

## Chapter 8

# Vector Spaces in Quantum Mechanics

We have seen in the previous Chapter that there is a sense in which the state of a quantum system can be thought of as being made up of other possible states. The aim here is to use the example of the Stern-Gerlach experiment to develop this idea further, and to show that the states of a quantum system can be represented by vectors in a complex vector space. To begin, we review some of the basic ideas of vectors, using the example of vectors in real two dimensional space.

### 8.1 Vectors in Two Dimensional Space

Below is a summary of the important properties of vectors in physical space based on their interpretation as mathematical objects that have both magnitude and direction. Position, velocity, force and so on are examples of such vectors. The intention is not to give a complete discussion, but to highlight a number of important properties of such vectors that have analogues in the case of quantum states, including the property that two vectors can be combined to produce another vector, and that ‘how much’ of one vector is contained in another can be measured via the inner product of two vectors.

#### 8.1.1 Linear Combinations of Vectors – Vector Addition

Consider two non-collinear vectors  $\hat{\mathbf{v}}_1$  and  $\hat{\mathbf{v}}_2$ , as illustrated in Fig. (8.1). Multiples of these pair of vectors can be added together in the fashion illustrated in Fig. (8.1) to form another vector. Conversely, any other vector  $\mathbf{v}$  can be expressed in terms of  $\hat{\mathbf{v}}_1$  and  $\hat{\mathbf{v}}_2$  using appropriate values for the components  $a$  and  $b$  of  $\mathbf{v}$ , i.e.

$$\mathbf{v} = a\hat{\mathbf{v}}_1 + b\hat{\mathbf{v}}_2. \quad (8.1)$$

The right hand side of this equation is known as a *linear combination* of the vectors  $\hat{\mathbf{v}}_1$  and  $\hat{\mathbf{v}}_2$ . The particular points to take away from this is that combining vectors produces other vectors, analogous to our observation above that combining states produces other states, and that the components  $a$  and  $b$  are a measure of how much of  $\hat{\mathbf{v}}_1$  and  $\hat{\mathbf{v}}_2$  respectively go towards making up the vector  $\mathbf{v}$ .

These vectors are *real* vectors in that the coefficients  $a$  and  $b$  are real numbers. We can readily generalize the ideas above by allowing  $a$  and  $b$  to be complex numbers. This makes

it difficult to draw figures such as Fig. (8.1), but the idea can be still retained that the absolute values  $|a|$  and  $|b|$  will then represent the extent to which  $\mathbf{v}$  is made up of the two vectors  $\mathbf{v}_1$  and  $\mathbf{v}_2$ .

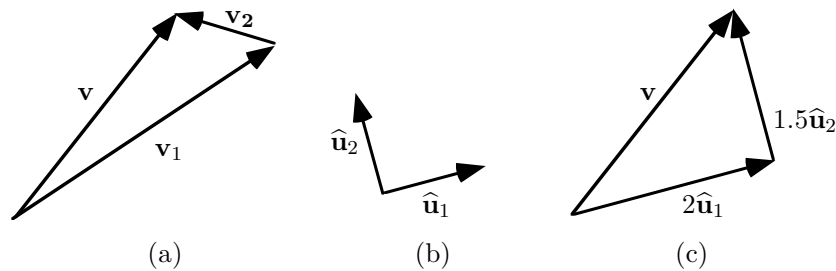


Figure 8.1: Examples of vector addition. (a) Two arbitrary basis vectors  $\mathbf{v}_1$  and  $\mathbf{v}_2$  combining to give  $\mathbf{v}$ ; (b) A pair of orthonormal basis vectors; (c) The vector  $\mathbf{v}$  expressed as a linear combination of the basis vectors  $\hat{\mathbf{u}}_1$  and  $\hat{\mathbf{u}}_2$ :  $\mathbf{v} = 2\hat{\mathbf{u}}_1 + 1.5\hat{\mathbf{u}}_2$ .

The two vectors  $\hat{\mathbf{v}}_1$  and  $\hat{\mathbf{v}}_2$  introduced above are arbitrary except insofar as they are not collinear. They are known as *basis vectors* in the sense that any vector can be written as a linear combination of them. There is effectively an infinite number of choices for the basis vectors, and in fact it is possible to choose three or more vectors to be basis vectors. But the minimum number is two, if we wish to be able to describe any vector in the plane as a linear combination of basis vectors. The collection of all the vectors that can be constructed by taking linear combinations of these basis vectors using any complex numbers  $a$  and  $b$  as components is known as a complex vector space, and since two basis vectors are needed, the vector space is said to be of dimension two.

This vector space possess more structure than that implied by simply forming various linear combinations. Vectors that can be drawn in a plane, as in Fig. (8.1), i.e. for which the coefficients  $a$  and  $b$  are real, can be clearly seen to have different lengths and relative orientations. These properties of vectors are encompassed in the definition of the inner, scalar or dot product of pairs of vectors.

### 8.1.2 Inner or Scalar Products

The inner or scalar product of two *real* vectors  $\mathbf{v}_1$  and  $\mathbf{v}_2$  is defined by

$$\mathbf{v}_1 \cdot \mathbf{v}_2 = v_1 v_2 \cos \theta \quad (8.2)$$

where  $v_1$  and  $v_2$  are the lengths of  $\mathbf{v}_1$  and  $\mathbf{v}_2$  respectively, and  $\theta$  is the angle between them.

Using the idea of an inner or scalar product  $\mathbf{v}_1 \cdot \mathbf{v}_2$  it is possible to introduce a particularly useful pair of basis vectors. To this end, consider two vectors  $\hat{\mathbf{u}}_1$  and  $\hat{\mathbf{u}}_2$  that satisfy

$$\hat{\mathbf{u}}_1 \cdot \hat{\mathbf{u}}_1 = \hat{\mathbf{u}}_2 \cdot \hat{\mathbf{u}}_2 = 1 \quad (8.3)$$

i.e. they have unit length, hence they are known as unit vectors, and

$$\hat{\mathbf{u}}_1 \cdot \hat{\mathbf{u}}_2 = 0 \quad (8.4)$$

i.e. they are orthogonal. This pair of vectors  $\hat{\mathbf{u}}_1$  and  $\hat{\mathbf{u}}_2$  is said to be orthonormal. As before, they form a basis in that multiples of each vector can be added together in the

fashion illustrated in Fig. (8.1) to form another vector. Conversely, any vector  $\mathbf{v}$  can be expressed using appropriate values for the components of  $\mathbf{v}$ , i.e.

$$\mathbf{v} = a\hat{\mathbf{u}}_1 + b\hat{\mathbf{u}}_2. \quad (8.5)$$

The components  $a$  and  $b$ , which represent ‘how much’ of the vector  $\mathbf{v}$  is made up of the vectors  $\hat{\mathbf{u}}_1$  and  $\hat{\mathbf{u}}_2$  are given by

$$a = \hat{\mathbf{u}}_1 \cdot \mathbf{v} \quad \text{and} \quad b = \hat{\mathbf{u}}_2 \cdot \mathbf{v} \quad (8.6)$$

