Lecture 3

Relevant sections in text: §1.2, 1.3

Spin states

We now construct a mathematical representation for 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 $\vec{S}$ along the unit vector $\hat{n}$ is known with certainty to be $\pm\hbar/2$ by $|\vec{S}\cdot\hat{n},\pm\rangle$. We define our Hilbert space of states as follows. We postulate that $\mathcal{H}$ is spanned by $|\vec{S}\cdot\hat{n},\pm\rangle$ for any particular choice of $\hat{n}$, with different choices of $\hat{n}$ just giving different bases. Thus, every vector $|\psi\rangle \in \mathcal{H}$ can be expanded via

$$|\psi\rangle = a_+|\vec{S}\cdot\hat{n},+\rangle + a_-|\vec{S}\cdot\hat{n},-\rangle. \tag{1}$$

Note: if we fix $\hat{n}$ once and for all, we might as well choose our z axis along $\hat{n}$. In this case we denote this basis by $|S_z,\pm\rangle \equiv |\pm\rangle$.

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

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

Since every vector can be expanded in terms of this basis, this defines the scalar product of any two vectors. Indeed, let

$$|\psi\rangle = a_+|\vec{S}\cdot\hat{n},+\rangle + a_-|\vec{S}\cdot\hat{n},-\rangle, \quad |\phi\rangle = b_+|\vec{S}\cdot\hat{n},+\rangle + b_-|\vec{S}\cdot\hat{n},-\rangle,$$

then (exercise)

$$\langle\psi|\phi\rangle = a_+^* b_+ + a_-^* b_-.$$

Note that the expansion coefficients in (1) can be computed by

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

This is just an instance of the general result for the expansion of a vector $|\psi\rangle$ in an orthonormal (ON) basis $|i\rangle$, $i = 1, 2, \ldots, n$, 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, $|\vec{S}\cdot\hat{n},\pm\rangle$, and we represent components of vectors as columns, then the basis has components

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

More generally, a vector with expansion

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

is represented by the column vector

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

Note that the pair of complex numbers which characterizes a ket will be different in different bases. The bra $\langle\psi|$ corresponding to $|\psi\rangle$ has components forming a row vector:

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

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 $A|\psi\rangle$. The "linear" requirement means

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

If you think of vectors as columns, then a linear operator is represented as a square matrix. I will explain this in detail momentarily.

Some really trivial (but useful) examples of linear operators are the *identity operator*, defined by

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

and the zero operator defined by

$$0|\psi\rangle = 0 \quad \leftarrow \text{ this is the zero vector.}$$

You should check via the definitions that these operators *are* linear.

The simplest non-trivial linear operator arises as follows. As you (should) 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. Using our bra-ket notation, 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 that A is defined as

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

You can easily check as an exercise that this is a linear operator. This operator is called the "outer product" or "tensor product" operator. As an important special case, if $|\alpha\rangle$ is normalized, *i.e.,* a unit vector: $\langle\alpha|\alpha\rangle = 1$, then the operator $|\alpha\rangle\langle\alpha|$ is a *projection operator* onto the 1-d vector space spanned by $|\alpha\rangle$.

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:

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

There is a zero operator defined to map any vector to the zero vector. Thus the set of linear operators forms a vector space! Moreover, you can check that the product of two operators, defined by

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

is a linear operator. Thus the set of linear operators forms an algebra. In general this algebra is *not* commutative since, in general $AB \neq BA$. You already know this from the point of view of matrices representing linear operators.

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:

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

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

A good example of this is the *identity operator* I, 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:

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

As mentioned earlier, the array of complex numbers A_{ij} is in fact the matrix representation of the linear operator A in the given basis. To see how this works, we expand in an orthonormal basis $|i\rangle$. Watch:

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

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 the product of two matrices gets defined via the product of linear operators. Consider the matrix elements of the operator AB:

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

Thus the familiar rules of matrix algebra arise the expression of linear operators in a given basis.