

Vectors for quantum mechanics¹

D. E. Soper²

University of Oregon

5 October 2011

I offer here some background for Chapter 1 of J. J. Sakurai, *Modern Quantum Mechanics*.

1 Vectors over the complex numbers

What is a vector? One can take two approaches, one very concrete, one abstract. Ultimately, the abstract approach is most useful and the concrete approach is even a bit misleading. However, both are useful.

We consider vectors ψ in an N -dimensional vector space over the complex numbers. In the concrete approach, such a vector is a list of N complex numbers:

$$\psi = \{\tilde{\psi}_1, \tilde{\psi}_2, \dots, \tilde{\psi}_N\} . \quad (1)$$

There is a special vector, the zero vector, defined by

$$0 = \{0, 0, 0, \dots, 0\} . \quad (2)$$

If c is a complex number, we can define multiplication by c as

$$c\psi = \{c\tilde{\psi}_1, c\tilde{\psi}_2, \dots, c\tilde{\psi}_N\} . \quad (3)$$

If ψ and $\phi = \{\tilde{\phi}_1, \tilde{\phi}_2, \dots, \tilde{\phi}_N\}$ are two vectors, we can define addition of these vectors as

$$\psi + \phi = \{\tilde{\psi}_1 + \tilde{\phi}_1, \tilde{\psi}_2 + \tilde{\phi}_2, \dots, \tilde{\psi}_N + \tilde{\phi}_N\} . \quad (4)$$

In the abstract approach, we say that an N -dimensional vector space \mathcal{V} over the complex numbers is a set of vectors $\psi \in \mathcal{V}$ together with two operations: multiplication by a complex number and addition of vectors. Thus we postulate that if $\psi \in \mathcal{V}$ and c is a complex number, then $c\psi \in \mathcal{V}$. Furthermore, if $\psi \in \mathcal{V}$ and $\phi \in \mathcal{V}$, then $\psi + \phi \in \mathcal{V}$. We also postulate that there is a vector $0 \in \mathcal{V}$ with $0\psi = 0$. Finally,

$$(c_1 c_2)\psi = c_1(c_2\psi) , \quad (5)$$

¹Copyright, 2011, D. E. Soper

²soper@uoregon.edu

$$(c_1 + c_2)\psi = c_1\psi + c_2\psi \quad (6)$$

and

$$c(\psi + \phi) = c\psi + c\phi \quad (7)$$

These properties say what a vector is, but do not say what “ N -dimensional” means. To define this, we first define “linearly independent” and “linearly dependent.” A set of vectors³ $\psi_1, \psi_2, \dots, \psi_n$ is linearly independent if, for any complex coefficients c_1, c_2, \dots, c_n ,

$$c_1\psi_1 + c_2\psi_2 + \dots + c_n\psi_n = 0 \quad (8)$$

only if

$$c_1 = c_2 = \dots = c_n = 0 \quad (9)$$

If a set of vectors is not linearly independent, then it is linearly dependent. Thus $\psi_1, \psi_2, \dots, \psi_n$ is linearly dependent if there are some coefficients c_1, c_2, \dots, c_n that are not all zero such that

$$c_1\psi_1 + c_2\psi_2 + \dots + c_n\psi_n = 0 \quad (10)$$

In this case, at least one of the coefficients, call it c_a , is non-zero. Then

$$\psi_a = \sum_{i \neq a} (c_i/c_a) \psi_i \quad (11)$$

That is, if $\psi_1, \psi_2, \dots, \psi_n$ are linearly dependent, then one of them can be expressed as a linear combination of the others. This gives us the needed definition: \mathcal{V} is N -dimensional if there is at least one set of N vectors $\psi_1, \psi_2, \dots, \psi_N$ that is linearly independent and if any set of $N + 1$ vectors is linearly dependent.

A set of N linearly independent vectors ψ_j in a vector space of dimension N is called a *basis* for \mathcal{V} . Once we have a basis, any other vector ϕ can be expressed as a linear combination of the basis vectors,

$$\phi = \sum_{i=1}^N c_i \psi_i \quad (12)$$

³I apologize that here ψ_1, ψ_2 , *etc.* are vectors, whereas in the concrete example I used a very similar notation $\tilde{\psi}_1, \tilde{\psi}_2$, *etc.* for complex numbers that are the components of a single vector. Fortunately, the bra-ket notation that we will use generally does not suffer from this notational difficulty.

A basis for our concrete example is

$$\begin{aligned}\psi_1 &= \{1, 0, 0, \dots, 0\} \ , \\ \psi_2 &= \{0, 1, 0, \dots, 0\} \ , \\ &\dots \\ \psi_N &= \{0, 0, 0, \dots, 1\} \ .\end{aligned}\tag{13}$$

In this course, we will (usually) use a notation for vectors in which a vector is represented as $|\psi\rangle$, called a ket-vector or just a ket. Here the “ ψ ” can be any name that distinguishes the vector from other vectors. Thus, for instance, if we have vectors $\psi_1, \psi_2, \dots, \psi_N$, we can denote them by kets $|1\rangle, |2\rangle, \dots, |N\rangle$.

2 Inner product

For quantum mechanics, we use a vector space \mathcal{V} over the complex numbers that has an inner product. For any two vectors ψ and ϕ , the inner product (ϕ, ψ) is a complex number. The inner product is linear in the first (right hand) factor and conjugate-linear in the second factor:

$$\begin{aligned}(\phi, c_1\psi_1 + c_2\psi_2) &= c_1(\phi, \psi_1) + c_2(\phi, \psi_2) \ , \\ (c_1\phi_1 + c_2\phi_2, \psi) &= c_1^*(\phi_1, \psi) + c_2^*(\phi_2, \psi) \ .\end{aligned}\tag{14}$$

