CHAPTER 3

FORMALISM

3.1 LINEAR ALGEBRA

The purpose of this chapter is to develop the *formalism* of quantum mechanics—terminology, notation, and mathematical background that illuminate the structure of the theory, facilitate practical calculations, and motivate a fundamental extension of the statistical interpretation. I begin with a brief survey of linear algebra.[1] Linear algebra abstracts and generalizes the arithmetic of ordinary vectors, as we encounter them in first-year physics. The generalization is in two directions: (1) We allow the scalars to be *complex*, and (2) we do not restrict ourselves to three dimensions (indeed, in Section 3.2 we shall be working with vectors that live in spaces of *infinite* dimension).

3.1.1 Vectors

A **vector space** consists of a set of **vectors** ($|\alpha\rangle$, $|\beta\rangle$, $|\gamma\rangle$, ...), together with a set of **scalars** (a, b, c, ...),[2] which are subject to two operations—vector addition and scalar multiplication:

[1] If you have already studied linear algebra, you should be able to skim this section quickly, but I wouldn't skip it altogether, because some of the notation may be unfamiliar. If, on the other hand, this material is new to you, be warned that I am only summarizing (often without proof) those aspects of the theory we will be needing later. For details, you should refer to a text on linear algebra, such as the classic by P. R. Halmos: *Finite Dimensional Vector Spaces*, 2nd ed. (Princeton, NJ: van Nostrand, 1958).

[2] For our purposes, the scalars will be ordinary complex numbers. Mathematicians can tell you about vector spaces over more exotic fields, but such objects play no role in quantum mechanics.

Vector addition. The "sum" of any two vectors is another vector:

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle. \tag{3.1}$$

Vector addition is **commutative**

$$|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle, \tag{3.2}$$

and **associative**

$$|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle. \tag{3.3}$$

There exists a **zero** (or **null**) **vector**,[3] $|0\rangle$, with the property that

$$|\alpha\rangle + |0\rangle = |\alpha\rangle, \tag{3.4}$$

for every vector $|\alpha\rangle$. And for every vector $|\alpha\rangle$ there is an associated **inverse vector** ($|-\alpha\rangle$), such that

$$|\alpha\rangle + |-\alpha\rangle = |0\rangle. \tag{3.5}$$

Scalar multiplication. The "product" of any scalar with any vector is another vector:

$$a|\alpha\rangle = |\gamma\rangle. \tag{3.6}$$

Scalar multiplication is **distributive** with respect to vector addition

$$a(|\alpha\rangle + |\beta\rangle) = a|\alpha\rangle + a|\beta\rangle \tag{3.7}$$

and with respect to scalar addition

$$(a+b)|\alpha\rangle = a|\alpha\rangle + b|\alpha\rangle. \tag{3.8}$$

It is also **associative** with respect to the ordinary multiplication of scalars:

$$a(b|\alpha\rangle) = (ab)|\alpha\rangle. \tag{3.9}$$

Multiplication by the scalars 0 and 1 has the effect you would expect:

$$0|\alpha\rangle = |0\rangle; \quad 1|\alpha\rangle = |\alpha\rangle. \tag{3.10}$$

Evidently $|-\alpha\rangle = (-1)|\alpha\rangle$.

There's a lot less here than meets the eye—all I have done is to write down in abstract language the familiar rules for manipulating vectors. The virtue of such abstraction is that we will be able to apply our knowledge and intuition about the behavior of ordinary vectors to other systems that happen to share the same formal properties.

[3] It is customary, where no confusion can arise, to write the null vector without the adorning bracket: $|0\rangle \to 0$.

A **linear combination** of the vectors $|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \ldots$ is an expression of the form

$$a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle + \cdots. \tag{3.11}$$

A vector $|\lambda\rangle$ is said to be **linearly independent** of the set $|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \ldots$ if it cannot be written as a linear combination of them. (For example, in three dimensions the unit vector $\hat{k}$ is linearly independent of $\hat{\imath}$ and $\hat{\jmath}$, but any vector in the xy-plane is linearly *dependent* on $\hat{\imath}$ and $\hat{\jmath}$.) By extension, a *set* of vectors is linearly independent if each one is linearly independent of all the rest. A collection of vectors is said to **span** the space if *every* vector can be written as a linear combination of the members of this set.[4] A set of *linearly independent* vectors that spans the space is called a **basis**. The number of vectors in any basis is called the **dimension** of the space. For the moment we shall assume that the dimension (n) is *finite*.

With respect to a prescribed basis

$$|e_1\rangle, \ |e_2\rangle, \ \ldots, \ |e_n\rangle, \tag{3.12}$$

any given vector

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \cdots + a_n|e_n\rangle \tag{3.13}$$

is uniquely represented by the (ordered) n-tuple of its **components**:

$$|\alpha\rangle \leftrightarrow (a_1, a_2, \ldots, a_n). \tag{3.14}$$

It is often easier to work with the components than with the abstract vectors themselves. To add vectors, you add their corresponding components:

$$|\alpha\rangle + |\beta\rangle \leftrightarrow (a_1 + b_1, a_2 + b_2, \ldots, a_n + b_n); \tag{3.15}$$

to multiply by a scalar you multiply each component:

$$c|\alpha\rangle \leftrightarrow (ca_1, ca_2, \ldots, ca_n); \tag{3.16}$$

the null vector is represented by a string of zeroes:

$$|0\rangle \leftrightarrow (0, 0, \ldots, 0); \tag{3.17}$$

and the components of the inverse vector have their signs reversed:

$$|-\alpha\rangle \leftrightarrow (-a_1, -a_2, \ldots, -a_n). \tag{3.18}$$

The only *dis*advantage of working with components is that you have to commit yourself to a particular basis, and the same manipulations will look very different to someone working in a different basis.

Problem 3.1 Consider the ordinary vectors in three dimensions ($a_x\hat{\imath} + a_y\hat{\jmath} + a_z\hat{k}$) with complex components.

[4] A set of vectors that spans the space is also called **complete**, though I personally reserve that word for the infinite-dimensional case, where subtle questions of convergence arise.

(a) Does the subset of all vectors with $a_z = 0$ constitute a vector space? If so, what is its dimension; if not, why not?

(b) What about the subset of all vectors whose z component is 1?

(c) How about the subset of vectors whose components are all equal?

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*Problem 3.2 Consider the collection of all polynomials (with complex coefficients) of degree $< N$ in x.

(a) Does this set constitute a vector space (with the polynomials as "vectors")? If so, suggest a convenient basis, and give the dimension of the space. If not, which of the defining properties does it lack?

(b) What if we require that the polynomials be *even* functions?

(c) What if we require that the leading coefficient (i.e., the number multiplying x^{N-1}) be 1?

(d) What if we require that the polynomials have the value 0 at $x = 1$?

(e) What if we require that the polynomials have the value 1 at $x = 0$?

Problem 3.3 Prove that the components of a vector with respect to a given basis are *unique*.

3.1.2 Inner Products

In three dimensions we encounter two kinds of vector products: the dot product and the cross product. The latter does not generalize in any natural way to n-dimensional vector spaces, but the former *does*—in this context it is usually called the **inner product**. The inner product of two vectors ($|\alpha\rangle$ and $|\beta\rangle$) is a complex number (which we write as $\langle\alpha|\beta\rangle$), with the following properties:

$$\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*, \tag{3.19}$$

$$\langle\alpha|\alpha\rangle \geq 0, \quad \text{and } \langle\alpha|\alpha\rangle = 0 \Leftrightarrow |\alpha\rangle = |0\rangle, \tag{3.20}$$

$$\langle\alpha|\left(b|\beta\rangle + c|\gamma\rangle\right) = b\langle\alpha|\beta\rangle + c\langle\alpha|\gamma\rangle. \tag{3.21}$$

Apart from the generalization to complex numbers, these axioms simply codify the familiar behavior of dot products. A vector space with an inner product is called an **inner product space**.

Because the inner product of any vector with itself is a nonnegative number (Equation 3.20), its square root is *real*—we call this the **norm** of the vector:

$$\|\alpha\| \equiv \sqrt{\langle\alpha|\alpha\rangle}; \tag{3.22}$$

it generalizes the notion of "length". A "unit" vector, whose norm is 1, is said to be **normalized** (the word should really be "normal", but I guess that sounds too anthropomorphic). Two vectors whose inner product is zero are called **orthogonal** (generalizing the notion of "perpendicular"). A collection of mutually orthogonal normalized vectors,

$$\langle\alpha_i|\alpha_j\rangle = \delta_{ij}, \tag{3.23}$$

is called an **orthonormal set**. It is always possible (see Problem 3.4), and almost always convenient, to choose an *orthonormal basis*; in that case the inner product of two vectors can be written very neatly in terms of their components:

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \cdots + a_n^* b_n, \tag{3.24}$$

the norm (squared) becomes

$$\langle\alpha|\alpha\rangle = |a_1|^2 + |a_2|^2 + \cdots + |a_n|^2, \tag{3.25}$$

and the components themselves are

$$a_i = \langle e_i|\alpha\rangle. \tag{3.26}$$

(These results generalize the familiar formulas $\mathbf{a} \cdot \mathbf{b} = a_x b_x + a_y b_y + a_z b_z$, $\mathbf{a} \cdot \mathbf{a} = a_x^2 + a_y^2 + a_z^2$, and $a_x = \hat{\imath} \cdot \mathbf{a}$, $a_y = \hat{\jmath} \cdot \mathbf{a}$, $a_z = \hat{k} \cdot \mathbf{a}$, for the three-dimensional orthonormal basis $\hat{\imath}$, $\hat{\jmath}$, $\hat{k}$.) From now on we shall *always* work in orthonormal bases unless it is explicitly indicated otherwise.

Another geometrical quantity one might wish to generalize is the *angle* between two vectors. In ordinary vector analysis $\cos\theta = (\mathbf{a} \cdot \mathbf{b})/|\mathbf{a}||\mathbf{b}|$. But because the inner product is in general a complex number, the analogous formula (in an arbitrary inner product space) does not define a (real) angle θ. Nevertheless, it is still true that the *absolute value* of this quantity is a number no greater than 1,

$$|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle. \tag{3.27}$$

(This important result is known as the **Schwarz inequality**; the proof is given in Problem 3.5.) So you can, if you like, define the angle between $|\alpha\rangle$ and $|\beta\rangle$ by the formula

$$\cos\theta = \sqrt{\frac{\langle\alpha|\beta\rangle\langle\beta|\alpha\rangle}{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle}}. \tag{3.28}$$

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*Problem 3.4 Suppose you start out with a basis ($|e_1\rangle, |e_2\rangle, \ldots, |e_n\rangle$) that is *not* orthonormal. The **Gram-Schmidt procedure** is a systematic ritual for generating from it an orthonormal basis ($|e_1'\rangle, |e_2'\rangle, \ldots, |e_n'\rangle$). It goes like this:

(i) Normalize the first basis vector (divide by its norm):

$$|e_1'\rangle = \frac{|e_1\rangle}{\|e_1\|}.$$

(ii) Find the projection of the second vector along the first, and subtract it off:

$$|e_2\rangle - \langle e_1'|e_2\rangle|e_1'\rangle.$$

This vector is orthogonal to $|e_1'\rangle$; normalize it to get $|e_2'\rangle$.