A well known example of a vector expressed as a linear combination of a pair of unit vectors is given by the position vector  $\mathbf{r}$  written with respect to the unit vectors  $\hat{\mathbf{i}}$  and  $\hat{\mathbf{j}}$ :

$$\mathbf{r} = x\hat{\mathbf{i}} + y\hat{\mathbf{j}}. \quad (8.7)$$

Once again, if we allow for the possibility of complex vectors, then the definition of the inner product is changed to allow for this. Thus the inner product of two vectors  $\mathbf{v}_1$  and  $\mathbf{v}_2$  is now  $\mathbf{v}_1^* \cdot \mathbf{v}_2$ , and orthonormal vectors satisfy

$$\begin{aligned} \mathbf{u}_1^* \cdot \mathbf{u}_1 &= \mathbf{u}_2^* \cdot \mathbf{u}_2 = 1 \\ \mathbf{u}_1^* \cdot \mathbf{u}_2 &= \mathbf{u}_2^* \cdot \mathbf{u}_1 = 0. \end{aligned} \quad (8.8)$$

Complex basis vectors are not exotic mathematical entities. A simple example is

$$\begin{aligned} \mathbf{u}_1 &= \frac{3\mathbf{i} + 4i\mathbf{j}}{5} \\ \mathbf{u}_2 &= \frac{4\mathbf{i} - 3i\mathbf{j}}{5} \end{aligned} \quad (8.9)$$

though it is true to say that they are not often encountered in mechanics, except at an advanced level, but are, as we shall see, routinely found in quantum mechanics. Because of that, it is convenient to introduce a new notation for inner product (one that is commonly used in pure mathematics) which is to write the inner product of two vectors  $\mathbf{v}_1$  and  $\mathbf{v}_2$  as  $(\mathbf{v}_1, \mathbf{v}_2)$ , so that we would have here

$$(\mathbf{v}_1, \mathbf{v}_2) = \mathbf{v}_1^* \cdot \mathbf{v}_2. \quad (8.10)$$

The value of this notation is simply that it is more general and does not tie us to the geometrical notion of inner product that we are used to using with position vectors, velocity vectors and the like.

## 8.2 Spin Half Quantum States as Vectors

We now need to examine the way in which the quantum states for a spin half system can be seen to fit in with the idea of being considered as vectors. To see how this comes about, we will show that there is a perfect analogy between Eqs. (7.30) and (7.31) and corresponding relationships for ordinary (complex) vectors. Returning to the Stern-Gerlach example discussed in the preceding Chapter we obtained there an expression Eq. (7.31)

$$|S\rangle = |+\rangle\langle +|S\rangle + |-\rangle\langle -|S\rangle.$$

for the state of a spin half atom expressed in terms of the states  $|\pm\rangle$ , which are states for which the atom has a  $z$  component of spin equal to  $\pm\frac{1}{2}\hbar$ , and  $\langle \pm|S\rangle$  are probability amplitudes (complex numbers) whose magnitude in some sense tells us ‘how much’ of the

states  $|\pm\rangle$  are to be found in the state  $|S\rangle$ . This result was obtained by ‘cancelling’ the common factor  $\langle S'|$  from the result

$$\langle S'|S\rangle = \langle S'|+\rangle\langle +|S\rangle + \langle S'|-\rangle\langle -|S\rangle.$$

What we should bear in mind here is that we can recover this relationship between probability amplitudes by reintroducing  $\langle S'|$  into Eq. (7.31) for any chosen final state, yielding an expression for the probability amplitudes as needed. Thus, as has been said before, Eq. (7.31) effectively represents a ‘template’ into which we insert the appropriate information in order to recover the required probability amplitudes. We can also note that there is nothing sacred about choosing to cancel the the common factor  $|S\rangle$  – we could equally as well cancel the factor  $|S\rangle$ , yielding

$$\langle S'| = \langle S'|+\rangle\langle +| + \langle S'|-\rangle\langle -|. \quad (8.11)$$

Having carried out this cancellation procedure, what has reappeared is the state of a quantum system i.e.  $|S\rangle$  which was introduced earlier in a different context, specifically as being nothing more than a way of writing down all that we knew about the state of a quantum system. There, the notation had no mathematical significance, but in the manner in which it appears here, it seems to have acquired a mathematical meaning of some kind. The aim is to see what this meaning might be, and in doing so, we will show that the expression for  $|S\rangle$  has many of the properties that we associate with expressing a vector as a sum of its components.

We begin by considering the probability amplitudes  $\langle S'|S\rangle$  themselves. These are complex numbers in general for arbitrary spin directions, (but they were real in the particular Stern-Gerlach example used above), such that their modulus squared  $|\langle S'|S\rangle|^2$  is the probability  $P(S'|S)$  of observing the spin to be in the state  $|S'\rangle$  given that it was in the state  $|S\rangle$ . In particular,  $\langle S|S\rangle$  is the probability amplitude of observing the spin to be in the state  $|S\rangle$  given that it was in the state  $|S\rangle$ . This will have to be unity, i.e.  $P(S|S) = |\langle S|S\rangle|^2 = 1$ . Thus we can conclude that

$$\langle S|S\rangle = e^{i\eta} \quad (8.12)$$

where  $\eta$  is an arbitrary phase. It turns out that this phase always cancels out in any calculation of observable quantities, so it is conventionally set to zero, and hence

$$\langle S|S\rangle = 1. \quad (8.13)$$

The state  $|S\rangle$  is said to be normalized to unity.

As a particular case, this last result implies that

$$\langle +|+\rangle = 1. \quad (8.14)$$

We can now consider the probability amplitude  $\langle +|S\rangle$  obtained by replacing  $S'$  by  $+$  in the above expression for  $\langle S'|S\rangle$ :

$$\langle +|S\rangle = \langle +|+\rangle\langle +|S\rangle + \langle +|-\rangle\langle -|S\rangle. \quad (8.15)$$

We have seen that we can put  $\langle +|+\rangle = 1$ , so we have

$$\langle +|-\rangle\langle -|S\rangle = 0 \quad (8.16)$$

which has to be true no matter what the state  $|S\rangle$  happens to be, i.e. no matter what value the probability amplitude  $\langle -|S\rangle$  is. Thus we conclude that

$$\langle +|-\rangle = 0. \quad (8.17)$$

Similarly we can show that

$$\langle -|- \rangle = 1 \quad \text{and} \quad \langle -|+ \rangle = 0. \quad (8.18)$$

Thus we can set up a comparison:

$$\begin{aligned} \langle +|+ \rangle = 1 &\longleftrightarrow \hat{\mathbf{u}}_1^* \cdot \hat{\mathbf{u}}_1 = 1 \\ \langle +|- \rangle = 0 &\longleftrightarrow \hat{\mathbf{u}}_2^* \cdot \hat{\mathbf{u}}_1 = 0 \\ \langle -|- \rangle = 1 &\longleftrightarrow \hat{\mathbf{u}}_2^* \cdot \hat{\mathbf{u}}_2 = 1 \\ \langle -|+ \rangle = 0 &\longleftrightarrow \hat{\mathbf{u}}_2^* \cdot \hat{\mathbf{u}}_1 = 0 \end{aligned} \quad (8.19)$$

where we have chosen to make the comparison between the probability amplitudes and the inner product of complex unit vectors as we are dealing with probability amplitudes that are, in general, complex numbers. This comparison implies the following correspondences:

$$\begin{aligned} |+\rangle &\longleftrightarrow \hat{\mathbf{u}}_1 & |-\rangle &\longleftrightarrow \hat{\mathbf{u}}_2 \\ \langle +| &\longleftrightarrow \hat{\mathbf{u}}_1^* & \langle -| &\longleftrightarrow \hat{\mathbf{u}}_2^* \end{aligned} \quad (8.20)$$