Furthermore

$$(\phi, \psi) = (\psi, \phi)^* \ .\tag{15}$$

Evidently, (ψ, ψ) is real. We postulate that

$$(\psi, \psi) \geq 0\tag{16}$$

and if $\psi \neq 0$,

$$(\psi, \psi) > 0 \ .\tag{17}$$

In our concrete example, the inner product could be

$$(\phi, \psi) = \sum_{j=1}^N \tilde{\phi}_j^* \tilde{\psi}_j \ .\tag{18}$$

In this course, we will usually use the notation

$$(\phi, \psi) = \langle \phi | \psi \rangle\tag{19}$$

for the inner product. We call $\langle\phi|$ a bra-vector, or just a bra. I usually think of bras as kets just written backwards so as to provide a convenient notation for inner products. Sakurai interprets the bras as belonging to a different space from the kets. Then there is a mapping that he calls “DC” that maps a ket $|\phi\rangle$ into its corresponding bra $\langle\phi|$. If you think of it that way, then the mapping is conjugate-linear: if

$$|\phi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle \quad , \quad (20)$$

then

$$\langle\phi| = c_1^*\langle\phi_1| + c_2^*\langle\phi_2| \quad . \quad (21)$$

With the bra-ket notation

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \quad . \quad (22)$$

With the bra-ket notation, the property that the inner product is linear in the ket vectors is stated as

$$\langle\phi|(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1\langle\phi|\psi_1\rangle + c_2\langle\phi|\psi_2\rangle \quad (23)$$

The property $(c_1\phi_1 + c_2\phi_2, \psi) = c_1^*(\phi_1, \psi) + c_2^*(\phi_2, \psi)$ is a little more awkward to state. If $|\phi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle$, then, using Eq. (21), we can write

$$\langle\phi|\psi\rangle = (c_1^*\langle\phi_1| + c_2^*\langle\phi_2|)|\psi\rangle = c_1^*\langle\phi_1|\psi\rangle + c_2^*\langle\phi_2|\psi\rangle \quad . \quad (24)$$

Thus the bra-ket notation makes it easy to get things right as long as we remember Eq. (21), although it is a little tricky to express what the postulates are.

With the bra-ket notation, the zero vector is usually represented as just 0 without a ket symbol. Thus we might write $|\phi\rangle + |\psi\rangle = 0$. We could write $|\phi\rangle + |\psi\rangle = |\text{zero}\rangle$, but people usually don't do that. One often sees a notation $|0\rangle$, but that can mean “ground state of a harmonic oscillator” or “vacuum state” or something else other than $|\text{zero}\rangle$.

3 Interpretation of the inner product

Suppose that $|\phi\rangle$ is a state vector normalized to $\langle\phi|\phi\rangle = 1$. Suppose further that we know how to measure whether our physical system is in state $|\phi\rangle$.

For instance, we can determine if an atom is in a state $|S_z, +\rangle$ by sending it through a Stern-Gerlach apparatus with its magnetic field in the z -direction and seeing whether its path is bent in the z -direction.

Suppose that $|\psi\rangle$ is a state vector normalized to $\langle\psi|\psi\rangle = 1$ and that we know how to prepare a system so that we know it is in state $|\psi\rangle$. For instance, we can prepare an atom in a state $|S_z, +\rangle$ by sending some atoms through a Stern-Gerlach apparatus with its magnetic field in the z -direction and selecting one whose path is bent in the z -direction.

Suppose in addition that $|\phi\rangle$ is a state vector normalized to $\langle\phi|\phi\rangle = 1$ and that we know how to measure whether the system is in state $|\phi\rangle$. For instance, we can measure whether an atom in a state $|S_x, +\rangle$ by sending the atom through a Stern-Gerlach apparatus with its magnetic field in the x -direction and seeing if the path of the atom is bent in the x -direction.

Then if we prepare a system in state $|\psi\rangle$, the probability that we will find upon the appropriate measurement that it is in state $|\phi\rangle$ is $|\langle\phi|\psi\rangle|^2$.

Note that to make this interpretation work, we always represent a system that is in a definite quantum state by a vector $|\psi\rangle$ with the normalization $\langle\psi|\psi\rangle = 1$.

4 Orthonormal basis

If $|1\rangle, |2\rangle, \dots, |N\rangle$ form a basis for our space, there is, *in general*, no particular behavior of the inner product $\langle i|j\rangle$. However, a basis can be “orthonormal”, which means that

$$\langle i|j\rangle = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} . \quad (25)$$

This connects to the physical interpretation. Suppose that we know how to prepare states represented by vectors $|i\rangle$ with the normalization $\langle i|i\rangle = 1$ for each i . Suppose further that experiment shows that if the system is prepared in state $|i\rangle$ and we measure whether it is in state $|j\rangle$ for $j \neq i$, then the probability that the system will be found to be in state $|j\rangle$ is zero. That means that $\langle i|j\rangle = 0$. That is, the vectors $|i\rangle$ form an orthonormal basis for the space of quantum states.

An example of this is the two states $|S_z, +\rangle$ and $|S_z, -\rangle$ describing the spin of an electron.

In Sakurai, the term “base kets” refers to an orthonormal basis. I will usually also be a little sloppy in language and refer to “basis kets $|i\rangle$ ” with $i = 1, \dots, N$ when I mean an orthonormal basis.

There is a useful relation for an orthonormal basis. Since it is a basis, any vector $|\phi\rangle$ can be expressed as a linear combination of the basis elements,

$$|\phi\rangle = \sum_{i=1}^N c_i |i\rangle . \quad (26)$$

From this, we can find the expansion coefficients. We have

$$\langle j|\phi\rangle = \sum_{i=1}^N c_i \langle j|i\rangle = c_j . \quad (27)$$

Thus the expansion can be written

$$|\phi\rangle = \sum_{i=1}^N \langle i|\phi\rangle |i\rangle . \quad (28)$$

We usually write this in the form

$$|\phi\rangle = \sum_{i=1}^N |i\rangle \langle i|\phi\rangle . \quad (29)$$

Notice how this works with the probabilistic interpretation of inner products. Let us assume that $|\phi\rangle$, normalized to $\langle\phi|\phi\rangle = 1$, represents a physical state. Suppose that the basis states $|i\rangle$ correspond to possible results of a measurement. For instance, the basis states could be $|S_x, +\rangle$ and $|S_x, -\rangle$. Recall that the condition $\langle i|j\rangle = 0$ when $i \neq j$ means that if measurement shows that our system is in state $|i\rangle$, then we are sure that it is not in state $|j\rangle$. For example, if we send an atom through a Stern-Gerlach apparatus, then if it went up, it did not go down and if it went down, it did not go up. Now the normalization condition $\langle\phi|\phi\rangle = 1$ gives

$$1 = \langle\phi|\phi\rangle = \langle\phi| \left(\sum_{i=1}^N |i\rangle \langle i|\phi\rangle \right) = \sum_{i=1}^N \langle\phi|i\rangle \langle i|\phi\rangle = \sum_{i=1}^N |\langle i|\phi\rangle|^2 . \quad (30)$$

This says that the sum of the probabilities to get the various results i is 1.