(iii) Subtract from $|e_3\rangle$ its projections along $|e_1'\rangle$ and $|e_2'\rangle$:

$$|e_3\rangle - \langle e_1'|e_3\rangle|e_1'\rangle - \langle e_2'|e_3\rangle|e_2'\rangle.$$

This is orthogonal to $|e_1'\rangle$ and $|e_2'\rangle$; normalize it to get $|e_3'\rangle$. And so on.

Use the Gram-Schmidt procedure to orthonormalize the three-space basis $|e_1\rangle = (1+i)\hat{\imath} + (1)\hat{\jmath} + (i)\hat{k}$, $|e_2\rangle = (i)\hat{\imath} + (3)\hat{\jmath} + (1)\hat{k}$, $|e_3\rangle = (0)\hat{\imath} + (28)\hat{\jmath} + (0)\hat{k}$.

Problem 3.5 Prove the Schwarz inequality (Equation 3.27). *Hint*: Let $|\gamma\rangle = |\beta\rangle - (\langle\alpha|\beta\rangle/\langle\alpha|\alpha\rangle)|\alpha\rangle$, and use $\langle\gamma|\gamma\rangle \geq 0$.

Problem 3.6 Find the angle (in the sense of Equation 3.28) between the vectors $|\alpha\rangle = (1+i)\hat{\imath} + (1)\hat{\jmath} + (i)\hat{k}$ and $|\beta\rangle = (4-i)\hat{\imath} + (0)\hat{\jmath} + (2-2i)\hat{k}$.

Problem 3.7 Prove the **triangle inequality**: $\|(|\alpha\rangle + |\beta\rangle)\| \leq \|\alpha\| + \|\beta\|$.

3.1.3 Linear Transformations

Suppose you take every vector (in three-space) and multiply it by 17, or you rotate every vector by 39° about the z-axis, or you reflect every vector in the xy-plane—these are all examples of **linear transformations**. A linear transformation[5] ($\hat{T}$) takes each vector in a vector space and "transforms" it into some other vector ($|\alpha\rangle \to |\alpha'\rangle = \hat{T}|\alpha\rangle$), with the proviso that the operation is *linear*:

$$\hat{T}(a|\alpha\rangle + b|\beta\rangle) = a(\hat{T}|\alpha\rangle) + b(\hat{T}|\beta\rangle), \qquad [3.29]$$

for any vectors $|\alpha\rangle$, $|\beta\rangle$ and any scalars a, b.

If you know what a particular linear transformation does to a set of *basis* vectors, you can easily figure out what it does to *any* vector. For suppose that

$$\begin{aligned}
\hat{T}|e_1\rangle &= T_{11}|e_1\rangle + T_{21}|e_2\rangle + \cdots + T_{n1}|e_n\rangle,\\
\hat{T}|e_2\rangle &= T_{12}|e_1\rangle + T_{22}|e_2\rangle + \cdots + T_{n2}|e_n\rangle,\\
&\cdots\\
\hat{T}|e_n\rangle &= T_{1n}|e_1\rangle + T_{2n}|e_2\rangle + \cdots + T_{nn}|e_n\rangle,
\end{aligned}$$

or, more compactly,

$$\hat{T}|e_j\rangle = \sum_{i=1}^{n} T_{ij}|e_i\rangle, \quad (j = 1, 2, \ldots, n). \qquad [3.30]$$

[5] In this chapter I'll use a hat (^) to denote linear transformations; this is not inconsistent with my earlier convention (putting hats on operators), for (as we shall see) our operators *are* linear transformations.

If $|\alpha\rangle$ is an arbitrary vector:

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \cdots + a_n|e_n\rangle = \sum_{j=1}^{n} a_j|e_j\rangle, \qquad [3.31]$$

then

$$\hat{T}|\alpha\rangle = \sum_{j=1}^{n} a_j(\hat{T}|e_j\rangle) = \sum_{j=1}^{n}\sum_{i=1}^{n} a_j T_{ij}|e_i\rangle = \sum_{i=1}^{n}\Big(\sum_{j=1}^{n} T_{ij}a_j\Big)|e_i\rangle. \qquad [3.32]$$

Evidently $\hat{T}$ takes a vector with components $a_1, a_2, \ldots, a_n$ into a vector with components[6]

$$a_i' = \sum_{j=1}^{n} T_{ij}a_j. \qquad [3.33]$$

Thus the n^2 **elements** T_{ij} uniquely characterize the linear transformation $\hat{T}$ (with respect to a given basis), just as the n components a_i uniquely characterize the vector $|\alpha\rangle$ (with respect to the same basis):

$$\hat{T} \leftrightarrow (T_{11}, T_{12}, \ldots, T_{nn}). \qquad [3.34]$$

If the basis is orthonormal, it follows from Equation 3.30 that

$$T_{ij} = \langle e_i|\hat{T}|e_j\rangle. \qquad [3.35]$$

It is convenient to display these complex numbers in the form of a **matrix**[7]:

$$\mathbf{T} = \begin{pmatrix} T_{11} & T_{12} & \cdots & T_{1n} \\ T_{21} & T_{22} & \cdots & T_{2n} \\ \vdots & \vdots & & \vdots \\ T_{n1} & T_{n2} & \cdots & T_{nn} \end{pmatrix}. \qquad [3.36]$$

The study of linear transformations, then, reduces to the theory of matrices. The *sum* of two linear transformations ($\hat{S} + \hat{T}$) is defined in the natural way:

$$(\hat{S} + \hat{T})|\alpha\rangle = \hat{S}|\alpha\rangle + \hat{T}|\alpha\rangle; \qquad [3.37]$$

this matches the usual rule for adding matrices (you add their corresponding elements):

$$\mathbf{U} = \mathbf{S} + \mathbf{T} \Leftrightarrow U_{ij} = S_{ij} + T_{ij}. \qquad [3.38]$$

[6] Notice the reversal of indices between Equations 3.30 and 3.33. This is not a typographical error. Another way of putting it (switching $i \leftrightarrow j$ in Equation 3.30) is that if the *components* transform with T_{ij}, the *basis* vectors transform with T_{ji}.

[7] I'll use boldface to denote matrices.

The *product* of two linear transformations ($\hat{S}\hat{T}$) is the net effect of performing them in succession—first $\hat{T}$, then $\hat{S}$:

$$|\alpha\rangle \rightarrow |\alpha'\rangle = \hat{T}|\alpha\rangle \rightarrow |\alpha''\rangle = \hat{S}|\alpha'\rangle = \hat{S}(\hat{T}|\alpha\rangle) = \hat{S}\hat{T}|\alpha\rangle. \quad [3.39]$$

What matrix **U** represents the combined transformation $\hat{U} = \hat{S}\hat{T}$? It's not hard to work it out:

$$a_i'' = \sum_{j=1}^{n} S_{ij}a_j' = \sum_{j=1}^{n} S_{ij}\left(\sum_{k=1}^{n} T_{jk}a_k\right) = \sum_{k=1}^{n}\left(\sum_{j=1}^{n} S_{ij}T_{jk}\right)a_k = \sum_{k=1}^{n} U_{ik}a_k.$$

Evidently

$$\mathbf{U} = \mathbf{ST} \Leftrightarrow U_{ik} = \sum_{j=1}^{n} S_{ij}T_{jk}; \quad [3.40]$$

this is the standard rule for matrix multiplication—to find the ik^{th} element of the product, you look at the i^{th} row of **S** and the k^{th} column of **T**, multiply corresponding entries, and add. The same procedure allows you to multiply *rectangular* matrices, as long as the number of columns in the first matches the number of rows in the second. In particular, if we write the n-tuple of components of $|\alpha\rangle$ as an $n \times 1$ **column matrix**

$$\mathbf{a} \equiv \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}, \quad [3.41]$$

the transformation rule (Equation 3.33) can be written

$$\mathbf{a}' = \mathbf{Ta}. \quad [3.42]$$

And now, some useful matrix terminology: The **transpose** of a matrix (which we shall write with a tilde: $\tilde{\mathbf{T}}$) is the same set of elements, but with rows and columns interchanged:

$$\tilde{\mathbf{T}} = \begin{pmatrix} T_{11} & T_{21} & \cdots & T_{n1} \\ T_{12} & T_{22} & \cdots & T_{n2} \\ \vdots & \vdots & & \vdots \\ T_{1n} & T_{2n} & \cdots & T_{nn} \end{pmatrix}. \quad [3.43]$$

Notice that the transpose of a *column* matrix is a **row matrix**:

$$\tilde{\mathbf{a}} = (a_1 \quad a_2 \quad \cdots \quad a_n). \quad [3.44]$$

A square matrix is **symmetric** if it is equal to its transpose (reflection in the **main diagonal**—upper left to lower right—leaves it unchanged); it is **antisymmetric** if this operation reverses the sign:

$$\text{SYMMETRIC: } \tilde{\mathbf{T}} = \mathbf{T}; \quad \text{ANTISYMMETRIC: } \tilde{\mathbf{T}} = -\mathbf{T}. \quad [3.45]$$

To construct the (complex) **conjugate** of a matrix (which we denote, as usual, with an asterisk: $\mathbf{T}^*$), you take the complex conjugate of every element:

$$\mathbf{T}^* = \begin{pmatrix} T_{11}^* & T_{12}^* & \cdots & T_{1n}^* \\ T_{21}^* & T_{22}^* & \cdots & T_{2n}^* \\ \vdots & \vdots & & \vdots \\ T_{n1}^* & T_{n2}^* & \cdots & T_{nn}^* \end{pmatrix}; \quad \mathbf{a}^* = \begin{pmatrix} a_1^* \\ a_2^* \\ \vdots \\ a_n^* \end{pmatrix}. \quad [3.46]$$

A matrix is **real** if all its elements are real and **imaginary** if they are all imaginary:

$$\text{REAL: } \mathbf{T}^* = \mathbf{T}; \quad \text{IMAGINARY: } \mathbf{T}^* = -\mathbf{T}. \quad [3.47]$$

The **Hermitian conjugate** (or **adjoint**) of a matrix (indicated by a dagger: $\mathbf{T}^\dagger$) is the transposed conjugate:

$$\mathbf{T}^\dagger \equiv \tilde{\mathbf{T}}^* = \begin{pmatrix} T_{11}^* & T_{21}^* & \cdots & T_{n1}^* \\ T_{12}^* & T_{22}^* & \cdots & T_{n2}^* \\ \vdots & \vdots & & \vdots \\ T_{1n}^* & T_{2n}^* & \cdots & T_{nn}^* \end{pmatrix}; \quad \mathbf{a}^\dagger \equiv \tilde{\mathbf{a}}^* = (a_1^* \quad a_2^* \quad \cdots \quad a_n^*). \quad [3.48]$$

A square matrix is **Hermitian** (or **self-adjoint**) if it is equal to its Hermitian conjugate; if Hermitian conjugation introduces a minus sign, the matrix is **skew Hermitian** (or **anti-Hermitian**):

$$\text{HERMITIAN: } \mathbf{T}^\dagger = \mathbf{T}; \quad \text{SKEW HERMITIAN: } \mathbf{T}^\dagger = -\mathbf{T}. \quad [3.49]$$

With this notation the inner product of two vectors (with respect to an orthonormal basis—Equation 3.24), can be written very neatly in matrix form:

$$\langle\alpha|\beta\rangle = \mathbf{a}^\dagger\mathbf{b}. \quad [3.50]$$

(Notice that each of the three operations discussed in this paragraph, if applied twice, returns you to the original matrix.)