We know that  $\langle +|S \rangle$  and  $\langle -|S \rangle$  are both just complex numbers, so call them  $a$  and  $b$  respectively. If we now write

$$|S \rangle = a|+\rangle + b|-\rangle \quad (8.21)$$

we establish a perfect correspondence with the expression

$$\mathbf{v} = a\hat{\mathbf{u}}_1 + b\hat{\mathbf{u}}_2. \quad (8.22)$$

On the basis of this result, we are then tempted to interpret the ket  $|S \rangle$  as a vector expressed as a linear combination of two orthonormal basis vectors  $|\pm \rangle$ . We can push the analogy further if we once again use the fact that  $\langle S|S \rangle = 1$ , so that

$$\langle S|S \rangle = 1 = \langle S|- \rangle \langle -|S \rangle + \langle S|+ \rangle \langle +|S \rangle \quad (8.23)$$

On the other hand, the total probability of observing the system in either of the states  $|\pm \rangle$  must add up to unity, which means that

$$P(+|S) + P(-|S) = |\langle +|S \rangle|^2 + |\langle -|S \rangle|^2 = 1. \quad (8.24)$$

By comparing the last two equations, and noting that

$$|\langle \pm|S \rangle|^2 = \langle \pm|S \rangle \langle \pm|S \rangle^* \quad (8.25)$$

we conclude that

$$\langle \pm|S \rangle = \langle S|\pm \rangle^*. \quad (8.26)$$

If we now consider

$$\langle S'| = \langle S'|+ \rangle \langle +| + \langle S'|- \rangle \langle -|$$

and use the result, Eq. (8.26),  $\langle \pm|S' \rangle = \langle S'|\pm \rangle^*$ , we can write this as

$$\langle S'| = \langle +|S' \rangle^* \langle +| + \langle -|S' \rangle^* \langle -| \quad (8.27)$$

or, expressed in terms of  $a' = \langle +|S' \rangle$  and  $b' = \langle -|S' \rangle$ , we have

$$\langle S'| = a'^* \langle +| + b'^* \langle -| \quad (8.28)$$

which has a perfect correspondence with an ordinary vector  $\hat{\mathbf{v}}'$  in the form

$$\mathbf{v}'^* = a'^* \hat{\mathbf{u}}_1^* + b'^* \hat{\mathbf{u}}_2^*. \quad (8.29)$$

So the bra  $\langle S'|$  is itself a vector, a bra vector, which can be thought of as being just the complex conjugate of the corresponding ket vector  $|S'\rangle$ . But while it is occasionally useful to think this way, it is not strictly true mathematically, and this way of viewing a bra vector will not be employed here. Instead, as will be shown shortly, an interpretation of ket vectors as column vectors leads to the interpretation of bra vectors as row vectors. A more mathematical standpoint also leads to interpretation of bra vectors as ‘linear functionals’, that is, a bra is a mathematical operator that acts on a ket vector to produce a complex number.

Finally, to complete the correspondence, we note that the probability amplitude  $\langle S'|S\rangle$  can be written

$$\langle S'|S\rangle = a'^*a + b'^*b \quad (8.30)$$

which can be compared with the inner product  $\mathbf{v}'^* \cdot \mathbf{v}$ , or written in the more formal notation:

$$(\mathbf{v}', \mathbf{v}) = a'^*a + b'^*b \quad (8.31)$$

which tells us that the probability amplitude can be considered as being simply the inner product of the two vectors  $|S'\rangle$  and  $|S\rangle$ , i.e.

$$\langle S'|S\rangle = (|S'\rangle, |S\rangle). \quad (8.32)$$

In other words, we have a perfect analogy between the two dimensional complex vector space formed by linear combinations of the unit vectors  $\hat{\mathbf{u}}_1$  and  $\hat{\mathbf{u}}_2$  discussed in Section 8.1 and a complex vector space consisting of all the linear combinations of the states  $|\pm\rangle$ . The ket vectors  $|\pm\rangle$  are referred to as *basis states*, analogous to  $\hat{\mathbf{u}}_1$  and  $\hat{\mathbf{u}}_2$  being referred to as basis vectors.

Different spin states can be constructed by forming linear combinations  $|S\rangle = a|+\rangle + b|-\rangle$  of these basis states, with  $a$  and  $b$  being allowed to range over all the complex numbers, though we have only been looking at linear combinations with real coefficients. By limiting  $a$  and  $b$  to be real numbers, we are constructing states whose measured component of spin all lie in the same plane, which, with the system of axes we have been using here, is the  $XZ$  plane. If the coefficients  $a$  and  $b$  are complex, the state  $|S\rangle$  represents a state in which the measured component  $S = \mathbf{S} \cdot \mathbf{n}$  is along a direction  $\hat{\mathbf{n}}$  that points out of this plane, though we will not attempt to prove this here (see Eq. (8.46)). So, any linear combination in which  $a$  and  $b$  are any complex numbers also defines a possible spin state of the spin half system. Thus all the possible linear combinations of  $|\pm\rangle$ , i.e. combinations of the form  $a|+\rangle + b|-\rangle$  where  $a$  and  $b$  are complex numbers form a *complex vector space* known as the *state space* of the system.

The quantum state vectors can also be ‘multiplied’ together – the inner product of the two vectors  $|S'\rangle$  and  $|S\rangle$  is just the probability amplitude  $\langle S'|S\rangle$ . In particular, the basis states are normalized to unity, i.e. they are unit vectors, and they are orthogonal to each other, i.e. they form a pair of *orthonormal basis states*.

The terminology often adopted is to say that the state vector  $|S\rangle = a|+\rangle + b|-\rangle$  is a ‘linear superposition’ of the two states  $|\pm\rangle$ . The probability amplitudes  $a = \langle +|S\rangle$  and  $b = \langle -|S\rangle$  represent ‘how much’ of the states  $|\pm\rangle$  are contained within the state  $|S\rangle$  to the extent that  $|\langle \pm|S\rangle|^2$  is the probability of the  $z$  component of spin being found to have the values  $\pm\frac{1}{2}\hbar$ .

