

Lecture 3

Relevant sections in text: §1.2, 1.3

Spin states

We now model the states of the spin 1/2 particle. As before, we denote a state of the particle in which the component of the spin vector \mathbf{S} along the unit vector \mathbf{n} is $\pm\hbar/2$ by $|\mathbf{S} \cdot \mathbf{n}, \pm\rangle$. We define our Hilbert space of states as follows. We postulate that \mathcal{H} is spanned by $|\mathbf{S} \cdot \mathbf{n}, \pm\rangle$ for any choice of \mathbf{n} , with different choices of \mathbf{n} just giving different bases. Thus, every vector $|\psi\rangle \in \mathcal{H}$ can be expanded via

$$|\psi\rangle = a_+|\mathbf{S} \cdot \mathbf{n}, +\rangle + a_-|\mathbf{S} \cdot \mathbf{n}, -\rangle. \quad (1)$$

We define the scalar product on \mathcal{H} by postulating that each set $|\mathbf{S} \cdot \mathbf{n}, \pm\rangle$ forms an *orthonormal basis*:

$$\langle \mathbf{S} \cdot \mathbf{n}, \pm | \mathbf{S} \cdot \mathbf{n}, \pm \rangle = 1, \quad \langle \mathbf{S} \cdot \mathbf{n}, \mp | \mathbf{S} \cdot \mathbf{n}, \pm \rangle = 0.$$

Since every vector can be expanded in terms of this basis, this defines the scalar product of any two vectors (exercise). Note that the expansion coefficients in (1) can be computed by

$$a_{\pm} = \langle \mathbf{S} \cdot \mathbf{n}, \pm | \psi \rangle.$$

This is just an instance of the general result for the expansion of a vector $|\psi\rangle$ in an orthonormal (ON) basis $|i\rangle$, $i = 1, 2, \dots, n$, where the ON property takes the form

$$\langle i | j \rangle = \delta_{ij}.$$

We have (exercise)

$$|\psi\rangle = \sum_i c_i |i\rangle, \quad c_i = \langle i | \psi \rangle.$$

We can therefore write

$$|\psi\rangle = \sum_i |i\rangle \langle i | \psi \rangle.$$

If we choose one of the spin bases, say, $|\mathbf{S} \cdot \mathbf{n}, \pm\rangle$, and we represent components of vectors as columns, then the basis has components

$$\langle \mathbf{S} \cdot \mathbf{n}, \pm | \mathbf{S} \cdot \mathbf{n}, + \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \langle \mathbf{S} \cdot \mathbf{n}, \pm | \mathbf{S} \cdot \mathbf{n}, - \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

More generally, a vector with expansion

$$|\psi\rangle = a_+|\mathbf{S} \cdot \mathbf{n}, +\rangle + a_-|\mathbf{S} \cdot \mathbf{n}, -\rangle$$

is represented by the column vector

$$\langle \mathbf{S} \cdot \mathbf{n}, \pm | \psi \rangle = \begin{pmatrix} a_+ \\ a_- \end{pmatrix}.$$

The bra $\langle \psi |$ corresponding to $|\psi\rangle$ has components forming a row vector:

$$\langle \psi | \mathbf{S} \cdot \mathbf{n}, \pm \rangle = (a_+^* \quad a_-^*).$$

Linear operators

Our next step in building a model of a spin 1/2 system using the rules of quantum mechanics is to represent the observables (S_x, S_y, S_z) by self-adjoint operators on the foregoing two-dimensional vector space. To do this we need to explain how to work with linear operators in our bra-ket notation.

A linear operator A is a linear mapping from \mathcal{H} to itself, that is, it associates to each vector $|\psi\rangle$ a vector $A|\psi\rangle$. This association (“mapping”, “operation”) is to be linear:

$$A(a|\alpha\rangle + b|\beta\rangle) = aA|\alpha\rangle + bA|\beta\rangle.$$

If you think of vectors as columns, then a linear operator is represented as a square matrix. I will explain this in detail momentarily. As you know, if you take a row vector and multiply it on the left with a column vector of the same size, you will get a square matrix, that is, a linear operator. More generally, given a ket $|\alpha\rangle$ and a bra $\langle\beta|$ we can define a linear operator via

$$A = |\alpha\rangle\langle\beta|.$$

What this means is

$$A|\psi\rangle = |\alpha\rangle\langle\beta|\psi\rangle.$$

You can easily check as an exercise that this is a linear operator. This operator is called the “outer product” or “tensor product” operator.

You can easily see that the sum of two linear operators, defined by,

$$(A + B)|\psi\rangle = A|\psi\rangle + B|\psi\rangle,$$

is a linear operator as is the scalar multiple:

$$(cA)|\psi\rangle = cA|\psi\rangle.$$

Thus the set of linear operators forms a vector space! Moreover, you can check that the product of two operators, defined by

$$(AB)|\psi\rangle = AB|\psi\rangle$$

is a linear operator. Thus the set of linear operators forms an algebra.