Matrix multiplication is not, in general, commutative ($\mathbf{ST} \neq \mathbf{TS}$); the difference between the two orderings is called the **commutator**:

$$[\mathbf{S}, \mathbf{T}] \equiv \mathbf{ST} - \mathbf{TS}. \quad [3.51]$$

The transpose of a product is the product of the transposes *in reverse order*:

$$\widetilde{(\mathbf{ST})} = \tilde{\mathbf{T}}\tilde{\mathbf{S}} \quad [3.52]$$

(see Problem 3.12), and the same goes for Hermitian conjugates:

$$(\mathbf{ST})^\dagger = \mathbf{T}^\dagger\mathbf{S}^\dagger. \quad [3.53]$$

The **unit matrix** (representing a linear transformation that carries every vector into itself) consists of ones on the main diagonal and zeroes everywhere else:

$$\mathbf{1} \equiv \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}. \qquad [3.54]$$

In other words,

$$\mathbf{1}_{ij} = \delta_{ij}. \qquad [3.55]$$

The **inverse** of a matrix (written $\mathbf{T}^{-1}$) is defined in the obvious way:

$$\mathbf{T}^{-1}\mathbf{T} = \mathbf{T}\mathbf{T}^{-1} = \mathbf{1}. \qquad [3.56]$$

A matrix has an inverse if and only if its **determinant**[8] is nonzero; in fact,

$$\mathbf{T}^{-1} = \frac{1}{\det \mathbf{T}}\tilde{\mathbf{C}}, \qquad [3.57]$$

where $\mathbf{C}$ is the matrix of **cofactors** [the cofactor of element T_{ij} is $(-1)^{i+j}$ times the determinant of the submatrix obtained from $\mathbf{T}$ by erasing the i^{th} row and the j^{th} column]. A matrix without an inverse is said to be **singular**. The inverse of a product (assuming it exists) is the product of the inverses *in reverse order*:

$$(\mathbf{ST})^{-1} = \mathbf{T}^{-1}\mathbf{S}^{-1}. \qquad [3.58]$$

A matrix is **unitary** if its inverse is equal to its Hermitian conjugate:

$$\text{UNITARY}: \mathbf{U}^{\dagger} = \mathbf{U}^{-1}. \qquad [3.59]$$

Assuming the basis is orthonormal, the columns of a unitary matrix constitute an orthonormal set, and so too do its rows (see Problem 3.16).

The components of a given vector depend on your (arbitrary) choice of basis, as do the elements in the matrix representing a given linear transformation. We might inquire how these numbers change when we switch to a different basis. The new basis vectors $|f_i\rangle$ are—like *all* vectors—linear combinations of the old ones:

$$\begin{aligned} |f_1\rangle &= S_{11}|e_1\rangle + S_{21}|e_2\rangle + \cdots + S_{n1}|e_n\rangle, \\ |f_2\rangle &= S_{12}|e_1\rangle + S_{22}|e_2\rangle + \cdots + S_{n2}|e_n\rangle, \\ &\cdots \\ |f_n\rangle &= S_{1n}|e_1\rangle + S_{2n}|e_2\rangle + \cdots + S_{nn}|e_n\rangle \end{aligned}$$

[8] I assume you know how to evaluate determinants. If not, see M. Boas, *Mathematical Methods in the Physical Sciences*, 2nd ed. (New York: John Wiley, 1983), Section 3.3.

(for some set of complex numbers S_{ij}), or, more compactly,

$$|f_j\rangle = \sum_{i=1}^{n} S_{ij}|e_i\rangle, \quad (j = 1, 2, \ldots, n). \qquad [3.60]$$

This is *itself* a linear transformation (compare Equation 3.30),[9] and we know immediately how the components transform:

$$a_i^f = \sum_{j=1}^{n} S_{ij} a_j^e \qquad [3.61]$$

(where the superscript indicates the basis). In matrix form

$$\mathbf{a}^f = \mathbf{S}\mathbf{a}^e. \qquad [3.62]$$

What about the matrix representing a given linear transformation $\hat{T}$—how is *it* modified by a change of basis? In the old basis we had (Equation 3.42)

$$\mathbf{a}^{e\prime} = \mathbf{T}^e\mathbf{a}^e,$$

and Equation 3.62—multiplying both sides by $\mathbf{S}^{-1}$—entails[10] $\mathbf{a}^e = \mathbf{S}^{-1}\mathbf{a}^f$, so

$$\mathbf{a}^{f\prime} = \mathbf{S}\mathbf{a}^{e\prime} = \mathbf{S}(\mathbf{T}^e\mathbf{a}^e) = \mathbf{S}\mathbf{T}^e\mathbf{S}^{-1}\mathbf{a}^f.$$

Evidently

$$\mathbf{T}^f = \mathbf{S}\mathbf{T}^e\mathbf{S}^{-1}. \qquad [3.63]$$

In general, two matrices ($\mathbf{T}_1$ and $\mathbf{T}_2$) are said to be **similar** if $\mathbf{T}_2 = \mathbf{S}\mathbf{T}_1\mathbf{S}^{-1}$ for some (nonsingular) matrix $\mathbf{S}$. What we have just found is that similar matrices represent the same linear transformation with respect to two different bases. Incidentally, if the first basis is orthonormal, the second will also be orthonormal if and only if the matrix $\mathbf{S}$ is *unitary* (see Problem 3.14). Since we always work in orthonormal bases, we are interested mainly in unitary similarity transformations.

While the *elements* of the matrix representing a given linear transformation may look very different in the new basis, two numbers associated with the matrix are unchanged: the determinant and the **trace**. For the determinant of a product is the product of the determinants, and hence

$$\det(\mathbf{T}^f) = \det(\mathbf{S}\,\mathbf{T}^e\mathbf{S}^{-1}) = \det(\mathbf{S})\det(\mathbf{T}^e)\det(\mathbf{S}^{-1}) = \det\mathbf{T}^e. \qquad [3.64]$$

[9] Notice, however, the radically different perspective: In this case we're talking about one and the same *vector*, referred to two different *bases*, whereas before we were thinking of a completely *different* vector, referred to the *same* basis.

[10] Note that $\mathbf{S}^{-1}$ certainly exists—if $\mathbf{S}$ were singular, the $|f_i\rangle$'s would not span the space, so they wouldn't constitute a basis.

And the trace, which is the sum of the diagonal elements,

$$\mathrm{Tr}(\mathbf{T}) \equiv \sum_{i=1}^{m} T_{ii}, \qquad [3.65]$$

has the property (see Problem 3.15) that

$$\mathrm{Tr}(\mathbf{T}_1\mathbf{T}_2) = \mathrm{Tr}(\mathbf{T}_2\mathbf{T}_1), \qquad [3.66]$$

(for any two matrices $\mathbf{T}_1$ and $\mathbf{T}_2$), so that

$$\mathrm{Tr}(\mathbf{T}^f) = \mathrm{Tr}(\mathbf{S}\mathbf{T}^e\mathbf{S}^{-1}) = \mathrm{Tr}(\mathbf{T}^e\mathbf{S}^{-1}\mathbf{S}) = \mathrm{Tr}(\mathbf{T}^e). \qquad [3.67]$$

Problem 3.8 Using the standard basis $(\hat{\imath}, \hat{\jmath}, \hat{k})$ for vectors in three dimensions:

(a) Construct the matrix representing a rotation through angle θ (counterclockwise, looking down the axis toward the origin) about the z-axis.

(b) Construct the matrix representing a rotation by 120° (counterclockwise, looking down the axis) about an axis through the point (1,1,1).

(c) Construct the matrix representing reflection in the xy-plane.

(d) Are **translations** ($x \to x + x_0$, $y \to y + y_0$, $z \to z + z_0$, for some constants x_0, y_0, z_0) linear transformations? If so, find the matrix which represents them; if not, explain why not.

*Problem 3.9 Given the following two matrices:

$$\mathbf{A} = \begin{pmatrix} -1 & 1 & i \\ 2 & 0 & 3 \\ 2i & -2i & 2 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 2 & 0 & -i \\ 0 & 1 & 0 \\ i & 3 & 2 \end{pmatrix},$$

compute (a) $\mathbf{A} + \mathbf{B}$, (b) $\mathbf{AB}$, (c) $[\mathbf{A}, \mathbf{B}]$, (d) $\tilde{\mathbf{A}}$, (e) $\mathbf{A}^*$, (f) $\mathbf{A}^\dagger$, (g) $\mathrm{Tr}(\mathbf{B})$, (h) $\det(\mathbf{B})$, and (i) $\mathbf{B}^{-1}$. Check that $\mathbf{B}\mathbf{B}^{-1} = \mathbf{1}$. Does $\mathbf{A}$ have an inverse?

*Problem 3.10 Using the square matrices in Problem 3.9 and the column matrices

$$\mathbf{a} = \begin{pmatrix} i \\ 2i \\ 2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 2 \\ (1-i) \\ 0 \end{pmatrix},$$

find (a) $\mathbf{Aa}$, (b) $\mathbf{a}^\dagger\mathbf{b}$, (c) $\tilde{\mathbf{a}}\mathbf{B}\mathbf{b}$, (d) $\mathbf{a}\mathbf{b}^\dagger$.

Problem 3.11 By explicit construction of the matrices in question, show that any matrix $\mathbf{T}$ can be written

(a) as the sum of a symmetric matrix $\mathbf{S}$ and an antisymmetric matrix $\mathbf{A}$;

(b) as the sum of a real matrix $\mathbf{R}$ and an imaginary matrix $\mathbf{I}$;

(c) as the sum of a Hermitian matrix $\mathbf{H}$ and a skew-Hermitian matrix $\mathbf{K}$.