One difference between ordinary vectors and quantum state vectors is the importance of the ‘normalization condition’, i.e. the requirement that  $\langle S|S\rangle = 1$ , which must hold true given the interpretation of the inner product as a probability amplitude. But how can this

be reconciled with the statement above that *any* linear combination of the basis states is a possible state of the system? How can a state vector such as  $|\tilde{S}\rangle = |+\rangle + |-\rangle$  which has the property

$$\langle\tilde{S}|\tilde{S}\rangle = 2 \quad (8.33)$$

be a physically acceptable state vector as it seems to be saying that the probability of finding the system in the state  $|\tilde{S}\rangle$  given that it is in the state  $|\tilde{S}\rangle$  is 4, which does not make sense. But, if we define a new vector  $|S\rangle$  by

$$|S\rangle = \frac{|\tilde{S}\rangle}{\sqrt{\langle\tilde{S}|\tilde{S}\rangle}} = \frac{1}{\sqrt{2}}|\tilde{S}\rangle \quad (8.34)$$

then automatically  $|S\rangle$  will have the required normalization property – it is said to be normalized to unity. So, rather than abandoning giving a physical interpretation of state vectors which are not normalized to unity, the approach adopted is that we can multiply any state vector by any factor and say that it still represents the same *physical* state, i.e.  $|S\rangle$  and  $|\tilde{S}\rangle = a|S\rangle$ , where  $a$  is any complex number, represent the same physical state. However, it is only the normalized state  $|S\rangle$  that should be used in any calculations in order to be certain that probability is properly accounted for.

This can be summarized in a table:

	Classical vector	Quantum state vector for spin half system
Basis Vectors	$\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2$	$ +\rangle,  -\rangle$
Inner Product	$(\mathbf{v}_1, \mathbf{v}_2) = \mathbf{v}_1^* \cdot \mathbf{v}_2$	$( S'\rangle,  S\rangle) = \langle S' S\rangle$
Orthonormality	$\hat{\mathbf{u}}_1^* \cdot \hat{\mathbf{u}}_1 = \hat{\mathbf{u}}_2^* \cdot \hat{\mathbf{u}}_2 = 1$ $\hat{\mathbf{u}}_1^* \cdot \hat{\mathbf{u}}_2 = \hat{\mathbf{u}}_2^* \cdot \hat{\mathbf{u}}_1 = 0$	$\langle + +\rangle = \langle - -\rangle = 1$ $\langle + -\rangle = \langle - +\rangle = 0$
Linear combination	$\hat{\mathbf{v}} = a\hat{\mathbf{u}}_1 + b\hat{\mathbf{u}}_2$ $a$ and $b$ complex numbers	$ S\rangle = a +\rangle + b -\rangle$ $a$ and $b$ complex numbers
Normalisation	—	$\langle S S\rangle = 1$

**A More Detailed Analysis** One of the important properties of vectors is that two or more of them can be combined as a ‘linear combination’ to produce a third. If we are to consider quantum states as vectors, then this very basic property must also be possessed by quantum states. In the above, we have not really shown that any linear combination of the basis states  $|\pm\rangle$ , does indeed represent a possible state of the system, even if we restrict ourselves to the case of the measuring spin components in the  $XZ$  plane. But a more detailed argument than that just presented can be used to strengthen this conclusion. To see how this comes about, we return to the above expression Eq. (7.25) for the probability amplitude  $\langle S_f = \frac{1}{2}\hbar | S_i = \frac{1}{2}\hbar \rangle$ :

$$\begin{aligned} \langle S_f = \frac{1}{2}\hbar | S_i = \frac{1}{2}\hbar \rangle &= \langle S_f = \frac{1}{2}\hbar | S_I = \frac{1}{2}\hbar \rangle \langle S_I = \frac{1}{2}\hbar | S_i = \frac{1}{2}\hbar \rangle \\ &+ \langle S_f = \frac{1}{2}\hbar | S_I = -\frac{1}{2}\hbar \rangle \langle S_I = -\frac{1}{2}\hbar | S_i = \frac{1}{2}\hbar \rangle. \end{aligned} \quad (8.35)$$

We can ‘cancel’  $\langle S_f = \frac{1}{2}\hbar |$  from this expression and write

$$|S_i = \frac{1}{2}\hbar\rangle = |S_I = \frac{1}{2}\hbar\rangle\langle S_I = \frac{1}{2}\hbar|S_i = \frac{1}{2}\hbar\rangle + |S_I = -\frac{1}{2}\hbar\rangle\langle S_I = -\frac{1}{2}\hbar|S_i = \frac{1}{2}\hbar\rangle \quad (8.36)$$

In Section 7.3, Eq. (7.17), the quantity  $\langle S_f = \frac{1}{2}\hbar|S_i = \frac{1}{2}\hbar\rangle$  was shown to be given by

$$\langle S_f = \frac{1}{2}\hbar|S_i = \frac{1}{2}\hbar\rangle = \cos[(\theta_f - \theta_i)/2]$$

with the phase factor  $\exp(i\Phi)$  put equal to unity, and with  $\hat{\mathbf{n}}$  and  $\hat{\mathbf{m}}$ , the directions of the magnetic fields, confined to the  $XZ$  plane. The probability amplitudes for the system to pass through the intermediate states  $|S_I = \pm\frac{1}{2}\hbar\rangle$ , that is,  $\langle S_I = \pm\frac{1}{2}\hbar|S_i = \frac{1}{2}\hbar\rangle$  are likewise given by

$$\begin{aligned} \langle S_I = \frac{1}{2}\hbar|S_i = \frac{1}{2}\hbar\rangle &= \cos[\frac{1}{2}(\theta_I - \theta_i)] \\ \langle S_I = -\frac{1}{2}\hbar|S_i = \frac{1}{2}\hbar\rangle &= \cos[\frac{1}{2}(\theta_I + \pi - \theta_i)] = -\sin[\frac{1}{2}(\theta_I - \theta_i)]. \end{aligned} \quad (8.37)$$

so that Eq. (8.36) becomes

$$|S_i = \frac{1}{2}\hbar\rangle = \cos[\frac{1}{2}(\theta_I - \theta_i)]|S_I = +\frac{1}{2}\hbar\rangle - \sin[\frac{1}{2}(\theta_I - \theta_i)]|S_I = -\frac{1}{2}\hbar\rangle. \quad (8.38)$$

To further simplify things, we will assume that  $\theta_I = 0$ , i.e. the  $\hat{\mathbf{1}}$  vector is in the  $z$  direction. In addition, we will make the notational simplification already used above defined by

$$\begin{aligned} |S_i = \frac{1}{2}\hbar\rangle &\rightarrow |S\rangle \\ |S_I = \pm\frac{1}{2}\hbar\rangle &\rightarrow |\pm\rangle \\ \langle S_I = \pm\frac{1}{2}\hbar|S_i = \frac{1}{2}\hbar\rangle &\rightarrow \langle\pm|S\rangle \end{aligned}$$

so that  $|\pm\rangle = |S_z = \pm\frac{1}{2}\hbar\rangle$ , and Eq. (8.36) becomes

$$|S\rangle = |+\rangle\langle +|S\rangle + |-\rangle\langle -|S\rangle. \quad (8.39)$$

or, using Eq. (8.37)

$$|S\rangle = \cos(\frac{1}{2}\theta_i)|+\rangle + \sin(\frac{1}{2}\theta_i)|-\rangle. \quad (8.40)$$

We are now at the point at which we can begin to supply an interpretation to this equation. What this equation is saying is that the combination  $\cos(\frac{1}{2}\theta_i)|+\rangle + \sin(\frac{1}{2}\theta_i)|-\rangle$ , and  $|S\rangle$ , both represent the same thing – the atomic spin is in a state for which  $S_i = \frac{1}{2}\hbar$ . In other words, if we were presented with the combination:

$$\frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle \quad (8.41)$$

we immediately see that  $\cos(\frac{1}{2}\theta_i) = 1/\sqrt{2}$  and  $\sin(\frac{1}{2}\theta_i) = 1/\sqrt{2}$ , and hence  $\theta_i = 90^\circ$ . Thus the magnetic field is pointing in the direction  $90^\circ$  to the  $z$  direction, i.e. in the  $x$  direction, and hence the spin state of the atom is the state  $|S\rangle = |S_x = \frac{1}{2}\hbar\rangle$ .

