say *a* choice, and not *the* choice, since the vector may be multiplied by a number of modulus unity without changing the norm. There is no universally accepted convention for eliminating this freedom, except perhaps to choose the vector with real components when possible.

Note that of the three simultaneous equations above, the first is not a real equation. In general, there will be only $(n-1)$ LI equations. This is the reason the norm of the vector is not fixed and, as shown in Appendix A.1, the reason the determinant vanishes.

Consider next the equations corresponding to $\omega = i$. The components of the eigenvector obey the equations

$$(1-i)x_1 = 0 \quad (\text{i.e., } x_1 = 0)$$

$$-ix_2 - x_3 = 0 \quad (\text{i.e., } x_2 = ix_3)$$

$$x_2 - ix_3 = 0 \quad (\text{i.e., } x_2 = ix_3)$$

Notice once again that we have only $n-1$ useful equations. A properly normalized solution to the above is

$$|\omega = i\rangle \leftrightarrow \frac{1}{2^{1/2}} \begin{bmatrix} 0 \\ i \\ 1 \end{bmatrix}$$

A similar procedure yields the third eigenvector:

$$|\omega = -i\rangle \leftrightarrow \frac{1}{2^{1/2}} \begin{bmatrix} 0 \\ -i \\ 1 \end{bmatrix} \quad \square$$

In the above example we have introduced a popular convention: labeling the eigenvectors by the eigenvalue. For instance, the ket corresponding to $\omega = \omega_i$ is labeled $|\omega = \omega_i\rangle$ or simply $|\omega_i\rangle$. This notation presumes that to each ω_i there is just one vector labeled by it. Though this is not always the case, only a slight change in this notation will be needed to cover the general case.

The phenomenon of a single eigenvalue representing more than one eigenvector is called *degeneracy* and corresponds to repeated roots for the characteristic polynomial. In the face of degeneracy, we need to modify not just the labeling, but also the procedure used in the example above for finding the eigenvectors. Imagine that instead of $R(\frac{1}{2}\pi i)$ we were dealing with another operator Ω on $\mathbb{V}^3(\mathcal{R})$ with roots ω_1 and $\omega_2 = \omega_3$. It appears as if we can get two eigenvectors, by the method described above, one for each distinct ω . How do we get a third? Or is there no third? These questions will be answered in all generality shortly when we examine the question of degeneracy in detail. We now turn our attention to two central theorems on Hermitian operators. These play a vital role in quantum mechanics.

Theorem 9. The eigenvalues of a Hermitian operator are real.

Proof. Let

$$\Omega|\omega\rangle = \omega|\omega\rangle$$

Dot both sides with $\langle\omega|$:

$$\langle\omega|\Omega|\omega\rangle = \omega\langle\omega|\omega\rangle \quad (1.8.11)$$

Take the adjoint to get

$$\langle\omega|\Omega^\dagger|\omega\rangle = \omega^*\langle\omega|\omega\rangle$$

Since $\Omega = \Omega^\dagger$, this becomes

$$\langle\omega|\Omega|\omega\rangle = \omega^*\langle\omega|\omega\rangle$$

Subtracting from Eq. (1.8.11)

$$0 = (\omega - \omega^*)\langle\omega|\omega\rangle$$

$$\omega = \omega^* \quad \text{Q.E.D.}$$