*Problem 3.12 Prove Equations 3.52, 3.53, and 3.58. Show that the product of two unitary matrices is unitary. Under what conditions is the product of two Hermitian matrices Hermitian? Is the sum of two unitary matrices unitary? Is the sum of two Hermitian matrices Hermitian?

Problem 3.13 In the usual basis $(\hat{\imath}, \hat{\jmath}, \hat{k})$, construct the matrix $\mathbf{T}_x$ representing a rotation through angle θ about the x-axis, and the matrix $\mathbf{T}_y$ representing a rotation through angle θ about the y-axis. Suppose now we change bases, to $\hat{\imath}' = \hat{\jmath}$, $\hat{\jmath}' = -\hat{\imath}$, $\hat{k}' = \hat{k}$. Construct the matrix $\mathbf{S}$ that effects this change of basis, and check that $\mathbf{S}\mathbf{T}_x\mathbf{S}^{-1}$ and $\mathbf{S}\mathbf{T}_y\mathbf{S}^{-1}$ are what you would expect.

Problem 3.14 Show that similarity preserves matrix multiplication (that is if $\mathbf{A}^e\mathbf{B}^e = \mathbf{C}^e$, then $\mathbf{A}^f\mathbf{B}^f = \mathbf{C}^f$). Similarity does *not*, in general, preserve symmetry, reality, or Hermiticity; show, however, that if $\mathbf{S}$ is *unitary*, and $\mathbf{H}^e$ is Hermitian, then $\mathbf{H}^f$ is Hermitian. Show that $\mathbf{S}$ carries an orthonormal basis into another orthonormal basis if and only if it is unitary.

*Problem 3.15 Prove that $\mathrm{Tr}(\mathbf{T}_1\mathbf{T}_2) = \mathrm{Tr}(\mathbf{T}_2\mathbf{T}_1)$. It follows immediately that $\mathrm{Tr}(\mathbf{T}_1\mathbf{T}_2\mathbf{T}_3) = \mathrm{Tr}(\mathbf{T}_2\mathbf{T}_3\mathbf{T}_1)$, but is it the case that $\mathrm{Tr}(\mathbf{T}_1\mathbf{T}_2\mathbf{T}_3) = \mathrm{Tr}(\mathbf{T}_2\mathbf{T}_1\mathbf{T}_3)$, in general? Prove it, or disprove it. *Hint*: The best disproof is always a counterexample—and the simpler the better!

Problem 3.16 Show that the rows and columns of a unitary matrix constitute orthonormal sets.

3.1.4 Eigenvectors and Eigenvalues

Consider the linear transformation in three-space consisting of a rotation, about some specified axis, by an angle θ. Most vectors will change in a rather complicated way (they ride around on a cone about the axis), but vectors that happen to lie *along* the axis have very simple behavior: They don't change at all ($\hat{T}|\alpha\rangle = |\alpha\rangle$). If θ is 180°, then vectors which lie in the the "equatorial" plane reverse signs ($\hat{T}|\alpha\rangle = -|\alpha\rangle$). In a complex vector space,[11] *every* linear transformation has "special" vectors like these, which are transformed into simple multiples of themselves:

$$\hat{T}|\alpha\rangle = \lambda|\alpha\rangle; \qquad [3.68]$$

[11] This is *not* always true in a *real* vector space (where the scalars are restricted to real values). See Problem 3.17.

they are called **eigenvectors** of the transformation, and the (complex) number λ is their **eigenvalue**. (The *null* vector doesn't count, even though, in a trivial sense, it obeys Equation 3.68 for *any* $\hat{T}$ and *any* λ; technically, an eigenvector is any *nonzero* vector satisfying Equation 3.68.) Notice that any (nonzero) multiple of an eigenvector is still an eigenvector with the same eigenvalue.

With respect to a particular basis, the eigenvector equation assumes the matrix form

$$\mathbf{Ta} = \lambda\mathbf{a} \qquad [3.69]$$

(for nonzero $\mathbf{a}$), or

$$(\mathbf{T} - \lambda\mathbf{1})\mathbf{a} = \mathbf{0}. \qquad [3.70]$$

(Here $\mathbf{0}$ is the **zero matrix**, whose elements are all zero.) Now, if the matrix $(\mathbf{T} - \lambda\mathbf{1})$ had an *inverse*, we could multiply both sides of Equation 3.70 by $(\mathbf{T} - \lambda\mathbf{1})^{-1}$, and conclude that $\mathbf{a} = \mathbf{0}$. But by assumption $\mathbf{a}$ is *not* zero, so the matrix $(\mathbf{T} - \lambda\mathbf{1})$ must in fact be singular, which means that its determinant vanishes:

$$\det(\mathbf{T} - \lambda\mathbf{1}) = \begin{vmatrix} (T_{11} - \lambda) & T_{12} & \cdots & T_{1n} \\ T_{21} & (T_{22} - \lambda) & \cdots & T_{2n} \\ \vdots & \vdots & & \vdots \\ T_{n1} & T_{n2} & \cdots & (T_{nn} - \lambda) \end{vmatrix} = 0. \qquad [3.71]$$

Expansion of the determinant yields an algebraic equation for λ:

$$C_n\lambda^n + C_{n-1}\lambda^{n-1} + \cdots + C_1\lambda + C_0 = 0, \qquad [3.72]$$

where the coefficients C_i depend on the elements of $\mathbf{T}$ (see Problem 3.19). This is called the **characteristic equation** for the matrix; its solutions determine the eigenvalues. Notice that it's an nth-order equation, so it has n (complex) roots.[12] However, some of these may be duplicates, so all we can say for certain is that an $n \times n$ matrix has *at least one* and *at most* n distinct eigenvalues. To construct the corresponding eigenvectors it is generally easiest simply to plug each λ back into Equation 3.69 and solve "by hand" for the components of $\mathbf{a}$. I'll show you how it goes by working out an example.

Example. Find the eigenvalues and eigenvectors of the following matrix:

$$\mathbf{M} = \begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}. \qquad [3.73]$$

The characteristic equation is

$$\begin{vmatrix} (2-\lambda) & 0 & -2 \\ -2i & (i-\lambda) & 2i \\ 1 & 0 & (-1-\lambda) \end{vmatrix} = -\lambda^3 + (1+i)\lambda^2 - i\lambda = 0, \qquad [3.74]$$

[12] It is here that the case of *real* vector spaces becomes more awkward, because the characteristic equation need not have any (real) solutions at all. See footnote 11 and Problem 3.17.

and its roots are 0, 1, and i. Call the components of the first eigenvector (a_1, a_2, a_3); then

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

which yields three equations:

$$\begin{aligned} 2a_1 - 2a_3 &= 0, \\ -2ia_1 + ia_2 + 2ia_3 &= 0, \\ a_1 - a_3 &= 0. \end{aligned}$$

The first determines a_3 (in terms of a_1): $a_3 = a_1$; the second determines a_2: $a_2 = 0$; and the third is redundant. We may as well pick $a_1 = 1$ (since any multiple of an eigenvector is still an eigenvector):

$$\mathbf{a}^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \text{ for } \lambda_1 = 0. \qquad [3.75]$$

For the second eigenvector (recycling the same notation for the components) we have

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 1\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix},$$

which leads to the equations

$$\begin{aligned} 2a_1 - 2a_3 &= a_1, \\ -2ia_1 + ia_2 + 2ia_3 &= a_2, \\ a_1 - a_3 &= a_3, \end{aligned}$$

with the solution $a_3 = (1/2)a_1$, $a_2 = [(1-i)/2]a_1$; this time we'll pick $a_1 = 2$, so that

$$\mathbf{a}^{(2)} = \begin{pmatrix} 2 \\ (1-i) \\ 1 \end{pmatrix}, \text{ for } \lambda_2 = 1. \qquad [3.76]$$

Finally, for the third eigenvector,

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = i\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} ia_1 \\ ia_2 \\ ia_3 \end{pmatrix},$$

which gives the equations

$$\begin{aligned} 2a_1 - 2a_3 &= ia_1, \\ -2ia_1 + ia_2 + 2ia_3 &= ia_2, \\ a_1 - a_3 &= ia_3, \end{aligned}$$

whose solution is $a_3 = a_1 = 0$, with a_2 undetermined. Choosing $a_2 = 1$, we conclude

$$\mathbf{a}^{(3)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \text{ for } \lambda_3 = i. \qquad [3.77]$$

If the eigenvectors span the space (as they do in the preceding example), we are free to use *them* as a basis:

$$\begin{aligned} \hat{T}|f_1\rangle &= \lambda_1|f_1\rangle, \\ \hat{T}|f_2\rangle &= \lambda_2|f_2\rangle, \\ &\cdots \\ \hat{T}|f_n\rangle &= \lambda_n|f_n\rangle. \end{aligned}$$

The matrix representing $\hat{T}$ takes on a very simple form in this basis, with the eigenvalues strung out along the main diagonal and all other elements zero:

$$\mathbf{T} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}. \qquad [3.78]$$

The (normalized) eigenvectors are equally simple:

$$\mathbf{a}^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \mathbf{a}^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \cdots, \quad \mathbf{a}^{(n)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}. \qquad [3.79]$$

A matrix that can be brought to **diagonal form** (Equation 3.78) by a change of basis is said to be **diagonalizable**. The similarity matrix that accomplishes the transformation can be constructed by using the eigenvectors (in the old basis) as the columns of $\mathbf{S}^{-1}$:

$$(\mathbf{S}^{-1})_{ij} = (\mathbf{a}^{(j)})_i. \qquad [3.80]$$

Example (cont'd). In the example,

$$\mathbf{S}^{-1} = \begin{pmatrix} 1 & 2 & 0 \\ 0 & (1-i) & 1 \\ 1 & 1 & 0 \end{pmatrix},$$

so (using Equation 3.57)

$$\mathbf{S} = \begin{pmatrix} -1 & 0 & 2 \\ 1 & 0 & -1 \\ (i-1) & 1 & (1-i) \end{pmatrix},$$

and you can check for yourself that

$$\mathbf{STS}^{-1} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{pmatrix}.$$

There is a great advantage in bringing a matrix to diagonal form—it's much easier to work with. Unfortunately, not every matrix *can* be diagonalized—the eigenvectors have to span the space. For an example of a matrix that *cannot* be diagonalized, see Problem 3.18.

***Problem 3.17** The 2×2 matrix representing a rotation of the xy-plane is

$$\mathbf{T} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

Show that (except for certain special angles—what are they?) this matrix has no real eigenvalues. (This reflects the *geometrical* fact that no vector in the plane is carried into itself under such a rotation; contrast rotations in *three* dimensions.) This matrix *does*, however, have *complex* eigenvalues and eigenvectors. Find them. Construct a matrix $\mathbf{S}$ which diagonalizes $\mathbf{T}$. Perform the similarity transformation $(\mathbf{STS}^{-1})$ explicitly, and show that it reduces $\mathbf{T}$ to diagonal form.