Exercise 1.1 Let us postulate that the state space for a spin 1/2 system is spanned by an orthonormal basis consisting of two basis vectors, $|S_z; +\rangle$ and $|S_z; -\rangle$. Define

$$\begin{aligned} |S_x; +\rangle &= \frac{1}{\sqrt{2}}|S_z; +\rangle + \frac{1}{\sqrt{2}}|S_z; -\rangle , \\ |S_x; -\rangle &= \frac{1}{\sqrt{2}}|S_z; +\rangle - \frac{1}{\sqrt{2}}|S_z; -\rangle . \end{aligned} \quad (31)$$

Show that the vectors $|S_x; +\rangle$ and $|S_x; -\rangle$ form an orthonormal basis.

Exercise 1.2 Since $|S_x; +\rangle$ and $|S_x; -\rangle$ form an orthonormal basis, we can expand $|S_z; +\rangle$ in this basis,

$$|S_z; +\rangle = c_{++}|S_x; +\rangle + c_{-+}|S_x; -\rangle . \quad (32)$$

Similarly, we can expand $|S_z; -\rangle$ in this basis,

$$|S_z; -\rangle = c_{+-}|S_x; +\rangle + c_{--}|S_x; -\rangle . \quad (33)$$

Use Eq. (29) to find the coefficients c_{ij} .

Exercise 1.3 Another basis for the state space for a spin 1/2 particle consists of the states

$$\begin{aligned} |S_y; +\rangle &= \frac{1}{\sqrt{2}}|S_z; +\rangle + \frac{i}{\sqrt{2}}|S_z; -\rangle , \\ |S_y; -\rangle &= \frac{1}{\sqrt{2}}|S_z; +\rangle - \frac{i}{\sqrt{2}}|S_z; -\rangle . \end{aligned} \quad (34)$$

These vectors can be written in terms of the basis vectors $|S_x; \pm\rangle$,

$$\begin{aligned} |S_y; +\rangle &= d_{++}|S_x; +\rangle + d_{-+}|S_x; -\rangle , \\ |S_y; -\rangle &= d_{+-}|S_x; +\rangle + d_{--}|S_x; -\rangle . \end{aligned} \quad (35)$$

Use Eq. (29) to find the coefficients d_{ij} .

I should point out that the sign conventions used in these exercises are from Sakurai (1.4.17). This agrees with Sakurai's tentative choice in (1.1.14) but not with the tentative choice in (1.1.9).

The states $|S_y, \pm\rangle$ can be prepared and measured with a Stern-Gerlach apparatus with magnetic field oriented along the y direction. Note that we need factors of i in the coefficient relating these vectors to $|S_x, \pm\rangle$. This illustrates why we choose a vector space over the complex numbers rather than over the real numbers for representing a quantum system.

5 Operators

A linear operator A on the space \mathcal{V} maps a vector $|\psi\rangle$ to another vector $|\psi'\rangle = A|\psi\rangle$. The mapping is linear,

$$A(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1A|\psi_1\rangle + c_2A|\psi_2\rangle . \quad (36)$$

Evidently, any linear combination of linear operators defines another linear operator:

$$(\alpha A + \beta B)|\psi\rangle = \alpha A|\psi\rangle + \beta B|\psi\rangle; . \quad (37)$$

There are two special operators, the null operator “0”,

$$0|\psi\rangle = 0 , \quad (38)$$

and the unit operator “1”,

$$1|\psi\rangle = |\psi\rangle . \quad (39)$$

One can define the product of two linear operators in a straightforward fashion: the product $C = AB$ is defined by $C|\psi\rangle = A(B|\psi\rangle)$. Note that in general AB and BA are not equal to each other.

The bra-ket notation provides a slick way to represent certain operators. We can interpret the symbol $|\psi\rangle\langle\phi|$ as an operator. If $A = |\phi_2\rangle\langle\phi_1|$, the action of A on a state ψ is

$$A|\psi\rangle = (|\phi_2\rangle\langle\phi_1|)|\psi\rangle = |\phi_2\rangle(\langle\phi_1|\psi\rangle) = |\phi_2\rangle\langle\phi_1|\psi\rangle . \quad (40)$$

For instance, if we have an orthonormal basis $|i\rangle$, then Eq. (29) gives us a way to write the unit operator

$$1 = \sum_i |i\rangle\langle i| . \quad (41)$$

We will use this often. A good example is to express the action of an arbitrary operator A in terms of an (orthonormal) basis with basis vectors $|i\rangle$. Let $A|\psi\rangle = |\phi\rangle$. Using the basis vectors $|i\rangle$, the j -component of $|\psi\rangle$ is

$$\tilde{\psi}_j = \langle j|\psi\rangle \quad (42)$$

and the i -component of $|\phi\rangle$ is

$$\tilde{\phi}_i = \langle i|\phi\rangle \quad (43)$$

These related by

$$\langle i|\phi\rangle = \langle i|A|\psi\rangle = \langle i|A|1|\psi\rangle = \sum_j \langle i|A|j\rangle \langle j|\psi\rangle \quad (44)$$

Then this has the form of a matrix multiplication,

$$\tilde{\phi}_i = \sum_j A_{ij} \tilde{\psi}_j \quad (45)$$

where the matrix elements are

$$A_{ij} = \langle i|A|j\rangle \quad (46)$$

We can also use the “unit operator insertion” method to find the matrix elements of a product of two operators

$$\langle i|AB|j\rangle = \langle i|A|1|B|j\rangle = \sum_k \langle i|A|k\rangle \langle k|B|j\rangle \quad (47)$$

That is, the matrix that represents AB is the matrix product of the two matrices that represent A and B .