But what if we were presented with the combination  $2|+\rangle + 2|-\rangle$ ? Here, we cannot find any angle  $\theta_i$ , so it appears that this combination is not a possible state of the atomic spin. But we can write this as

$$2\sqrt{2}\left[\frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle\right] \quad (8.42)$$

which we can now understand as representing  $2\sqrt{2}|S_x = \frac{1}{2}\hbar\rangle$ . Is  $2\sqrt{2}|S_x = \frac{1}{2}\hbar\rangle$  a different physical state of the system to  $|S_x = \frac{1}{2}\hbar\rangle$ ? Well, it is our notation, so we can say what we like, and what turns out to be preferable is to say that  $\alpha|S\rangle$  describes the same physical



state as  $|S\rangle$ , for any value of the constant  $\alpha$ . Thus, we can say that  $2|+\rangle + 2|-\rangle$  is also a state of the system, namely  $2\sqrt{2}|S_x = \frac{1}{2}\hbar\rangle$ , which represents the same physical information about the state of the system as  $|S_x = \frac{1}{2}\hbar\rangle$ .

Thus any combination  $C_+|+\rangle + C_-|-\rangle$  where  $C_{\pm}$  are real numbers will always represent some state of the system, in general given by

$$\sqrt{C_+^2 + C_-^2} |S_i = \frac{1}{2}\hbar\rangle \quad (8.43)$$

where

$$S_i = \mathbf{S} \cdot \hat{\mathbf{n}} \quad (8.44)$$

and where  $\hat{\mathbf{n}}$  is a unit vector in the direction defined by the angle

$$\theta_i = 2 \tan^{-1} \left( \frac{C_-}{C_+} \right). \quad (8.45)$$

Conversely, given any state of the system, we can work out how to write it in the form  $C_+|+\rangle + C_-|-\rangle$ . Further, we can repeat the whole of the above discussion for any other choice of the intermediate states  $|S_I = \pm\frac{1}{2}\hbar\rangle$ .

It is this last fact that a state  $|S\rangle$  can be written as the linear combination or linear superposition  $C_+|+\rangle + C_-|-\rangle$  of two other states, analogous to Eq. (8.1) for the arbitrary vector  $\mathbf{v}$ , and conversely that any linear superposition of states is itself another state is the essential property that these states need to possess in order for them to be interpreted as vectors belonging to some vector space, specifically here a real vector space.

In the more general case of the magnetic fields vectors not all being in the  $XZ$  plane, the probability amplitudes  $\langle \pm|S\rangle$  will be, in general, complex numbers. For instance, it can be shown that the state  $|S\rangle = |S_n = \frac{1}{2}\hbar\rangle$  where  $S_n = \mathbf{S} \cdot \hat{\mathbf{n}}$ , and where  $\hat{\mathbf{n}} = \sin\theta \cos\phi \hat{\mathbf{i}} + \sin\theta \sin\phi \hat{\mathbf{j}} + \cos\theta \hat{\mathbf{k}}$  is a unit vector oriented in a direction defined by the spherical polar angles  $\theta, \phi$ , is given by

$$|S\rangle = \cos(\frac{1}{2}\theta)|+\rangle + e^{i\phi} \sin(\frac{1}{2}\theta)|-\rangle \quad (8.46)$$

Nevertheless, the arguments presented above continue to apply. In particular *any* linear combination  $C_-|-\rangle + C_+|+\rangle$ , where  $C_{\pm}$  are complex numbers, will be a possible spin state of an atom. But since the coefficients are complex numbers, the vector space, or state space, is a *complex* vector space. This more general case, is what is usually encountered in quantum mechanics and below, we will assume that the probability amplitudes are, in general, complex.

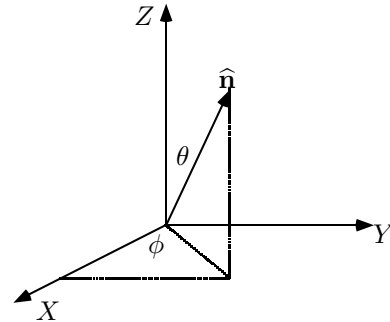


Figure 8.2: Polar angles for defining direction of unit vector  $\hat{\mathbf{n}}$

### 8.3 The General Case of Many Intermediate States

The above results were based on the particular case of a spin half system which could pass through two possible intermediate spin states, and was developed, at least in part, by analogy with the two slit experiment where a particle could pass through two possible intermediate states defined by the positions of the slits. We can generalize these results

to apply to situations in which the system can pass through any number of intermediate states, and where the intermediate states can be more general states of quantum systems. So, suppose we have some unspecified system which is prepared initially in some state  $|\psi\rangle$ , and we are interested in finding it in some other state  $|\phi\rangle$ . Further suppose that the system can pass through any of a set of intermediate states  $\{|\varphi_n\rangle; n = 1, 2, \dots\}$  where these states form a set of orthonormal basis states, i.e.

$$\begin{aligned}\langle\varphi_m|\varphi_n\rangle &= \delta_{mn} = 1 & n = m \\ &= 0 & n \neq m\end{aligned}\quad (8.47)$$

where  $\delta_{mn}$  is known as the Kronecker delta. Then

1.  $\langle\phi|\psi\rangle$  = the probability amplitude of the system being found in the state  $|\phi\rangle$  given that it was in state  $|\psi\rangle$ .
2.  $|\langle\phi|\psi\rangle|^2$  = the probability of the system being found in the state  $|\phi\rangle$  given that it was in state  $|\psi\rangle$ .
3. The *closure relation*:

$$\langle\phi|\psi\rangle = \sum_n \langle\phi|\varphi_n\rangle\langle\varphi_n|\psi\rangle \quad (8.48)$$

which tells us that the total probability amplitude of finding the system in the final state  $|\phi\rangle$  is just the sum of the probability amplitudes of the system passing through any of the intermediate states  $\{|\varphi_n\rangle; n = 1, 2, \dots\}$ .

4. The completeness relations:

$$|\psi\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle \quad (8.49)$$

$$\langle\phi| = \sum_n \langle\phi|\varphi_n\rangle\langle\varphi_n| \quad (8.50)$$

which tells us that either the initial or final states can be expressed as a linear combination of the intermediate states  $\{|n\rangle; n = 1, 2, \dots\}$ .