Problem 3.18 Find the eigenvalues and eigenvectors of the following matrix:

$$\mathbf{M} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}.$$

Can this matrix be diagonalized?

Problem 3.19 Show that the first, second, and last coefficients in the characteristic equation (Equation 3.72) are

$$C_n = (-1)^n, \; C_{n-1} = (-1)^{n-1}\mathrm{Tr}(\mathbf{T}), \text{ and } C_0 = \det(\mathbf{T}). \qquad [3.81]$$

For a 3×3 matrix with elements T_{ij}, what is C_1?

Problem 3.20 It is pretty obvious that the trace of a *diagonal* matrix is the sum of its eigenvalues, and its determinant is their product (see Equation 3.78). It follows (from Equations 3.64 and 3.67) that the same holds for any *diagonalizable* matrix. Prove that

$$\det(\mathbf{T}) = \lambda_1\lambda_2\cdots\lambda_n, \quad \mathrm{Tr}(\mathbf{T}) = \lambda_1 + \lambda_2 + \cdots + \lambda_n \qquad [3.82]$$

for *any* matrix. (The λ's are the n solutions to the characteristic equation—in the case of multiple roots, there may be fewer linearly independent eigen*vectors* than there

are solutions, but we still count each λ as many times as it occurs.) *Hint*: Write the characteristic equation in the form

$$(\lambda_1 - \lambda)(\lambda_2 - \lambda)\cdots(\lambda_n - \lambda) = 0,$$

and use the result of Problem 3.19.

3.1.5 Hermitian Transformations

In Equation 3.48 I defined the Hermitian conjugate (or "adjoint") of a *matrix* as its transpose conjugate: $\mathbf{T}^\dagger = \tilde{\mathbf{T}}^*$. Now I want to give you a more fundamental definition for the Hermitian conjugate of a *linear transformation*: It is that transformation $\hat{T}^\dagger$ which, when applied to the *first* member of an inner product, gives the same result as if $\hat{T}$ itself had been applied to the *second* vector:

$$\langle \hat{T}^\dagger \alpha | \beta \rangle = \langle \alpha | \hat{T}\beta \rangle \qquad [3.83]$$

(for all vectors $|\alpha\rangle$ and $|\beta\rangle$).[13] [I have to warn you that although everybody uses it, this is lousy notation. For α and β are not *vectors* (the *vectors* are $|\alpha\rangle$ and $|\beta\rangle$), they are *labels*—serial numbers ("F43A-9GT"), or names ("Charlie"), or bar codes—anything you care to use to identify the different vectors. In particular, they are endowed with no mathematical properties at all, and the expression "$\hat{T}\beta$" is literally *nonsense*: linear transformations act on *vectors*, not *labels*. But it's pretty clear what the notation *means*: $|\hat{T}\beta\rangle$ means $\hat{T}|\beta\rangle$, and $\langle \hat{T}^\dagger \alpha | \beta \rangle$ means the inner product of the vector $\hat{T}^\dagger|\alpha\rangle$ with the vector $|\beta\rangle$. Notice in particular that

$$\langle \alpha | c\beta \rangle = c\langle \alpha | \beta \rangle, \qquad [3.84]$$

but

$$\langle c\alpha | \beta \rangle = c^* \langle \alpha | \beta \rangle \qquad [3.85]$$

for any scalar c.] If you're working in an orthonormal basis (as we always shall), the Hermitian conjugate of a linear transformation is represented by the Hermitian conjugate of the corresponding matrix (so the terminology is consistent); for (using Equations 3.50 and 3.53),

$$\langle \alpha | \hat{T}\beta \rangle = \mathbf{a}^\dagger \mathbf{T}\mathbf{b} = (\mathbf{T}^\dagger \mathbf{a})^\dagger \mathbf{b} = \langle \hat{T}^\dagger \alpha | \beta \rangle. \qquad [3.86]$$

In quantum mechanics, a fundamental role is played by Hermitian transformations ($\hat{T}^\dagger = \hat{T}$). The eigenvectors and eigenvalues of a Hermitian transformation have three crucial properties:

[13] If you're wondering whether such a transformation necessarily *exists*, you should have been a math major. Still, it's a good question, and the answer is yes. See, for instance, Halmos, (footnote 1), Section 44.

1. The eigenvalues of a Hermitian transformation are real.

Proof: Let λ be an eigenvalue of $\hat{T}$: $\hat{T}|\alpha\rangle = \lambda|\alpha\rangle$, with $|\alpha\rangle \neq |0\rangle$. Then

$$\langle \alpha | \hat{T}\alpha \rangle = \langle \alpha | \lambda\alpha \rangle = \lambda \langle \alpha | \alpha \rangle.$$

Meanwhile, if $\hat{T}$ is Hermitian, then

$$\langle \alpha | \hat{T}\alpha \rangle = \langle \hat{T}\alpha | \alpha \rangle = \langle \lambda\alpha | \alpha \rangle = \lambda^* \langle \alpha | \alpha \rangle.$$

But $\langle \alpha | \alpha \rangle \neq 0$ (Equation 3.20), so $\lambda = \lambda^*$, and hence λ is real. QED

2. The eigenvectors of a Hermitian transformation belonging to distinct eigenvalues are orthogonal.

Proof: Suppose $\hat{T}|\alpha\rangle = \lambda|\alpha\rangle$ and $\hat{T}|\beta\rangle = \mu|\beta\rangle$, with $\lambda \neq \mu$. Then

$$\langle \alpha | \hat{T}\beta \rangle = \langle \alpha | \mu\beta \rangle = \mu \langle \alpha | \beta \rangle,$$

and if $\hat{T}$ is Hermitian,

$$\langle \alpha | \hat{T}\beta \rangle = \langle \hat{T}\alpha | \beta \rangle = \langle \lambda\alpha | \beta \rangle = \lambda^* \langle \alpha | \beta \rangle.$$

But $\lambda = \lambda^*$ (from property 1), and $\lambda \neq \mu$, by assumption, so $\langle \alpha | \beta \rangle = 0$. QED

3. The eigenvectors of a Hermitian transformation span the space.

Comment: If all the n roots of the characteristic equation are distinct, then (by property 2) we have n mutually orthogonal eigenvectors, so they *obviously* span the space. But what if there are duplicate roots (or, as they are called, in this context, **degenerate** eigenvalues)? Suppose λ is m-fold degenerate; any *linear combination* of two eigenvectors belonging to the same eigenvalue is still an eigenvector (with the same eigenvalue)—what we must show is that there are m *linearly independent* eigenvectors with eigenvalue λ. The proof is given in most books on linear algebra,[14] and I shall not repeat it here. These eigenvectors can be orthogonalized by the Gram-Schmidt procedure (see Problem 3.4), so in fact the eigenvectors of a Hermitian transformation can always be taken to constitute an orthonormal basis. It follows, in particular, that *any Hermitian matrix can be diagonalized by a similarity transformation, with* $\mathbf{S}$ *unitary*. This rather technical result is, in a sense, the mathematical support on which much of quantum mechanics leans. As we shall see, it turns out to be a thinner reed than one might have hoped.

[14] I like the treatment in F. W. Byron, Jr., and R. W. Fuller, *Mathematics of Classical and Quantum Physics* (Reading, MA: Addison-Wesley, 1969), Vol. I, Section 4.7.

Problem 3.21 A Hermitian linear transformation must satisfy $\langle\alpha|\hat{T}\beta\rangle = \langle\hat{T}\alpha|\beta\rangle$ for all vectors $|\alpha\rangle$ and $|\beta\rangle$. Prove that it is (surprisingly) sufficient that $\langle\gamma|\hat{T}\gamma\rangle = \langle\hat{T}\gamma|\gamma\rangle$ for all vectors $|\gamma\rangle$. Suppose you could show that $\langle e_n|\hat{T}e_n\rangle = \langle\hat{T}e_n|e_n\rangle$ for every member of an orthonormal basis. Does it necessarily follow that $\hat{T}$ is Hermitian? *Hint*: First let $|\gamma\rangle = |\alpha\rangle + |\beta\rangle$, and then let $|\gamma\rangle = |\alpha\rangle + i|\beta\rangle$.

*Problem 3.22 Let

$$\mathbf{T} = \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix}.$$

(a) Verify that **T** is Hermitian.

(b) Find its eigenvalues (note that they are real).

(c) Find and normalize the eigenvectors (note that they are orthogonal).

(d) Construct the unitary diagonalizing matrix **S**, and check explicitly that it diagonalizes **T**.

(e) Check that det(**T**) and Tr(**T**) are the same for **T** as they are for its diagonalized form.

**Problem 3.23 Consider the following Hermitian matrix:

$$\mathbf{T} = \begin{pmatrix} 2 & i & 1 \\ -i & 2 & i \\ 1 & -i & 2 \end{pmatrix}.$$

(a) Calculate det(**T**) and Tr(**T**).

(b) Find the eigenvalues of **T**. Check that their sum and product are consistent with (a), in the sense of Equation 3.82. Write down the diagonalized version of **T**.

(c) Find the eigenvectors of **T**. Within the degenerate sector, construct two linearly independent eigenvectors (it is this step that is always possible for a *Hermitian* matrix, but not for an *arbitrary* matrix—contrast Problem 3.18). Orthogonalize them, and check that both are orthogonal to the third. Normalize all three eigenvectors.

(d) Construct the unitary matrix **S** that diagonalizes **T**, and show explicitly that the similarity transformation using **S** reduces **T** to the appropriate diagonal form.

Problem 3.24 A *unitary* linear transformation is one for which $\hat{U}^\dagger\hat{U} = 1$.

(a) Show that unitary transformations preserve inner products, in the sense that $\langle\hat{U}\alpha|\hat{U}\beta\rangle = \langle\alpha|\beta\rangle$, for all vectors $|\alpha\rangle$, $|\beta\rangle$.

(b) Show that the eigenvalues of a unitary transformation have modulus 1.

(c) Show that the eigenvectors of a unitary transformation belonging to distinct eigenvalues are orthogonal.

3.2 FUNCTION SPACES

We are ready now to apply the machinery of linear algebra to the interesting and important case of **function spaces**, in which the "vectors" are (complex) functions of x, inner products are integrals, and derivatives appear as linear transformations.