Exercise 1.4 The operators that represent the three components of spin for a spin $1/2$ system are S_x , S_y and S_z . The matrix elements of these operators in the $|S_z, \pm\rangle$ basis are

$$\begin{aligned} \langle S_z, i|S_x|S_z, j\rangle &= \frac{1}{2} (\sigma_x)_{ij} \quad , \\ \langle S_z, i|S_y|S_z, j\rangle &= \frac{1}{2} (\sigma_y)_{ij} \quad , \\ \langle S_z, i|S_z|S_z, j\rangle &= \frac{1}{2} (\sigma_z)_{ij} \quad , \end{aligned} \quad (48)$$

where (displaying the $i = +$ elements first and the $i = -$ elements second)

$$\begin{aligned}\sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \\ \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \\ \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .\end{aligned}\tag{49}$$

Define the “comutator” of S_x with S_y by $[S_x, S_y] = S_x S_y - S_y S_x$. Show that $[S_x, S_y] = iS_z$. What is $[S_y, S_z]$? What is $[S_z, S_x]$?

6 The adjoint of an operator

Suppose that A is a linear operator. Then we can define another operator A^\dagger , called the adjoint of A . We say that A^\dagger applied to a state $|\phi\rangle$ gives another state $|\phi'\rangle = A^\dagger|\phi\rangle$. To say what $|\phi'\rangle$ is, we give its inner product $\langle\phi'|\psi\rangle$ with *any* state $|\psi\rangle$:

$$\langle\phi'|\psi\rangle = \langle\phi|A|\psi\rangle .\tag{50}$$

If we use our alternative notation for vectors and inner products, the definition is

$$(A^\dagger\phi, \psi) = (\phi, A\psi) .\tag{51}$$

Unfortunately, the bra-ket notation does not allow us to write the definition of the adjoint of an operator in this simple way. The best that we can do is to use

$$\langle\psi|A^\dagger|\phi\rangle = \langle\phi|A|\psi\rangle^* .\tag{52}$$

Note that taking the adjoint twice is the same as doing nothing:

$$\langle\psi|(A^\dagger)^\dagger|\phi\rangle = \langle\phi|A^\dagger|\psi\rangle^* = (\langle\psi|A|\phi\rangle^*)^* = \langle\psi|A|\phi\rangle ,\tag{53}$$

for every pair of vectors $|\psi\rangle$ and $|\phi\rangle$, so

$$(A^\dagger)^\dagger = A .\tag{54}$$

If we have two operators A and B and define $C = AB$, then what is C^\dagger ? We have

$$(C^\dagger\phi, \psi) = (\phi, C\psi) = (\phi, AB\psi) = (A^\dagger\phi, B\psi) = (B^\dagger A^\dagger\phi, \psi) ,\tag{55}$$

so

$$C^\dagger = B^\dagger A^\dagger . \quad (56)$$

There is a simple relation between the matrix elements of A and those of A^\dagger . Using Eq. (52), we have

$$\langle i | A^\dagger | j \rangle = \langle j | A | i \rangle^* . \quad (57)$$

Thus the matrix elements of A^\dagger are the complex conjugates of the matrix elements of A with the indices reversed.

When we use the bra-ket notation, we can say that an operator A can act backward on a bra,

$$\langle \phi | A = \langle \phi' | . \quad (58)$$

The new bra vector $\langle \phi' |$ is defined by Eq. (50). Then the corresponding ket vector is $|\phi'\rangle = A^\dagger |\phi\rangle$. Thus also if

$$|\phi'\rangle = A |\phi\rangle \quad (59)$$

then

$$\langle \phi' | = \langle \phi | A^\dagger . \quad (60)$$

An operator A is self-adjoint (or “hermitian”) if

$$A^\dagger = A . \quad (61)$$

An operator U is “unitary” if $U^\dagger = U^{-1}$, that is if

$$U^\dagger U = 1 . \quad (62)$$

We will explore self-adjoint operators and unitary operators in subsequent sections.

7 Unitary operators

Suppose that $|\psi\rangle$ and $|\phi\rangle$ are two vectors and that U is a unitary operator. Define $|\psi'\rangle = U|\psi\rangle$ and $|\phi'\rangle = U|\phi\rangle$. Then

$$\langle \phi' | \psi' \rangle = \langle \phi | U^\dagger U | \psi \rangle = \langle \phi | 1 | \psi \rangle = \langle \phi | \psi \rangle . \quad (63)$$

That is, a unitary operator preserves inner products.

For this reason, we use unitary operators to represent symmetry operations. For instance, there will be a unitary operator to represent the effect of rotating a system about the y -axis through an angle $\pi/3$ (say). If we rotate $|\psi\rangle$ and $|\phi\rangle$, we don't get the same states. We get different states $|\psi'\rangle$ and $|\phi'\rangle$. However, $\langle\phi|\psi\rangle$ has a physical meaning: its square is the probability for $|\phi\rangle$ to look like $|\psi\rangle$ if we perform the appropriate measurement. It should not matter whether we perform the $|\phi\rangle$ measurement on state $|\psi\rangle$ or we rotate $|\psi\rangle$ to get $|\psi'\rangle$ and perform the rotated measurement, corresponding to $|\phi'\rangle$. Thus the rotation should be represented by a unitary operator. We will investigate rotation operators in some detail later in this course.

We can also use a unitary operator to represent any change of basis. Suppose that the vectors $|A, i\rangle$, $i = 1, \dots, N$ form an orthonormal basis, the A basis, for the space of states of a quantum system. Suppose that the vectors $|B, i\rangle$, $i = 1, \dots, N$ form another basis. Define a linear operator U by

$$U|A, i\rangle = |B, i\rangle . \quad (64)$$

With this definition, we do not know at the moment whether U is unitary. Let us investigate this question.