5.  $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$ .
6. The normalization condition:

$$\langle\psi|\psi\rangle = \sum_n \langle\psi|\varphi_n\rangle\langle n|\psi\rangle = \sum_n |\langle\varphi_n|\psi\rangle|^2 = 1. \quad (8.51)$$

This last result tells us that the probability of finding the system in any of the states  $|n\rangle$  adds up to unity. Moreover, we know that  $\langle\varphi_m|\varphi_n\rangle = 0$  if  $n \neq m$  so that a system in state  $|\varphi_n\rangle$  can never be found in some other state  $|\varphi_m\rangle$ . Consequently, the set of states  $\{|\varphi_n\rangle; n = 1, 2, \dots\}$  represent a complete set of possible alternative final states, complete in the sense that the total probability of ending up in any of the mutually exclusive possible final states  $|\varphi_n\rangle$  adds up to unity – there is nowhere else for the system to be found. Thus the set of states  $\{|\varphi_n\rangle; n = 1, 2, \dots\}$  is known as a *complete set of orthonormal basis states*. It is one of the major tasks in dealing with a quantum system of identifying a set of basis states.

## 8.4 General Mathematical Description of a Quantum System

Most of the discussion above has been developed on the basis of studying the properties of systems that can pass through different intermediate states, leading to the idea of summing the probability amplitudes associated with the different ‘paths’ that the system can pass along between the initial and observed final state. The preceding section extended this perspective to apply to arbitrary systems with arbitrary numbers of intermediate states.

But it was also shown that the mathematical description of this sum of probability amplitudes admits an interpretation of the state of the system as being a vector in a complex vector space, the state space of the system. It is this mathematical picture that is summarized here. This idea that the state of a quantum system is to be considered a vector belonging to a complex vector space, which we have developed here in the case of a spin half system, and which has its roots in the sum over paths point of view, is the basis of all of modern quantum mechanics and is used to describe any quantum mechanical system. Below is a summary of the main points as they are used for a general quantum system whose state spaces are of arbitrary dimension (including state spaces of infinite dimension). The emphasis here is on the mathematical features of the theory, removing it from being couched in the language of probability amplitudes for different intermediate states.

### 8.4.1 State Space

We have indicated a number of times that in quantum mechanics, the state of a physical system is represented by a vector belonging to a complex vector space known as the state space of the system. Here we will give a list of the defining conditions of a state space, though we will not be concerning ourselves too much with the formalities.

The following definitions and concepts set up the state space of a quantum system.

1. Every physical state of a quantum system is specified by a vector called a state vector, ket vector, or sometimes just state and written  $|\dots\rangle$  where  $\dots$  is a label specifying the physical information known about the state. An arbitrary state is written  $|\psi\rangle$ , or  $|\phi\rangle$  and so on. The set of all state vectors describing a given physical system forms a complex vector space (or Hilbert space)  $\mathcal{H}$  also known as the state space or ket space for the system.
2. Every linear superposition of two or more state vectors  $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \dots$ , is also a state of the quantum system i.e. the state  $|\psi\rangle$  given by

$$|\psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + c_3|\phi_3\rangle + \dots$$

is a state of the system for all complex numbers  $c_1, c_2, c_3, \dots$

These last two points amount to saying that every physical state of a system is represented by a vector in the state space of the system, and every vector in the state space represents a possible physical state of the system. To guarantee this, the following condition is also imposed:

3. If a state of the system is represented by a vector  $|\psi\rangle$ , then the same state is represented by the vector  $c|\psi\rangle$  where  $c$  is any non-zero complex number.

Finally, we need the concept of a set of basis states, and of the dimension of the state space.

4. A set of vectors  $\{|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, \dots\}$  is said to form a basis for the state space if every state of the quantum system can be represented as a linear superposition of the  $|\varphi_i\rangle$ 's i.e. for any state  $|\psi\rangle$  we can write

$$|\psi\rangle = \sum_i c_i |\varphi_i\rangle.$$

The set of vectors  $\{|\varphi_i\rangle, i = 1, 2, \dots\}$  are said to *span* the vector space. The vectors are also termed the *base* states for the vector space. They are also said to be *complete*. What this means, mathematically, is that for every state  $|\phi\rangle$  say, at least one of the inner products  $\langle\varphi_n|\phi\rangle$  will be non-zero, or conversely, there does not exist a state  $|\xi\rangle$  for which  $\langle\varphi_n|\xi\rangle = 0$  for all the basis states  $|\varphi_n\rangle$ . Completeness clearly means that no more basis states are needed to describe any possible physical state of a system. It is guaranteed for state spaces of finite dimension, but not guaranteed for state spaces of infinite dimension.

For example, returning to the spin half system, the two states  $|\pm\rangle$  are all that is needed to describe any state of the system, i.e. there are no spin states that cannot be described in terms of these basis states. Thus, these states are said to be complete.

5. The minimum number of vectors needed to form a complete set of basis states is known as the dimension of the state space. [In many, if not most cases of interest in quantum mechanics, the dimension of the state space is infinite.]

It should be noted that there is an infinite number of possible sets of basis states for any state space. Often the choice of basis states is suggested by the physics (such as the set of eigenstates of an observable, see Chapter 9).

### 8.4.2 Probability Amplitudes and the Inner Product of State Vectors

We obtained a number of properties of probability amplitudes when looking at the case of a spin half system. Some of the results obtained there, and a few more that were not, are summarized in the following.

If  $|\phi\rangle$  and  $|\psi\rangle$  are any two state vectors belonging to the state space  $\mathcal{H}$ , then

1.  $\langle\phi|\psi\rangle$ , a complex number, is the probability amplitude of observing the system to be in the state  $|\phi\rangle$  given that it is in the state  $|\psi\rangle$ .
2. The probability of observing the system to be in the state  $|\phi\rangle$  given that it is in the state  $|\psi\rangle$  is  $|\langle\phi|\psi\rangle|^2$ .

The probability amplitude  $\langle\phi|\psi\rangle$ , can then be shown to have the properties

3.  $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$ .
4.  $(\langle\phi|\{c_1|\psi_1\rangle + c_2|\psi_2\rangle\}) = c_1\langle\phi|\psi_1\rangle + c_2\langle\phi|\psi_2\rangle$  where  $c_1$  and  $c_2$  are complex numbers.

5.  $\langle\psi|\psi\rangle \geq 0$ . If  $\langle\psi|\psi\rangle=0$  then  $|\psi\rangle = 0$ , the zero vector.

This last statement is related to the physically reasonable requirement that the probability of a system being found in a state  $|\psi\rangle$  given that it is in the state  $|\psi\rangle$  has to be unity, i.e.  $|\langle\psi|\psi\rangle|^2 = 1$  which means that  $\langle\psi|\psi\rangle = \exp(i\eta)$ . We now *choose*  $\eta = 0$  so that  $\langle\psi|\psi\rangle = 1$ , which is bigger than zero. But recall that any multiple of a state vector still represents the same physical state of the system, i.e.  $|\tilde{\psi}\rangle = a|\psi\rangle$  still represents the same physical state as  $|\psi\rangle$ . However, in this case,  $\langle\tilde{\psi}|\tilde{\psi}\rangle = |a|^2$  which is not necessarily unity, but is certainly bigger than zero.

6. The quantity  $\sqrt{\langle\psi|\psi\rangle}$  is known as the *length* or *norm* of  $|\psi\rangle$ .
7. A state  $|\phi\rangle$  is normalized, or normalized to unity, if  $\langle\phi|\phi\rangle = 1$ .