3.2.1 Functions as Vectors

Do functions really behave as vectors? Well, is the sum of two functions a function? Sure. Is addition of functions commutative and associative? Indeed. Is there a "null" function? Yes: $f(x) \equiv 0$. If you multiply a function by a complex number, do you get another function? Of course. Now, the set of *all* functions is a bit unwieldy—we'll be concerned with special *classes* of functions, such as the set of all polynomials of degree $< N$ (Problem 3.2), or the set of all odd functions that go to zero at $x = 1$, or the set of all periodic functions with period π. Of course, when you start imposing conditions like this, you've got to make sure that you still meet the requirements for a vector space. For example, the set of all functions whose maximum value is 3 would *not* constitute a vector space (multiplication by 2 would give you functions with maximum value 6, which are outside the space).

The inner product of two functions [$f(x)$ and $g(x)$] is defined by the integral

$$\langle f|g\rangle = \int f(x)^* g(x)\, dx \qquad [3.87]$$

(the limits will depend on the domain of the functions in question). You can check for yourself that it satisfies the three conditions (Equations 3.19, 3.20, and 3.21) for an inner product. Of course, this integral may not *converge*, so if we want a function space with an inner product, we must restrict the class of functions so as to ensure that $\langle f|g\rangle$ is always well defined. It is clearly *necessary* that every admissible function be **square integrable**:

$$\int |f(x)|^2\, dx < \infty \qquad [3.88]$$

(otherwise the inner product of f with *itself* wouldn't even exist). As it turns out,

Table 3.1: The first few Legendre polynomials, $P_n(x)$.

$P_0 = 1$
$P_1 = x$
$P_2 = \frac{1}{2}(3x^2 - 1)$
$P_3 = \frac{1}{2}(5x^3 - 3x)$
$P_4 = \frac{1}{8}(35x^4 - 30x^2 + 3)$
$P_5 = \frac{1}{8}(63x^5 - 70x^3 + 15x)$

this restriction is also *sufficient*—if f and g are both square integrable, then the integral in Equation 3.87 is necessarily finite.[15]

For example, consider the set $P(N)$ of all *polynomials* of degree $< N$:

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{N-1} x^{N-1}, \qquad [3.89]$$

on the interval $-1 \leq x \leq 1$. They are certainly square integrable, so this is a bona fide inner product space. An obvious basis is the set of powers of x:

$$|e_1\rangle = 1, \ |e_2\rangle = x, \ |e_3\rangle = x^2, \ \ldots, \ |e_N\rangle = x^{N-1}; \qquad [3.90]$$

evidently it's an N-dimensinal vector space. This is *not*, however, an *orthonormal* basis, for

$$\langle e_1|e_1\rangle = \int_{-1}^{1} 1 \, dx = 2, \quad \langle e_1|e_3\rangle = \int_{-1}^{1} x^2 \, dx = 2/3,$$

and so on. If you apply the Gram-Schmidt procedure, to orthonormalize this basis (Problem 3.25), you get the famous **Legendre polynomials**, $P_n(x)$ (except that Legendre, who had other things on his mind, didn't normalize them properly):

$$|e_n'\rangle = \sqrt{n - (1/2)}\, P_{n-1}(x), \quad (n = 1, 2, \ldots, N). \qquad [3.91]$$

In Table 3.1 I have listed the first few Legendre polynomials.

***Problem 3.25** Orthonormalize the powers of x, on the interval $-1 \leq x \leq 1$, to obtain the first four Legendre polynomials (Equation 3.91).

***Problem 3.26** Let $T(N)$ be the set of all trigonometric functions of the form

$$f(x) = \sum_{n=0}^{N-1} [a_n \sin(n\pi x) + b_n \cos(n\pi x)], \qquad [3.92]$$

[15] There is a quick phoney "proof" of this, based on the Schwarz inequality (Equation 3.27). The trouble is, we *assumed* the existence of the inner product in proving the Schwarz inequality (Problem 3.5), so the logic is circular. For a legitimate proof, see F. Riesz and B. Sz.-Nagy, *Functional Analysis* (New York: Unger, 1955), Section 21.

on the interval $-1 \leq x \leq 1$. Show that

$$|e_n\rangle = \frac{1}{\sqrt{2}} e^{in\pi x}, \quad (n = 0, \pm 1, \ldots, \pm(N-1)) \qquad [3.93]$$

constitutes an orthonormal basis. What is the dimension of this space?

Problem 3.27 Consider the set of all functions of the form $p(x)e^{-x^2/2}$, where $p(x)$ is again a polynomial of degree $< N$ in x, on the interval $-\infty < x < \infty$. Check that they constitute an inner product space. The "natural" basis is

$$|e_1\rangle = e^{-x^2/2}, \ |e_2\rangle = xe^{-x^2/2}, \ |e_3\rangle = x^2 e^{-x^2/2}, \ \ldots, \ |e_N\rangle = x^{N-1} e^{-x^2/2}.$$

Orthonormalize the first four of these, and comment on the result.

3.2.2 Operators as Linear Transformations

In function spaces *operators* (such as d/dx, d^2/dx^2, or simply x) behave as linear transformations, provided that they carry functions in the space into other functions in the space and satisfy the linearity condition (Equation 3.29). For example, in the polynomial space $P(N)$ the derivative operator ($\hat{D} \equiv d/dx$) is a linear transformation, but the operator $\hat{x}$ (multiplication by x)[16] is *not*, for it takes $(N-1)$th-order polynomials into Nth-order polynomials, which are no longer in the space.

In a function space, the eigenvectors of an operator $\hat{T}$ are called **eigenfunctions**:

$$\hat{T}f(x) = \lambda f(x). \qquad [3.94]$$

For example, the eigenfunctions of $\hat{D}$ are

$$f_\lambda(x) = Ae^{\lambda x}. \qquad [3.95]$$

Evidently this operator has only *one* eigenfunction (the one with $\lambda = 0$) in the space $P(N)$.

A Hermitian operator is one that satisfies the defining condition (Equation 3.83):

$$\langle f|\hat{T}g\rangle = \langle \hat{T}f|g\rangle, \qquad [3.96]$$

for all functions $f(x)$ and $g(x)$ in the space. Is the derivative operator Hermitian? Well, using integration by parts, we get

$$\langle f|\hat{D}g\rangle = \int_a^b f^* \frac{dg}{dx} dx = (f^*g)\Big|_a^b - \int_a^b \frac{df^*}{dx} g \, dx = (f^*g)\Big|_a^b - \langle \hat{D}f|g\rangle. \qquad [3.97]$$

[16] For consistency, I'll put a hat on x when I'm emphasizing its role as an operator, but you're welcome to ignore it if you think I'm being too fastidious.

It's *close*, but the sign is wrong, and there's an unwanted boundary term. The sign is easily disposed of: $\hat{D}$ itself is (except for the boundary term) *skew* Hermitian, so $i\hat{D}$ would be Hermitian—complex conjugation of the i compensates for the minus sign coming from integration by parts. As for the boundary term, it will go away if we restrict ourselves to functions which have the same value at the two ends:

$$f(b) = f(a). \qquad [3.98]$$

In practice, we shall almost always be working on the *infinite* interval ($a = -\infty$, $b = +\infty$), where square integrability (Equation 3.88) guarantees that $f(a) = f(b) = 0$, and hence that $i\hat{D}$ is Hermitian. But $i\hat{D}$ is *not* Hermitian in the polynomial space $P(N)$.

By now you will realize that when dealing with operators you must always keep in mind the function space you're working in—an innocent-looking operator may not be a legitimate linear transformation, because it carries functions out of the space; the eigenfunctions of an operator may not reside in the space; and an operator that's Hermitian in one space may *not* be Hermitian in another. However, these are relatively harmless problems—they can startle you, if you're not expecting them, but they don't bite. A much more dangerous snake is lurking here, but it only inhabits vector spaces of infinite dimension. I noted a moment ago that $\hat{x}$ is not a linear transformation in the space $P(N)$ (multiplication by x increases the order of the polynomial and hence takes functions outside the space). However, it *is* a linear transformation on $P(\infty)$, the space of *all* polynomials on the interval $-1 \leq x \leq 1$. In fact, it's a *Hermitian* transformation, since (obviously)

$$\int_{-1}^{1} [f(x)]^*[xg(x)]\,dx = \int_{-1}^{1} [xf(x)]^*[g(x)]\,dx.$$

But what are its eigenfunctions? Well,

$$x(a_0 + a_1x + a_2x^2 + \cdots) = \lambda(a_0 + a_1x + a_2x^2 + \cdots),$$

for all x, means

$$\begin{aligned} 0 &= \lambda a_0, \\ a_0 &= \lambda a_1, \\ a_1 &= \lambda a_2, \end{aligned}$$

and so on. If $\lambda = 0$, then all the components are zero, and that's not a legal eigenvector; but if $\lambda \neq 0$, the first equation says $a_0 = 0$, so the second gives $a_1 = 0$, and the third says $a_2 = 0$, and so on, and we're back in the same bind. *This* Hermitian operator doesn't have a complete set of eigenfunctions—in fact it doesn't have *any at all!* Not, at any rate, in $P(\infty)$.

What *would* an eigenfunction of $\hat{x}$ look like? If

$$xg(x) = \lambda g(x), \qquad [3.99]$$

where λ, remember, is a constant, then everywhere *except* at the one point $x = \lambda$ we must have $g(x) = 0$. Evidently the eigenfunctions of $\hat{x}$ are Dirac delta functions:

$$g_\lambda(x) = B\delta(x - \lambda), \qquad [3.100]$$

and since delta functions are certainly not polynomials, it is no wonder that the operator $\hat{x}$ has no eigenfunctions in $P(\infty)$.

The moral of the story is that whereas the first two theorems in Section 3.1.5 are completely general (the eigenvalues of a Hermitian operator are real, and the eigenvectors belonging to different eigenvalues are orthogonal), the third one (completeness of the eigenvectors) is valid (in general) only for finite-dimensional spaces. In infinite-dimensional spaces some Hermitian operators have complete sets of eigenvectors (see Problem 3.32d for an example), some have *in*complete sets, and some (as we just saw) have no eigenvectors (in the space) at all.[17] Unfortunately, the completeness property is absolutely essential in quantum mechanical applications. In Section 3.3 I'll show you how we manage this problem.

Problem 3.28 Show that $\exp(-x^2/2)$ is an eigenfunction of the operator $Q = (d^2/dx^2) - x^2$, and find its eigenvalue.

***Problem 3.29**

(a) Construct the matrix **D** representing the derivative operator $\hat{D} = d/dx$ with respect to the (nonorthonormal) basis (Equation 3.90) in $P(N)$.

(b) Construct the matrix representing $\hat{D}$ with respect to the (orthonormal) basis (Equation 3.93) in the space $T(N)$ of Problem 3.26.

(c) Construct the matrix **X** representing the operator $\hat{x} = x$ with respect to the basis (Equation 3.90) in $P(\infty)$. If this is a Hermitian operator (and it *is*), how come the matrix is not equal to its transpose conjugate?