If

$$|\psi\rangle = \sum c_i |A, i\rangle , \quad (65)$$

we have

$$U|\psi\rangle = \sum c_i U|A, i\rangle = \sum c_i |B, i\rangle . \quad (66)$$

Similarly, for any other vector $|\phi\rangle$ with

$$|\phi\rangle = \sum d_i |A, i\rangle , \quad (67)$$

we have

$$U|\phi\rangle = \sum d_i |B, i\rangle . \quad (68)$$

The inner product between $U|\psi\rangle$ and $U|\phi\rangle$ is

$$\begin{aligned} \langle\phi|U^\dagger U|\psi\rangle &= \sum_{i,j} d_i^* c_j \langle B, i|B, j\rangle \\ &= \sum_{i,j} d_i^* c_j \delta_{i,j} \\ &= \sum_{i,j} d_i^* c_j \langle A, i|A, j\rangle \\ &= \langle\phi|\psi\rangle . \end{aligned} \quad (69)$$

Thus if we define $|\Psi\rangle = U^\dagger U |\psi\rangle$, we have $\langle\phi|\Psi\rangle = \langle\phi|\psi\rangle$ for *every* vector $|\phi\rangle$. Thus $\langle\phi|(|\Psi\rangle - |\psi\rangle) = 0$ for *every* vector $|\phi\rangle$. Taking $|\phi\rangle = (|\Psi\rangle - |\psi\rangle)$, we have

$$(\langle\Psi| - \langle\psi|)(|\Psi\rangle - |\psi\rangle) = 0 \quad . \quad (70)$$

However, the inner product of a vector with itself can be zero only if the vector is zero. Thus $|\Psi\rangle - |\psi\rangle = 0$. That is

$$U^\dagger U |\psi\rangle = |\psi\rangle \quad (71)$$

for every vector $|\psi\rangle$. This means that $U^\dagger U = 1$. That is, the operator U that takes one orthonormal basis into another is unitary.

8 Self-adjoint operators

Physical quantities like angular momentum, energy, momentum, and position are represented in quantum mechanics by self-adjoint operators. Thus we should know some properties of self-adjoint or “hermitian” operators.

The spectral theorem. Let A be a linear operator on the space of quantum states of a system and let A be self-adjoint: $A^\dagger = A$. Then there is an orthonormal basis $|i\rangle$ such that the vectors $|i\rangle$ are *eigenvectors* of A ,

$$A|i\rangle = a_i|i\rangle \quad . \quad (72)$$

Here a_i is a real number, the *eigenvalue* of A corresponding to the eigenvector $|i\rangle$.

This theorem has an immediate consequence,

$$A = A 1 = A \sum_i |i\rangle\langle i| = \sum_i a_i |i\rangle\langle i| \quad . \quad (73)$$

This gives us the spectral representation of A :

$$A = \sum_i a_i |i\rangle\langle i| \quad . \quad (74)$$

This theorem is pretty easy to prove, but we will not do it in these notes. Instead, let us look at a couple of the ingredients. Suppose that we look for eigenvectors $|i\rangle$ of A and their corresponding eigenvalues a_i . We can choose

to normalize all eigenvectors that we find to $\langle i|i \rangle = 1$. We see immediately that any eigenvalue must be real:

$$\begin{aligned} a_i^* &= a_i^* \langle i|i \rangle = (\langle i|A^\dagger)|i \rangle = \langle i|A^\dagger|i \rangle \\ &= \langle i|A|i \rangle = \langle i|(A|i) \rangle = a_i \langle i|i \rangle \\ &= a_i \quad . \end{aligned} \tag{75}$$

Furthermore, eigenvectors corresponding to different eigenvalues must be orthogonal:

$$(a_i - a_j) \langle i|j \rangle = (\langle i|A)|j \rangle - \langle i|(A|j) \rangle = \langle i|A - A|j \rangle = 0 \quad . \tag{76}$$

If $(a_i - a_j) \neq 0$ then we must have $\langle i|j \rangle = 0$. Furthermore, if there are several eigenvectors $|i\rangle$ that correspond to the same eigenvalue, then any linear combination of these eigenvectors will also be an eigenvector with this same eigenvalue. Thus the eigenvectors with this eigenvalue form a vector space that is a subspace of the complete space. We can choose any orthonormal basis that we like for this subspace. That is, we can simply choose eigenvectors with a given eigenvalue to be orthogonal to each other. These remarks prove part of the theorem. It remains to be proved that there are enough eigenvectors so that they form a basis for the complete space.

The spectral theorem is important for the interpretation of quantum mechanics. We often associate a *measurement* with a self-adjoint operator. To see how this association works, consider a self-adjoint operator A that is associated with a certain measurement. (For example, we might measure the y -component of the spin of a particle.)

If we have a state $|\psi\rangle$ and we make a measurement that corresponds to the operator

$$A = \sum_i a_i |i\rangle \langle i| \quad , \tag{77}$$

then we do not know to start with what result we will get. The possible results are the eigenvalues a_i . If the state happens to be $|i\rangle$, then the result of measuring A is certainly a_i . Conversely, if the result of the measurement is a_i , then the state after the measurement⁴ is $|i\rangle$. In general, we have

$$|\psi\rangle = \sum_i \langle i|\psi \rangle |i\rangle \quad . \tag{78}$$

⁴This is the standard principle and applies to our Stern-Gerlach examples. However, one needs to be a little careful. We should be sure that nothing happened after the measurement that could change the state.

The probability that we will find $|\psi\rangle$ in the state $|i\rangle$ and thus get a measurement a_i is $|\langle i|\psi\rangle|^2$. As we have earlier seen with a simple calculation, these probabilities sum to 1.

Exercise 1.5 Let us postulate that the state space for a spin 1/2 system is spanned by an orthonormal basis consisting of two basis vectors, $|S_z; +\rangle$ and $|S_z; -\rangle$ and that the phases of these vectors are defined using the standard convention such that the matrix elements of S_x and S_y in this basis are given by 1/2 times the standard Pauli spin matrices, Eq. (49).