Normalized states are states for which probability is properly taken into account. It is mathematically convenient to permit the use of states whose norms are not equal to unity, but it is necessary in order to make use of the probability interpretation to deal only with that state which has norm of unity. Any state that cannot be normalized to unity (i.e. it is of infinite length) cannot represent a physically acceptable state.

8. Two states  $|\phi\rangle$  and  $|\psi\rangle$  are orthogonal if  $\langle\phi|\psi\rangle = 0$ .

The physical significance of two states being orthogonal should be understood: for a system in a certain state, there is zero probability of it being observed in a state with which it is orthogonal. In this sense, two orthogonal states are as distinct as it is possible for two states to be.

Finally, a set of orthonormal basis vectors  $\{|\varphi_n\rangle; n = 1, 2, \dots\}$  will have the property

9.  $\langle\varphi_m|\varphi_n\rangle = \delta_{mn}$  where  $\delta_{mn}$  is known as the Kronecker delta, and equals unity if  $m = n$  and zero if  $m \neq n$ .

All the above conditions satisfied by probability amplitudes were to a greater or lesser extent physically motivated, but it nevertheless turns out that these conditions are identical to the conditions that are used to define the inner product of two vectors in a complex vector space, in this case, the state space of the system, i.e. we could write, using the usual mathematical notation for an inner product,  $\langle\phi|\psi\rangle = (|\phi\rangle, |\psi\rangle)$ .

It is usually required in quantum mechanics that certain convergency criteria, defined in terms of the norms of sequences of vectors belonging to the state space, must be satisfied. This is not of any concern for spaces of finite dimension, but are important for spaces of infinite dimension. If these criteria are satisfied then the state space is said to be a Hilbert space. Thus rather than referring to the state space of a system, reference is made to the Hilbert space of the system.

Recognizing that a probability amplitude is nothing but an inner product on the state space of the system, leads to a more general way of defining what is meant by a bra vector. The following discussion emphasizes the fact that a bra vector, while it shares many characteristics of a ket vector, is actually a different mathematical entity.

### Bra Vectors

We have consistently used the notation  $\langle\phi|\psi\rangle$  to represent a probability amplitude, but we have just seen that this quantity is in fact nothing more than the inner product of two state vectors, which can be written in a different notation,  $(|\phi\rangle, |\psi\rangle)$ , that is more commonly used in pure mathematics. But the inner product can be viewed in another way, which leads to a new interpretation of the expression  $\langle\phi|\psi\rangle$ , and the introduction of a new class of state vectors.

We will arrive at this new interpretation by considering the specific example of a spin half system. Turning to the equation

$$\langle S'|S\rangle = (|S'\rangle, |S\rangle) \quad (8.52)$$

and ‘cancelling’ the  $|S\rangle$ , we get the result

$$\langle S'| \bullet = (|S'\rangle, \bullet) \quad (8.53)$$

where the ‘ $\bullet$ ’ is inserted, temporarily, to remind us that in order to complete the equation, a ket vector has to be inserted. By carrying out this procedure, we have introduced a new quantity  $\langle S'|$  which is known as a bra or bra vector, essentially because  $\langle S'|S\rangle$  looks like quantities enclosed between a pair of ‘bra(c)kets’. Written in this way, a bra vector takes on the character of a function which acts on a ket vector to produce a complex number, much as the symbol  $f(\bullet)$  acts on a number  $x$  to produce another number  $f(x)$ . In this instance, the bra vector is referred to in mathematical texts as a ‘linear functional’.

It is a vector because, as can be readily shown, the collection of all possible bras form a vector space. For instance, by the properties of the inner product, if

$$|S\rangle = C_+|+\rangle + C_-|-\rangle \quad (8.54)$$

then

$$(|S\rangle, \bullet) = \langle S| \bullet = (C_+|+\rangle + C_-|-\rangle, \bullet) \quad (8.55)$$

$$= C_+^*(|+\rangle, \bullet) + C_-^*(|-\rangle, \bullet) = C_+^*\langle +| \bullet + C_-^*\langle -| \bullet \quad (8.56)$$

i.e., dropping the ‘ $\bullet$ ’ symbols, we have

$$\langle S| = C_+^*\langle +| + C_-^*\langle -| \quad (8.57)$$

so that a linear combination of two bras is also a bra, from which follows (after a bit more work checking that the other requirements of a vector space are also satisfied) the result that the set of all bras is a vector space. Incidentally, this last calculation above shows, once again, that if  $|S\rangle = C_+|+\rangle + C_-|-\rangle$  then the corresponding bra is  $\langle S| = C_+^*\langle +| + C_-^*\langle -|$ . So, in a sense, the bra vectors are the ‘complex conjugates’ of the ket vectors.

The vector space of all bra vectors is obviously closely linked to the vector space of all the kets  $\mathcal{H}$ , and is in fact usually referred to as the dual space, and represented by  $\mathcal{H}^*$ . To each ket vector  $|\psi\rangle$  belonging to  $\mathcal{H}$ , there is then an associated bra vector  $\langle\psi|$  belonging to the dual space  $\mathcal{H}^*$ . However, the reverse is not necessarily true: there are bra vectors that do not necessarily have a corresponding ket vector, and therein lies the difference between bras and kets. It turns out that the difference only matters for Hilbert spaces of infinite dimension, in which case there can arise bra vectors whose corresponding ket vector is of infinite length, i.e. has infinite norm, and hence cannot be normalized to unity. Such

ket vectors can therefore never represent a possible physical state of a system. But these issues will not arise here, so will not be of any concern.

The point to be taken away from all this is that a bra vector is not the same kind of mathematical object as a ket vector. It is a linear functional, and as such has the attributes of an operator in the sense that it acts on a ket vector to produce a complex number, this complex number being given by the appropriate inner product. This is in contrast to the more usual sort of operators encountered in quantum mechanics, as we will see later, that act on ket vectors to produce other ket vectors. Nevertheless, in spite of the mathematical distinction that can be made between bra and ket vectors, the correspondence between the two kinds of vectors is in most circumstances so complete that a bra vector equally well represents the state of a quantum system as a ket vector. Thus, we can and do talk of a system being in the state  $\langle S|$ .

We can summarize all this in the general case as follows: The inner product  $(|\psi\rangle, |\phi\rangle)$  defines, for all states  $|\psi\rangle$ , the set of functions (or linear functionals)  $(|\psi\rangle, \ )$ . The linear functional  $(|\psi\rangle, \ )$  maps any ket vector  $|\phi\rangle$  into the complex number given by the inner product  $(|\psi\rangle, |\phi\rangle)$ .