****Problem 3.30** Construct the matrices **D** and **X** in the (orthonormal) basis (Equation 3.91) for $P(\infty)$. You will need to use two recursion formulas for Legendre polynomials:

$$xP_n(x) = \frac{1}{(2n+1)}[(n+1)P_{n+1}(x) + nP_{n-1}(x)]; \qquad [3.101]$$

$$\frac{dP_n}{dx} = \sum_{k=0}(2n - 4k - 1)P_{n-2k-1}(x), \qquad [3.102]$$

---

[17] In an n-dimensional vector space, every linear transformation can be represented (with respect to a particular basis) by an $n \times n$ matrix, and as long as n is finite, the characteristic Equation 3.71 is guaranteed to deliver at least one eigenvalue. But if n is *infinite*, we can't take the determinant, there *is* no characteristic equation, and hence there is no assurance that even a *single* eigenvector exists.

where the sum cuts off at the first term with a negative index. Confirm that $\mathbf{X}$ is Hermitian but $i\mathbf{D}$ is not.

Problem 3.31 Consider the operator $\hat{D}^2 = d^2/dx^2$. Under what conditions (on the admissable functions) is it a Hermitian operator? Construct the matrix representing $\hat{D}^2$ in $P(N)$ (with respect to the basis Equation 3.90), and confirm that it is the square of the matrix representing $\hat{D}$ (Problem 3.29a).

Problem 3.32

(a) Show that $i\hat{D}$ is Hermitian in the space $T(N)$ of Problem 3.26.

(b) What are its eigenvalues and (normalized) eigenfunctions, in $T(N)$?

(c) Check that your results in (b) satisfy the three theorems in Section 3.1.5.

(d) Confirm that $i\hat{D}$ has a complete set of eigenfunctions in $T(\infty)$ (quote the pertinent theorem from Fourier analysis).

3.2.3 Hilbert Space

To construct the real number system, mathematicians typically begin with the *integers*, and use them to define the *rationals* (ratios of integers). They proceed to show that the rational numbers are "dense," in the sense that between any two of them (no matter how close together they are) you can always find another one (in fact, infinitely many of them). And yet, the set of all rational numbers has "gaps" in it, for you can easily think of infinite *sequences* of rational numbers whose *limit* is *not* a rational number. For example,

$$A_N = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots \pm \frac{1}{N} \qquad [3.103]$$

is a rational number for any finite integer N, but its limit (as $N \to \infty$) is $\ln 2$, which is *not* a rational number. So the final step in constructing the real numbers is to "fill in the gaps", or "complete" the set, by including the limits of all convergent sequences of rational numbers. (Of course, some sequences don't *have* limits, and those we do not include. For example, if you change the minus signs in Equation 3.103 to plus signs, the sequence does not converge, and it doesn't correspond to *any* real number.)

The same thing happens with function spaces. For example, the set of all polynomials, $P(\infty)$, includes functions of the form

$$f_N(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \frac{x^4}{4!} + \cdots + \frac{x^N}{N!} \qquad [3.104]$$

(for finite N), but it does *not* include the limit as $N \to \infty$:

$$1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \cdots = \sum_{n=0}^{\infty} \frac{x^n}{n!} = e^x. \qquad [3.105]$$

For e^x is not itself a polynomial, although it *is* the limit of a *sequence* of polynomials. To *complete* the space, we would like to include all such functions. Of course, some sequences of polynomials don't have limits, or have them only for a restricted range of x. For example, the series

$$1 + x + x^2 + x^3 + \cdots = \frac{1}{1-x}$$

converges only for $|x| < 1$. And even if the sequence does have a limit, the limit function may not be square integrable, so we can't include it in an inner product space. To complete the space, then, we throw in all square-integrable convergent sequences of functions in the space. Notice that completing a space does not involve the introduction of any new basis vectors; it is just that we now allow linear combinations involving an infinite number of terms,

$$|\alpha\rangle = \sum_{j=1}^{\infty} a_j |e_j\rangle, \qquad [3.106]$$

provided $\langle\alpha|\alpha\rangle$ is finite—which is to say (if the basis is orthonormal), provided

$$\sum_{j=1}^{\infty} |a_j|^2 < \infty. \qquad [3.107]$$

A **complete**[18] inner product space is called a **Hilbert space.**[19] The completion of $P(\infty)$ is easy to characterize: It is nothing less than the set of *all* square-integrable functions on the interval $-1 < x < +1$; we call it $L_2(-1, +1)$. More generally, the set of all square-integrable functions on the interval $a < x < b$ is $L_2(a, b)$. We shall be concerned primarily with the Hilbert space $L_2(-\infty, +\infty)$ (or L_2, for short), because this is where quantum mechanical wave functions live. Indeed, to physicists L_2 is practically synonymous with "Hilbert space".

The eigenfunctions of the Hermitian operators $i\hat{D} = id/dx$ and $\hat{x} = x$ are of particular importance. As we have already found (Equations 3.95 and 3.100), they take the form

$$f_\lambda(x) = A_\lambda e^{-i\lambda x}, \quad \text{and} \quad g_\lambda(x) = B_\lambda \delta(x - \lambda),$$

respectively. Note that there is no restriction on the eigenvalues—*every* real number is an eigenvalue of $i\hat{D}$, and *every* real number is an eigenvalue of $\hat{x}$. The set of all eigenvalues of a given operator is called its **spectrum**; $i\hat{D}$ and $\hat{x}$ are operators with **continuous spectra**, in contrast to the **discrete spectra** we have encountered

[18] Note the two entirely different uses of the word "complete": a *set of vectors* is complete if it spans the space; an *inner product space* is complete if it has no "holes" in it (i.e., it includes all its limits).

[19] Every finite-dimensional inner product space is trivially complete, so they're all technically Hilbert spaces, but the term is usually reserved for *infinite*-dimensional spaces.

heretofore. Unfortunately, these eigenfunctions *do not lie in Hilbert space*, and hence, in the strictest sense, do not count as vectors at all. For neither of them is square-integrable:

$$\int_{-\infty}^{\infty} f_\lambda(x)^* f_\lambda(x)\,dx = |A_\lambda|^2 \int_{-\infty}^{\infty} e^{i\lambda x} e^{-i\lambda x}\,dx = |A_\lambda|^2 \int_{-\infty}^{\infty} 1\,dx \to \infty,$$

and

$$\int_{-\infty}^{\infty} g_\lambda(x)^* g_\lambda(x)\,dx = |B_\lambda|^2 \int_{-\infty}^{\infty} \delta(x-\lambda)\delta(x-\lambda)\,dx = |B_\lambda|^2 \delta(\lambda-\lambda) \to \infty.$$

Nevertheless, they do satisfy a kind of orthogonality condition:

$$\int_{-\infty}^{\infty} f_\lambda(x)^* f_\mu(x)\,dx = A_\lambda^* A_\mu \int_{-\infty}^{\infty} e^{i\lambda x} e^{-i\mu x}\,dx = |A_\lambda|^2 2\pi\delta(\lambda-\mu)$$

(see Equation 2.126), and

$$\int_{-\infty}^{\infty} g_\lambda(x)^* g_\mu(x)\,dx = B_\lambda^* B_\mu \int_{-\infty}^{\infty} \delta(x-\lambda)\delta(x-\mu)\,dx = |B_\lambda|^2 \delta(\lambda-\mu).$$

It is customary to "normalize" these (unnormalizable) functions by picking the constant so as to leave an unadorned Dirac delta function on the right side (replacing the *Kronecker* delta in the usual orthonormality condition; Equation 3.23).[20] Thus

$$f_\lambda(x) = \frac{1}{\sqrt{2\pi}} e^{-i\lambda x}, \text{ with } \langle f_\lambda | f_\mu \rangle = \delta(\lambda-\mu), \qquad [3.108]$$

are the "normalized" eigenfunctions of $i\hat{D}$, and

$$g_\lambda(x) = \delta(x-\lambda), \text{ with } \langle g_\lambda | g_\mu \rangle = \delta(\lambda-\mu), \qquad [3.109]$$

are the "normalized" eigenfunctions of $\hat{x}$.[21]

What if we use the "normalized" eigenfunctions of $i\hat{D}$ and $\hat{x}$ as bases for L_2?[22] Because the spectrum is continuous, the linear combination becomes an integral:

$$|f\rangle = \int_{-\infty}^{\infty} a_\lambda |f_\lambda\rangle\,d\lambda; \quad |f\rangle = \int_{-\infty}^{\infty} b_\lambda |g_\lambda\rangle\,d\lambda. \qquad [3.110]$$

[20] I'll call this "normalization" (in quotes) so you won't confuse it with the real thing.

[21] We are engaged here in a dangerous stretching of the rules, pioneered by Dirac (who had a kind of inspired confidence that he could get away with it) and disparaged by von Neumann (who was more sensitive to mathematical niceties), in their rival classics (P. A. M. Dirac, *The Principles of Quantum Mechanics*, first published in 1930, 4th ed., Oxford (Clarendon Press) 1958, and J. von Neumann, *The Mathematical Foundations of Quantum Mechanics*, first published in 1932, revised by Princeton Univ. Press, 1955). **Dirac notation** invites us to apply the language and methods of linear algebra to functions that lie in the "almost normalizable" suburbs of Hilbert space. It turns out to be powerful and effective beyond any reasonable expectation.

[22] That's right: We're going to use, as bases, sets of functions none of which is actually in the space! They may not be normalizable, but they *are* complete, and that's all we need.

Taking the inner product with $|f_\mu\rangle$, and exploiting the "orthonormality" of the basis (Equation 3.108), we obtain the "components" a_λ:

$$\langle f_\mu | f \rangle = \int_{-\infty}^{\infty} a_\lambda \langle f_\mu | f_\lambda \rangle\,d\lambda = \int_{-\infty}^{\infty} a_\lambda \delta(\mu-\lambda)\,d\lambda = a_\mu.$$

So

$$a_\lambda = \langle f_\lambda | f \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\lambda x} f(x)\,dx = F(-\lambda); \qquad [3.111]$$

evidently the $-\lambda$ "component" of the vector $|f\rangle$, in the basis of eigenfunctions of $i\hat{D}$, is the *Fourier transform* (Equation 2.85) of the function $f(x)$. Likewise,

$$b_\lambda = \langle g_\lambda | f \rangle = \int_{-\infty}^{\infty} \delta(x-\lambda) f(x)\,dx = f(\lambda), \qquad [3.112]$$

so the λ "component" of the vector $|f\rangle$ in the *position* basis is $f(\lambda)$ itself. [If that sounds like double-talk, remember that $|f\rangle$ is an abstract vector, which can be expressed with respect to any basis you like; in this sense the *function* $f(x)$ is merely the collection of its "components" in the particular basis consisting of eigenvectors of the position operator.] Meanwhile, we can no longer represent operators by matrices because the basis vectors are labeled by a nondenumerable index. Nevertheless, we are still interested in quantities of the form

$$\langle f_\lambda | \hat{T} | f_\mu \rangle,$$

which, by force of habit, we shall call the λ, μ **matrix element** of the operator $\hat{T}$.