Show that the vectors $|S_x, \pm\rangle$ given by Eq. (31) are eigenvectors of S_x :

$$S_x |S_x, \pm\rangle = \pm \frac{1}{2} |S_x, \pm\rangle . \quad (79)$$

Show that the vectors $|S_y, \pm\rangle$ given by Eq. (34) are eigenvectors of S_y :

$$S_y |S_y, \pm\rangle = \pm \frac{1}{2} |S_y, \pm\rangle . \quad (80)$$

I recommend using a matrix notation in which the $|S_z; \pm\rangle$ vectors are represented by

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \quad (81)$$

Exercise 1.6 Let us again postulate that the state space for a spin 1/2 system is spanned by an orthonormal basis consisting of two basis vectors, $|S_z; +\rangle$ and $|S_z; -\rangle$ and that the phases of these vectors are defined using the standard convention such that the matrix elements of S_x and S_y in this basis are given by 1/2 times the standard Pauli spin matrices.

Consider the operator

$$\vec{S} \cdot \vec{n} = \cos \theta S_z + \sin \theta S_x . \quad (82)$$

This is the operator that measures spin in the direction of a vector \vec{n} that lies in the z - x plane and makes an angle θ with the z -axis.

Find the eigenvalues of $\vec{S} \cdot \vec{n}$ and the corresponding eigenvectors, expressed as linear combinations of $|S_z; +\rangle$ and $|S_z; -\rangle$:

$$|\vec{S} \cdot \vec{n}; i\rangle = \sum_j c(i, j) |S_z; j\rangle . \quad (83)$$

I recommend using a matrix notation in which the $|S_z; \pm\rangle$ vectors are represented as in the previous problem. Then you need to solve a 2×2 matrix eigenvalue equation, which I presume that you know how to do.

Exercise 1.7 Suppose that we send a spin-1/2 atom through a Stern-Gerlach apparatus that measures spin in the direction \vec{n} , as in Exercise 1.6. Suppose that we select an atom that goes in the $+\vec{n}$ direction. That is, the value of $\vec{S} \cdot \vec{n}$ for this atom is $+1/2$. Now we send this atom through a Stern-Gerlach apparatus that measures spin in the \hat{x} direction. What is the probability that when we measure $\vec{S} \cdot \hat{x}$ for this atom, the value $\vec{S} \cdot \hat{x}$ will be $-1/2$?

One often speaks of the “expectation value” $\langle A \rangle$ of A in the state $|\psi\rangle$. The definition is

$$\langle A \rangle \equiv \sum_i a_i \text{Probability}_i = \sum_i a_i |\langle i | \psi \rangle|^2 . \quad (84)$$

We can evaluate this to obtain a very simple expression,

$$\langle A \rangle = \sum_i a_i \langle \psi | i \rangle \langle i | \psi \rangle = \langle \psi | \left(\sum_i a_i |i\rangle \langle i| \right) | \psi \rangle = \langle \psi | A | \psi \rangle . \quad (85)$$

9 More about self-adjoint operators

We can look at this more closely by introducing another concept. Consider the operator

$$P_i = |i\rangle \langle i| . \quad (86)$$

If $|\psi\rangle = \alpha|i\rangle$, then $P_i|\psi\rangle = |\psi\rangle$. If $|\phi\rangle$ is orthogonal to $|i\rangle$, *i.e.* $\langle i|\phi\rangle = 0$, then $P_i|\phi\rangle = 0$. If $|\Psi\rangle = \alpha|i\rangle + |\phi\rangle$, then $P_i|\Psi\rangle = \alpha|i\rangle$. That is P_i picks out

the part of $|\Psi\rangle$ that is proportional to $|i\rangle$. We call P_i the projection operator onto the space spanned by the vector $|i\rangle$.

More generally, suppose \mathcal{M} is a subspace of the complete vector space \mathcal{V} that we are using to describe our quantum states. That is, \mathcal{M} is a subset of \mathcal{V} and is itself a vector space in the sense that if $|\psi_1\rangle$ and $|\psi_2\rangle$ are in \mathcal{M} , then so is $\alpha_1|\psi_1\rangle + \alpha_2|\psi_2\rangle$.

Then there is a complementary vector space \mathcal{M}_\perp that consists of vectors $|\phi\rangle$ such that $\langle\phi|\psi\rangle = 0$ for *every* vector $|\psi\rangle$ in \mathcal{M} . Every vector $|\Psi\rangle$ can be written as the sum of a vector in \mathcal{M} and a vector in \mathcal{M}_\perp . To see this, choose an orthonormal basis of vectors $|\psi_i\rangle$ in \mathcal{M} . Define

$$|\psi\rangle = \sum_i |\psi_i\rangle \langle\psi_i|\Psi\rangle . \quad (87)$$

Further define

$$|\phi\rangle = |\Psi\rangle - |\psi\rangle . \quad (88)$$

Then

$$\langle\psi_j|\phi\rangle = \langle\psi_j|\Psi\rangle - \sum_i \langle\psi_j|\psi_i\rangle \langle\psi_i|\Psi\rangle = \langle\psi_j|\Psi\rangle - \langle\psi_j|\Psi\rangle = 0 . \quad (89)$$

Therefore $|\phi\rangle$ is in \mathcal{M}_\perp . Thus

$$|\Psi\rangle = |\psi\rangle + |\phi\rangle , \quad (90)$$

where $|\psi\rangle$ is in \mathcal{M} and $|\phi\rangle$ is in \mathcal{M}_\perp , as claimed.

Choose an orthonormal basis of vectors $|\psi_i\rangle$ in \mathcal{M} and an orthonormal basis of vectors $|\phi_j\rangle$ in \mathcal{M}_\perp . Then it follows from the construction above that the decomposition of a general vector Ψ into a part in \mathcal{M} and a part in \mathcal{M}_\perp is

$$|\Psi\rangle = \sum_i |\psi_i\rangle \langle\psi_i|\Psi\rangle + \sum_j |\phi_j\rangle \langle\phi_j|\Psi\rangle . \quad (91)$$

This leads us to define the operator that projects onto \mathcal{M} by

$$P(\mathcal{M}) = \sum_i |\psi_i\rangle \langle\psi_i| \quad (92)$$

and the operator that projects onto \mathcal{M}_\perp by

$$P(\mathcal{M}_\perp) = \sum_j |\phi_j\rangle \langle\phi_j| . \quad (93)$$

We have

$$\begin{aligned} P(\mathcal{M})|\Psi\rangle &= |\psi\rangle , \\ P(\mathcal{M}_\perp)|\Psi\rangle &= |\phi\rangle . \end{aligned} \tag{94}$$

This may all seem a little abstract, but once you get used to it, I think that you will find it very helpful to think about subspaces using these ideas. You may want to draw little pictures of the subspaces, even though you are pretty much limited to two or three real dimensions and you might want many complex dimensions instead.