1. The set of all linear functionals  $(|\psi\rangle, \ )$  forms a complex vector space  $\mathcal{H}^*$ , the dual space of  $\mathcal{H}$ .
2. The linear functional  $(|\psi\rangle, \ )$  is written  $\langle\psi|$  and is known as a bra vector.
3. To each ket vector  $|\psi\rangle$  there corresponds a bra vector  $\langle\psi|$  such that if  $|\phi_1\rangle \rightarrow \langle\phi_1|$  and  $|\phi_2\rangle \rightarrow \langle\phi_2|$  then

$$c_1|\phi_1\rangle + c_2|\phi_2\rangle \rightarrow c_1^*\langle\phi_1| + c_2^*\langle\phi_2|.$$

## 8.5 Constructing a State Space

Constructing a state space for a physical system can be carried out by recognizing the intermediate states through which a system can pass as it makes its way from some initial state to some observed final state. Thus, in the two slit example, the two possible intermediate states are those for which the particle is to be found at the position of either of the two slits. In the spin half example, the two intermediate states are those in which the spin is observed to have either of the two values  $S_z = \pm\frac{1}{2}\hbar$ ; these are the states we have been calling  $|\pm\rangle$ . Some more examples follow:

**Negatively Charged Ions** Here the system is a molecule which has acquired an extra electron, which, as an approximation, can be assumed to be found only on any one of the atoms making up the molecule. A simple example is the  $\text{O}_2^-$  ion in which the electron can be found on one or the other of the oxygen atoms. The two possibilities are considered to be two distinct orthonormal states which can be labelled, for instance, by the position of the two atomic nuclei with respect to the midpoint between them, say  $|-a\rangle$  and  $|a\rangle$ , where  $2a$  is the separation between the atoms. The state space for the system is therefore spanned by the orthonormal basis states  $|-a\rangle$  and  $|a\rangle$ , so that the state space is of dimension 2.

This kind of model can be generalized to situations involving different geometries, such as atoms arranged in a ring (e.g. the benzene molecule) which gives rise to results that serve as an approximate treatment of angular momentum in quantum mechanics.

A further generalization of this model is the following.

**The Tight-Binding Model of a Crystalline Metal** In the free electron model of a conducting solid, the conduction electrons are assumed to be able to move freely through the crystal, i.e. the effects of the background positive potentials of the positive ions left is ignored. A further development of this model is to take into account the fact that the electrons will experience some attraction to the periodically positioned positive ions, and so there will be a tendency for the electrons to be found in the neighbourhood of these ions. The resultant model – with the basis states consisting of a conduction electron being found on any one of the ion sites – is obviously similar to the one above for the molecular ion. Here however, the number of basis states is infinite (for an infinite crystal), so the state space is of infinite dimension. Representing the set of basis states by  $\{|n\rangle, n = 0, \pm 1, \pm 2, \dots\}$  where  $na$  is the position of the  $n^{\text{th}}$  atom, and  $a$  is the separation between neighbouring atoms, then any state of the system can then be written as

$$|\psi\rangle = \sum_{n=-\infty}^{n=+\infty} c_n |n\rangle. \quad (8.58)$$

If the basis states are orthonormal and the coefficients  $c_n$  satisfy

$$\sum_{n=-\infty}^{+\infty} |c_n|^2 < \infty \quad (8.59)$$

i.e. the probabilities  $|c_n|^2$  form a convergent infinite series, then the state  $|\psi\rangle$  can be normalized to unity. This shows that there are some linear combination of states that do not belong to the Hilbert space  $\mathcal{H}$  of the system, i.e. the Hilbert space consists only of those states for which the coefficients  $c_n$  satisfy Eq. (8.59).<sup>1</sup>

By taking into account the fact that the electrons can make their way from an ion to one of its neighbours, much of the band structure of semiconducting solids can be obtained.

**Particle in an Infinitely Deep Potential Well** We saw in Section 5.3 that a particle of mass  $m$  in an infinitely deep potential well of width  $L$  can have the energies  $E_n = n^2\pi^2\hbar^2/2mL^2$  where  $n$  is a positive integer. This suggests that the basis states of the particle in the well be the states  $|n\rangle$  such that if the particle is in state  $|n\rangle$ , then it has energy  $E_n$ . The probability amplitude of finding the particle at position  $x$  when in state  $|n\rangle$  is then  $\langle x|n\rangle$  which, from Section 5.3 we can identify with the wave function  $\psi_n$ , i.e.

$$\begin{aligned} \psi_n(x) = \langle x|n\rangle &= \sqrt{\frac{2}{L}} \sin(n\pi x/L) & 0 < x < L \\ &= 0 & x < 0, \quad x > L. \end{aligned} \quad (8.60)$$

<sup>1</sup>Note however, that we can still construct a bra vector

$$\langle\psi| = \sum_{n=-\infty}^{n=+\infty} c_n \langle n|$$

without placing any restrictions on the convergence of the  $c_n$ 's such as the one in Eq. (8.59). The corresponding ket cannot then represent a possible state of the system, but such inner products as  $\langle\psi|\phi\rangle$  where  $|\phi\rangle$  is a normalized ket can still be evaluated. The point being made here is that if  $\mathcal{H}$  is of infinite dimension, the dual space  $\mathcal{H}^*$  can also include bra vectors that do not correspond to normalized ket vectors in  $\mathcal{H}$ , which emphasizes the fact that  $\mathcal{H}^*$  is defined as a set of linear functionals, and not simply as a 'complex conjugate' version of  $\mathcal{H}$ . The distinction is important in some circumstances, but we will not have to deal with such cases.



The state space is obviously of infinite dimension. The particle can then be prepared in a state such as

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|1\rangle + |2\rangle] \quad (8.61)$$

the time dependent properties of which were discussed in Section 5.3.1.

**Spin Flipping** In this case, we have a spin half particle (for instance) in a constant magnetic field, so the two possible states are the familiar spin up or spin down states. If, in addition, we add a *rotating* magnetic field at right angles to the constant field, there arises a time dependent probability of the spin flipping from one orientation to the other. As the spin up and spin down states are of different energies, this represents a change in energy of the particle, a change that can be detected, and is the basis of the electron spin and nuclear magnetic resonance imaging much used in medical work. Obviously this is a state space of dimension two.

**The Qubit** Any two state system can be used to represent the quantum version of a binary numbers: spin up and spin down, an atom excited or not, and so on. Overall the two states can be represented by  $|0\rangle$  and  $|1\rangle$ , corresponding to the two binary numbers 0 and 1. A linear combination

$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle.$$

can be formed which represents the possibility of a memory registering a bit of information, not as either a 0 or a 1, which is all that can happen classically, but simultaneously, registering both possibilities of 0 or 1. Such a state is known as a *qubit*. Obviously, the state space is of dimension two, and much that we have said above about spin half systems applies. Quantum computation then involves manipulating the whole state  $|\psi\rangle$ , which, in effect, amounts to performing two calculations at once, differing by the initial setting of the memory bit.

The idea introduced above can be readily extended. Thus, if we have two two level atoms, we have such possibilities as  $|00\rangle$ ,  $|01\rangle$ ,  $|10\rangle$ , and  $|11\rangle$  where, for instance,  $|10\rangle$  is the state in which the first atom is in its excited state and the second is in its ground state. Obviously, the state  $|00\rangle$  represents the number zero,  $|01\rangle$  the number one,  $|10\rangle$  the number two, and  $|11\rangle$  the number three. We now have two qubits, and a state space of dimension four, and we can set up linear combinations such as

$$|\psi\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle \quad (8.62)$$

and we can then perform calculations making use, simultaneously, of four different possible values for whatever quantity the states are intended to represent. With three atoms, or four and so on, the state space becomes much larger: of dimension  $2^N$  in fact where  $N$  is the number of qubits, and the basis states represent the numbers ranging from 0 to  $2^N - 1$  in binary notation.