Problem 3.33

(a) Show that any linear combination of two functions in $L_2(a,b)$ is still in $L_2(a,b)$. If this *weren't* true, of course, $L_2(a,b)$ wouldn't be a vector space at all.

(b) For what range of (real) ν is the function $f(x) = |x|^\nu$ in $L_2(-1,+1)$?

(c) For what range of a is the function $f(x) = 1 - x + x^2 - x^3 + \cdots$ in $L_2(-a,+a)$?

(d) Show that the function $f(x) = e^{-|x|}$ is in L_2, and find its "components" in the basis (Equation 3.108).

(e) Find the matrix elements of the operator $\hat{D}^2$ with respect to the basis (Equation 3.108) of L_2.

Problem 3.34 $L_2(-1,+1)$ includes *discontinuous* functions [such as the step function, $\theta(x)$, Equation [2.125], which are not differentiable. But functions expressible as Taylor series ($f(x) = a_0 + a_1 x + a_2 x^2 + \cdots$) must be *infinitely* differentiable. How, then, can $\theta(x)$ be the limit of a sequence of polynomials? *Note*: This is not a difficult problem, once you see the light, but it is very subtle, so don't waste a lot of time on it if you're not getting anywhere.

3.3 THE GENERALIZED STATISTICAL INTERPRETATION

My next project is to recast the fundamental principles of quantum mechanics (as developed in Chapters 1 and 2) into the more elegant language of linear algebra. Remember that the state of a particle is represented by its wave function, $\Psi(x, t)$, whose absolute square is the probability density for finding the particle at point x, at time t. It follows that Ψ must be *normalized*, which is possible (by dividing off a constant) if and only if it is square integrable. Thus

1. The state of a particle is represented by a normalized vector ($|\Psi\rangle$) in the Hilbert space L_2.

Classical dynamical quantities (such as position, velocity, momentum and kinetic energy) can be expressed as functions of the "canonical" variables x and p (and, in rare cases, t): $Q(x, p, t)$. To each such classical observable we associate a quantum-mechanical *operator*, $\hat{Q}$, obtained from Q by the substitution

$$p \to \frac{\hbar}{i}\frac{\partial}{\partial x}. \qquad [3.113]$$

The expectation value of Q, in the state Ψ, is

$$\langle Q \rangle = \int \Psi(x, t)^* \hat{Q} \Psi(x, t)\, dx,$$

which we now write as an inner product:[23]

$$\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle. \qquad [3.114]$$

Now, the expectation value of an observable quantity has got to be a *real* number (after all, it corresponds to actual measurements in the laboratory, using rulers and clocks and meters), so

$$\langle \Psi | \hat{Q} \Psi \rangle = \langle \Psi | \hat{Q} \Psi \rangle^* = \langle \hat{Q} \Psi | \Psi \rangle, \qquad [3.115]$$

for all vectors $|\Psi\rangle$. It follows (see Problem 3.21) that $\hat{Q}$ must be a *Hermitian* operator. Thus

2. Observable quantities, $Q(x, p, t)$, are represented by Hermitian operators, $\hat{Q}(x, \frac{\hbar}{i}\frac{\partial}{\partial x}, t)$; the expectation value of Q, in the state $|\Psi\rangle$, is $\langle \Psi | \hat{Q} \Psi \rangle$.

[23] The "lousy notation" I warned you about on page 92 is not so bad in this context, for we are using the function Ψ *itself* to label the vector $|\Psi\rangle$, and the expression $\hat{Q}\Psi$ is perfectly self-explanatory.

In general, identical measurements on identically prepared systems (all in the same state Ψ) do not yield reproducible results; however, *some* states are **determinate**, for a particular observable, in the sense that they always give the same result. [A competent measurement of the total energy of a particle in the ground state of the harmonic oscillator, for example, will always return the value $(1/2)\hbar\omega$.] For a determinate state of observable Q, the standard deviation is zero:

$$0 = \sigma_Q^2 = \langle (\hat{Q} - \langle Q \rangle)^2 \rangle = \langle \Psi | (\hat{Q} - \langle Q \rangle)^2 \Psi \rangle$$
$$= \langle (\hat{Q} - \langle Q \rangle)\Psi | (\hat{Q} - \langle Q \rangle)\Psi \rangle = \| (\hat{Q} - \langle Q \rangle)|\Psi\rangle \|^2. \qquad [3.116]$$

[I used the fact that the operator $(\hat{Q} - \langle Q \rangle)$ is Hermitian to peel it off the second member of the inner product and attach it to the first member.] But the only vector with norm zero is the *null* vector (Equation 3.20), so $(\hat{Q} - \langle Q \rangle)|\Psi\rangle = 0$, or

$$\hat{Q}|\Psi\rangle = \langle Q \rangle |\Psi\rangle. \qquad [3.117]$$

Evidently determinate states are *eigenvectors* of $\hat{Q}$. Thus

3. A measurement of the observable Q on a particle in the state $|\Psi\rangle$ is *certain* to return the value λ if and only if $|\Psi\rangle$ is an eigenvector of $\hat{Q}$, with eigenvalue λ.

For example, the time-independent Schrödinger equation (Equation 2.11),

$$\hat{H}\psi = E\psi,$$

is nothing but an eigenvalue equation for the Hamiltonian operator, and the solutions are states of determinate energy (as we noted long ago).

Up to this point I have added nothing *new* to the statistical interpretation; I have merely explored its implications in the language of linear algebra. But there is a missing part to the story: Although we can calculate the *average* result of any measurement, we still cannot say what the probability of getting a *particular* result would be if we were to measure a given observable Q on a particle in an arbitrary state $|\Psi\rangle$ (except for the special case of *position* for which the original statistical interpretation supplies the answer). To finish the job, we need the following **generalized statistical interpretation**, which is inspired by postulate 3 above, and subsumes it as a special case:

3′. If you measure an observable Q on a particle in the state $|\Psi\rangle$, you are *certain* to get *one of the eigenvalues* of $\hat{Q}$. The probability of getting the particular eigenvalue λ is equal to the absolute square of the λ component of $|\Psi\rangle$, when expressed in the orthonormal basis of eigenvectors.[24]

[24] Notice that we could calculate from this the expectation value of Q, and it is important to check that the result is consistent with postulate 2 above. See Problem 3.35(c).

To sustain this postulate, it is essential that the eigenfunctions of $\hat{Q}$ span the space. As we have seen, in the *finite*-dimensional case the eigenvectors of a Hermitian operator *always* span the space. But this theorem fails in the infinite-dimensional case—we have encountered examples of Hermitian operators that have no eigenfunctions at all, or for which the eigenfunctions lie outside the Hilbert space. *We shall take it as a restriction on the subset of Hermitian operators that are* **observable**, *that their eigenfunctions constitute a complete set* (though they need not fall inside L_2).[25]

Now, there are two kinds of eigenvectors, which we need to treat separately. If the spectrum is *discrete* (with the distinct eigenvalues separated by finite gaps), we can label the eigenvectors with an integer n:

$$\hat{Q}|e_n\rangle = \lambda_n|e_n\rangle, \quad \text{with } n = 1, 2, 3, \ldots; \tag{3.118}$$

the eigenvectors are orthonormal (or rather, they can always be *chosen* so):

$$\langle e_n|e_m\rangle = \delta_{nm}; \tag{3.119}$$

the completeness relation takes the form of a *sum*:

$$|\Psi\rangle = \sum_{n=1}^{\infty} c_n|e_n\rangle; \tag{3.120}$$

the components are given by "Fourier's trick":

$$c_n = \langle e_n|\Psi\rangle, \tag{3.121}$$

and the probability of getting the particular eigenvalue λ_n is

$$\boxed{|c_n|^2 = |\langle e_n|\Psi\rangle|^2.} \tag{3.122}$$

On the other hand, if the spectrum is *continuous*, the eigenvectors are labeled by a continuous variable (k):

$$\hat{Q}|e_k\rangle = \lambda_k|e_k\rangle, \quad \text{with } -\infty < k < \infty; \tag{3.123}$$

the eigenfunctions are *not* normalizable (so they do not lie in L_2, and do not themselves represent possible particle states), but they satisfy a sort of "orthonormality" condition

$$\langle e_k|e_l\rangle = \delta(k - l) \tag{3.124}$$

[25] Some authors, following Dirac, take this to be an *axiom* of quantum mechanics, but it seems to me peculiar to use that term for something that is *provable* in many particular instances; I prefer to regard it as a part of what it *means* to be "observable".

(or rather, they can always be *chosen* so); the completeness relation takes the form of an *integral*:

$$|\Psi\rangle = \int_{-\infty}^{\infty} c_k|e_k\rangle\, dk; \tag{3.125}$$

the "components" are given by "Fourier's trick":

$$c_k = \langle e_k|\Psi\rangle, \tag{3.126}$$

and the probability of getting an eigenvalue in the *range* dk about λ_k is

$$\boxed{|c_k|^2\, dk = |\langle e_k|\Psi\rangle|^2\, dk.} \tag{3.127}$$

The generalized statistical interpretation makes no reference to the observable x; it treats *all* observables on an equal footing. But it includes the "original" form (Equation 1.3) as a special case. The "orthonormal" eigenfunctions of the position operator are

$$e_{x'}(x) = \delta(x - x'), \tag{3.128}$$

and the eigenvalue (x') can take on any value between $-\infty$ and $+\infty$. The x' "component" of $|\Psi\rangle$ is

$$c_{x'} = \langle e_{x'}|\Psi\rangle = \int_{-\infty}^{\infty} \delta(x - x')\Psi(x, t)\, dx = \Psi(x', t), \tag{3.129}$$

so the probability of finding the particle in the range dx' about x' is

$$|c_{x'}|^2\, dx' = |\Psi(x', t)|^2\, dx', \tag{3.130}$$

which is the original statistical interpretation of Ψ.

A more illuminating example is provided by the momentum operator. Its "orthonormal" eigenfunctions are (see Problem 3.37)

$$e_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}, \tag{3.131}$$

and the eigenvalue (p) can take on any value in the range $-\infty < p < \infty$. The p "component" of $|\Psi\rangle$ is

$$\boxed{c_p = \langle e_p|\Psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x, t)\, dx \equiv \Phi(p, t).} \tag{3.132}$$

We call $\Phi(p, t)$ the **momentum-space wave function**—it is (apart from the factors of $\hbar$) the *Fourier transform* of the "position-space" wave function $\Psi(x, t)$. Evidently the probability of getting a momentum in the range dp is

$$|\Phi(p, t)|^2\, dp. \tag{3.133}$$