With this notation, we can consider again our self-adjoint operator A again. There could be more than one eigenvector $|i\rangle$ with a given eigenvalue a . In this case, we say that the eigenvalue is *degenerate*. We can define a projection operator

$$P(a) = \sum_i \Theta(a_i = a) |i\rangle\langle i| . \tag{95}$$

Here $\Theta(a_i = a) = 1$ if $|i\rangle$ has eigenvalue a_i equal to a and $\Theta(a_i = a) = 0$ if $|i\rangle$ has eigenvalue a_i not equal to a . Thus only eigenvectors whose eigenvalues equal a are included in the sum. The operator $P(a)$ projects onto the subspace consisting of vectors that are eigenvectors of A with eigenvalue a . We can write the spectral theorem as

$$A = \sum_a a P(a) . \tag{96}$$

Here we sum over the distinct eigenvalues a of A . This form of the spectral theorem has the advantage that the operator A uniquely determines the eigenvalues a and the subspaces projected by $P(a)$. In each subspace, we can find an orthonormal basis of eigenvectors with eigenvalue a , but it is our choice which basis to pick. If the eigenvalue a is degenerate, someone else might pick a different basis.

Here is an important application. Suppose that we have two self-adjoint operators A and B . Suppose further that $AB = BA$, that is

$$[A, B] = 0 . \tag{97}$$

Then we can “diagonalize” A and B at the same time. That is, there is an orthonormal basis $|i\rangle$ such that

$$\begin{aligned} A|i\rangle &= a_i|i\rangle , \\ B|i\rangle &= b_i|i\rangle . \end{aligned} \tag{98}$$

Thus

$$\begin{aligned} A &= \sum_i a_i |i\rangle\langle i| , \\ B &= \sum_i b_i |i\rangle\langle i| . \end{aligned} \tag{99}$$

The proof of this uses what we have learned in this section. Since A is self-adjoint, we can find subspaces $\mathcal{M}(a)$ consisting of eigenvectors of A with eigenvalues a :

$$A = \sum_a a P(a) . \tag{100}$$

Let $|\psi\rangle$ be a vector in $\mathcal{M}(a)$. Consider the vector $B|\psi\rangle$. We have

$$AB|\psi\rangle = BA|\psi\rangle = aB|\psi\rangle . \tag{101}$$

Thus $B|\psi\rangle$ is in $\mathcal{M}(a)$. We can thus consider B to be an operator just on the subspace $\mathcal{M}(a)$. Since it is self-adjoint, there is an orthonormal basis of vectors $|i\rangle$ in $\mathcal{M}(a)$ that are eigenvectors of B . Of course, these vectors are also eigenvectors of A . We construct eigenvectors of B in each subspace $\mathcal{M}(a)$. In this way we construct a basis for the whole space \mathcal{V} such that the basis vectors are eigenvectors of both A and B .

We will find in this course that it happens pretty frequently that we want to find eigenvectors of some operator A and that is another operator B that commutes with A , so that we can find eigenvectors of A and B together. This helps in the problem of finding the eigenvectors of A . In fact, there may be more than two operators, all of which commute with each other. Then, with an evident extension of the results of this section, there is a basis of eigenvectors of all of the operators.

Exercise 1.8 Suppose a self-adjoint linear operator is represented by the matrix

$$A = \begin{pmatrix} 8 & 2 & 2 \\ 2 & 8 & 2 \\ 2 & 2 & 8 \end{pmatrix} . \tag{102}$$

Suppose another self-adjoint linear operator acting on the same space is represented by the matrix

$$B = \begin{pmatrix} 11 & -1 & 2 \\ -1 & 11 & 2 \\ 2 & 2 & 8 \end{pmatrix} . \tag{103}$$

Show that these operators commute. Since they commute, you should be able to find an orthonormal basis consisting of three eigenvectors $\psi(i)$, $i = 1, 2, 3$, which might conveniently be written as column vectors

$$\psi(i) = \begin{pmatrix} \psi_1(i) \\ \psi_2(i) \\ \psi_3(i) \end{pmatrix} , \quad (104)$$

such that these vectors are eigenvectors of both A and B :

$$\begin{aligned} A\psi(i) &= a_i\psi(i) , \\ B\psi(i) &= b_i\psi(i) . \end{aligned} \quad (105)$$

Find the eigenvectors $\psi(i)$ and the corresponding eigenvalues a_i and b_i .

10 Trace and determinant

In calculations, one often needs the trace and the determinant of an operator A .

The trace of A is defined by using the matrix representation of A in an orthonormal basis,

$$\text{tr}[A] = \sum_i \langle i|A|i\rangle . \quad (106)$$

The trace has the important property

$$\text{tr}[AB] = \text{tr}[BA] . \quad (107)$$

To see this, write

$$\begin{aligned} \text{tr}[AB] &= \sum_i \langle i|AB|i\rangle = \sum_{i,j} \langle i|A|j\rangle \langle j|B|i\rangle \\ &= \sum_{i,j} \langle j|B|i\rangle \langle i|A|j\rangle = \sum_j \langle j|BA|j\rangle = \text{tr}[BA] . \end{aligned} \quad (108)$$

What if we use a different basis, $|\text{new}, i\rangle$? Then

$$\text{tr}_{\text{new}}[A] = \sum_i \langle \text{new}, i|A|\text{new}, i\rangle . \quad (109)$$

Let $|\text{new}, i\rangle = U|i\rangle$. As we have seen, U is unitary. We have

$$\text{tr}_{\text{new}}[A] = \sum_i \langle i|U^{-1}AU|i\rangle = \text{tr}[U^{-1}AU] . \quad (110)$$

Using Eq. (107), this is

$$\text{tr}_{\text{new}} [A] = \text{tr}[U^{-1}AU] = \text{tr}[UU^{-1}A] = \text{tr}[A] . \quad (111)$$

Thus we get the same result no matter which basis we use.