It is not hard to see that every linear operator can be written in terms of an orthonormal basis (ONB) $|i\rangle$ as

$$A = \sum_i A_{ij} |i\rangle \langle j|,$$

where

$$A_{ij} = \langle i|A|j\rangle$$

are called the *matrix elements* of A in the basis provided by $|i\rangle$.^{*} To see this, simply expand the vectors $|\psi\rangle$ and $A|\psi\rangle$ in the ONB:

$$A|\psi\rangle = \sum_i |i\rangle \langle i|A|\psi\rangle = \sum_{ij} |i\rangle \langle i|A|j\rangle \langle j|\psi\rangle = \sum_{ij} A_{ij} |i\rangle \langle j|\psi\rangle.$$

A very important example of this is the identity operator, defined by,

$$I|\psi\rangle = |\psi\rangle, \quad \forall |\psi\rangle.$$

It has the decomposition (good exercise!)

$$I = \sum_i |i\rangle \langle i|. \tag{2}$$

This “resolution of the identity” is used all the time to manipulate various equations. Don’t forget it! As a simple example, you can use (2) to view the expansion in a basis formula as a pretty trivial identity:

$$|\psi\rangle = I|\psi\rangle = \left(\sum_i |i\rangle \langle i| \right) |\psi\rangle = \sum_i |i\rangle \langle i|\psi\rangle !$$

The array A_{ij} is in fact the matrix representation of the linear operator A in the given basis. To see how this works, we consider the action of a linear operator on a vector and see the familiar rules of matrix multiplication coming into play when we expand in an orthonormal basis $|i\rangle$. Watch:

$$\begin{aligned} \langle i|A|\psi\rangle &= \langle i| \sum_{jk} A_{jk} |j\rangle \langle k|\psi\rangle \\ &= \sum_{jk} A_{jk} \langle i|j\rangle \langle k|\psi\rangle \\ &= \sum_k A_{ik} \langle k|\psi\rangle. \end{aligned}$$

* More generally, any scalar of the form $\langle \alpha|A|\beta\rangle$ is called a matrix element.

The final line shows how the i^{th} component of $A|\psi\rangle$ — the i^{th} entry of the column vector representing $A|\psi\rangle$ — is given by matrix multiplication of the array A_{ik} with the column vector $\langle k|\psi\rangle$. We can equally well see how matrix multiplication gets defined via the product of linear operators. Consider the matrix elements of the operator AB :

$$\begin{aligned}\langle i|AB|k\rangle &= \sum_j \langle i|A|j\rangle \langle j|B|k\rangle \\ &= \sum_j A_{ij} B_{jk}.\end{aligned}$$

Given a linear operator A we recall the notion of eigenvectors and eigenvalues. They are solutions λ and $|\lambda\rangle$ to the equation

$$A|\lambda\rangle = \lambda|\lambda\rangle.$$

The zero vector is not considered an eigenvector. Note that the eigenvector $|\lambda\rangle$ corresponding to an eigenvalue λ is not unique, since any scalar multiple of the eigenvector will also be an eigenvector with the same eigenvalue. However, note that such eigenvectors are not linearly dependent. It may or may not happen that there is more than one linearly independent eigenvector for a given eigenvalue. When there is, one says that the eigenvalue is *degenerate*. Note also that the number of eigenvalues and the dimension of the eigenspace can range from 0 to the (still finite) dimension of the Hilbert space.

Finally, let us note that a linear operator A on \mathcal{H} also defines a linear operation on the dual vector space, *i.e.*, the space of bras. This operation is denoted

$$\langle\psi| \rightarrow \langle\psi|A.$$

To define $\langle\psi|A$ we should tell how it acts (as a linear function) on kets; the definition is

$$(\langle\psi|A)|\phi\rangle = \langle\psi|A|\phi\rangle.$$

As an exercise you should check that $\langle\psi|A$ so-defined is indeed a linear function, *i.e.*, a bra and that A is a linear operation on bras.

Self-adjoint operators

A linear operator A on a finite-dimensional Hilbert space defines an operator A^\dagger called the *adjoint* of A . It is defined by demanding that, for all kets, we have

$$\langle\psi|A^\dagger|\phi\rangle = \langle\phi|A|\psi\rangle^*.$$

Note that this is equivalent to defining A^\dagger as the operator whose matrix elements are the complex conjugate-transpose of those of A :

$$(A^\dagger)_{ij} = (A_{ji})^*.$$

If

$$A^\dagger = A$$

we say that A is *self-adjoint* or *Hermitian*.

It is a standard result from linear algebra that a Hermitian operator has real eigenvalues and that eigenvectors corresponding to *distinct* eigenvalues must be orthogonal. See your text for the elementary proofs. An extremely important theorem from linear algebra says that a Hermitian operator always admits an orthonormal basis of eigenvectors. Typically, we will use a notation such as

$$A|i\rangle = a_i|i\rangle$$

to denote the eigenvalues and eigenvectors.