Note that if A is self-adjoint, then $\text{tr}[A]$ is the sum of the eigenvalues of A .

We can also define the determinant of an operator A by using the matrix elements of A in some basis:

$$\det[A] = \sum_{\{i\}} \epsilon(i_1, i_2, \dots, i_N) \langle 1|A|i_1\rangle \langle 2|A|i_2\rangle \cdots \langle N|A|i_N\rangle . \quad (112)$$

Here N is the dimension of our vector space and $\epsilon(i_1, i_2, \dots, i_N)$ is defined by two properties: $\epsilon(1, 2, \dots, N) = 1$ and $\epsilon(i_1, i_2, \dots, i_N)$ is antisymmetric under exchange of any two of its indices. Thus $\epsilon(i_1, i_2, \dots, i_N) = 0$ if any two of the indices are the same. The only way that $\epsilon(i_1, i_2, \dots, i_N)$ can be non-zero is if $\{i_1, i_2, \dots, i_N\}$ is one of the $N!$ permutations of $\{1, 2, \dots, N\}$. Then $\epsilon(i_1, i_2, \dots, i_N)$ is 1 if $\{i_1, i_2, \dots, i_N\}$ is an even permutation $\{1, 2, \dots, N\}$ and $\epsilon(i_1, i_2, \dots, i_N)$ is -1 if $\{i_1, i_2, \dots, i_N\}$ is an odd permutation $\{1, 2, \dots, N\}$. Notice that

$$\det[1] = 1 . \quad (113)$$

We can also write

$$\sum_{\{i\}} \epsilon(i_1, \dots, i_N) \langle j_1|A|i_1\rangle \cdots \langle j_N|A|i_N\rangle = \epsilon(j_1, \dots, j_N) \det[A] \quad (114)$$

and

$$\sum_{\{j\}} \epsilon(j_1, \dots, j_N) \langle j_1|A|i_1\rangle \cdots \langle j_N|A|i_N\rangle = \epsilon(i_1, \dots, i_N) \det[A] \quad (115)$$

and also

$$\sum_{\{i\}} \sum_{\{j\}} \epsilon(i_1, \dots, i_N) \epsilon(j_1, \dots, j_N) \langle j_1|A|i_1\rangle \cdots \langle j_N|A|i_N\rangle = N! \det[A] . \quad (116)$$

To prove these, we can first note that Eq. (114) follows in a straightforward fashion from the definition, Eq. (112). Then Eq. (116) follows by multiplying Eq. (114) by $\epsilon(j_1, \dots, j_N)$ and summing. Finally, to derive Eq. (115), we can note that the left hand side of Eq. (115) is completely antisymmetric in the indices i_n , so the left hand side has to be $\epsilon(i_1, \dots, i_N)$ times something, call it X . To find out what X is, we can multiply by $\epsilon(i_1, \dots, i_N)$ and sum over the indices i_n . The left hand side of the resulting equation is now the left hand side of Eq. (116), while the right hand side is $N! X$. We thus find that $X = \det[A]$.

The determinant has the important property

$$\det[AB] = \det[A] \det[B] . \quad (117)$$

To see this, write

$$\begin{aligned} \det[AB] &= \frac{1}{N!} \sum_{\{i\}} \sum_{\{j\}} \epsilon(i_1, \dots, i_N) \epsilon(j_1, \dots, j_N) \langle j_1 | AB | i_1 \rangle \cdots \langle j_N | AB | i_N \rangle \\ &= \frac{1}{N!} \sum_{\{i\}} \sum_{\{j\}} \epsilon(i_1, \dots, i_N) \epsilon(j_1, \dots, j_N) \\ &\quad \sum_{\{k\}} \langle j_1 | A | k_1 \rangle \langle k_1 | B | i_1 \rangle \cdots \langle j_N | A | k_N \rangle \langle k_N | B | i_N \rangle \\ &= \frac{1}{N!} \sum_{\{k\}} \\ &\quad \sum_{\{i\}} \epsilon(j_1, \dots, j_N) \langle j_1 | A | k_1 \rangle \cdots \langle j_N | A | k_N \rangle \\ &\quad \sum_{\{j\}} \epsilon(i_1, \dots, i_N) \langle k_1 | B | i_1 \rangle \cdots \langle k_N | B | i_N \rangle \\ &= \frac{1}{N!} \sum_{\{k\}} \epsilon(k_1, \dots, k_N) \det[A] \epsilon(k_1, \dots, k_N) \det[B] \\ &= \det[A] \det[B] . \end{aligned} \quad (118)$$

What if we use a different basis, $|\text{new}, i\rangle$ with $|\text{new}, i\rangle = U|i\rangle$. Then

$$\begin{aligned} \det_{\text{new}}[A] &= \det[U^{-1}AU] = \det[A] \det[U] \det[U^{-1}] \\ &= \det[A] \det[UU^{-1}] = \det[A] \det[1] = \det[A] . \end{aligned} \quad (119)$$

Thus we get the same result no matter which basis we use.

Note that if A is self-adjoint, then $\det[A]$ is the product of the eigenvalues of A . One simple application of this is that if we call the eigenvalues a_i and the eigenvectors $|i\rangle$, we can write, for any number λ ,

$$A - \lambda 1 = \sum_i (a_i - \lambda) |i\rangle \langle i| . \quad (120)$$

Thus

$$\det[A - \lambda 1] = \prod_i (a_i - \lambda) . \quad (121)$$

This is an N th order polynomial function of λ that vanishes when λ equals any eigenvalue of A . Thus to find the eigenvalues, we simply need to calculate $\det[A - \lambda 1]$ and find where it vanishes.