Chapter 9

General Mathematical Description of a Quantum System

It was shown in preceding Chapter 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 in the general case introduced there. 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.

9.1 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 symbol knonw as a *ket* written $|\ldots\rangle$ where $\ldots$ is a label specifying the physical information known about the state. An arbitrary state is written $|\psi\rangle$, or $|\phi\rangle$ and so on.

2. The set of all state vectors describing a given physical system forms a complex inner product space $\mathcal{H}$ (actually a Hilbert space, see Sec. 9.2) also known as the state space or ket space for the system. A ket is also referred to as a state vector, ket vector, or sometimes just state.

   Thus every linear combination (or superposition) of two or more state vectors $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle, \ldots$, is also a state of the quantum system i.e. the state $|\psi\rangle$ given by

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

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

This last point amounts 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 physical state of the system is represented by a vector $|\psi\rangle$, then the same physical state is represented by the vector $c|\psi\rangle$ where c is any non-zero complex number.

Next, we need the concept of *completeness*:

4. A set of vectors $|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, \ldots$ is said to be complete if every state of the quantum system can be represented as a linear combination of the $|\varphi_i\rangle$'s, i.e. for any state $|\psi\rangle$ we can write

$$|\psi\rangle = \sum_i c_1|\varphi_i\rangle.$$

The set of vectors $|\varphi_i\rangle$ are said to *span* the space.

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.

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

5. A set of vectors $\{|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, \ldots\}$ is said to form a basis for the state space if the set of vectors is complete, and if they are linearly independent. The vectors are also termed the *base* states for the vector space.

   Linear independence means that if $\sum_i c_i|\varphi_i\rangle = 0$ then $c_i = 0$ for all i.

The states $|\pm\rangle$ for a spin half system can be shown to be linearly independent, and thus form a basis for the state space of the system.

6. 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. The arguments presented in the preceding Chapter by which we arrive at a set of basis states serves as a physically motivated starting point to construct the state space for the system. But once we have defined the state space in this way, there is no reason why we cannot, at least mathematically, construct other sets of basis states. These basis states that we start with are particularly useful as they have an immediate physical meaning; this might not be the case for an arbitrary basis set. But there are other means by which other physically meaningful basis states can be determined: often the choice of basis states is suggested by the physics (such as the set of eigenstates of an observable, see Chapter 11).

9.2 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 $\langle\psi|\psi\rangle = 1$. But recall that any multiple of a state vector still represents the same physical state of the system, i.e. $|\widetilde{\psi}\rangle = a|\psi\rangle$ still represents the same physical state as $|\psi\rangle$. However, in this case, $\langle\widetilde{\psi}|\widetilde{\psi}\rangle = |a|^2$ which is not necessarily unity, but is 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 $|\psi\rangle$ is normalized, or normalized to unity, if $\langle\psi|\psi\rangle = 1$.

Normalized states are states which have a direct probability interpretation. 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 the normalized 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 δ_{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, $\langle\phi|\psi\rangle = (|\phi\rangle, |\psi\rangle)$. The state space of a physical system is thus more than just a complex vector space, it is a vector space on which there is defined an inner product, and so is more correctly termed a complex 'inner product' space. Further, 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.

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 important to recognize that all the vectors belonging to a Hilbert space have finite norm, or, putting it another way, all the state vectors can be normalized to unity – this state of affairs is physically necessary if we want to be able to apply the probability interpretation in a consistent way. However, as we shall see, we will encounter states which do not have a finite norm and hence neither represent physically realizable states, nor do they belong to the state or Hilbert space of the system. Nevertheless, with proper care regarding their use and interpretation, such states turn out to be essential, and play a crucial role throughout quantum mechanics.

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 characteristices of a ket vector, is actually a different mathematical entity.

9.2.1 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 encountered 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. If we consider the equation

$$\langle\phi|\psi\rangle = (|\phi\rangle, |\psi\rangle) \tag{9.1}$$

and 'cancel' the $|\psi\rangle$, we get the result

$$\langle\phi|\bullet = (|\phi\rangle,\ \bullet) \tag{9.2}$$

where the '•' 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 $\langle\phi|$ which is known as a bra or bra vector, essentially because $\langle\phi|\psi\rangle$ looks like quantities enclosed between a pair of 'bra(c)kets'. 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

$$|\psi\rangle = a_1|\varphi_1\rangle + a_2|\varphi_2\rangle \tag{9.3}$$

then

$$(|\psi\rangle,\ \bullet) = \langle\psi|\bullet = (a_1|\varphi_1\rangle + a_2|\varphi_2\rangle,\ \bullet) \tag{9.4}$$

$$= a_1^*(|\varphi_1\rangle,\ \bullet) + a_2^*(|\varphi_2\rangle,\ \bullet) = a_1^*\langle\varphi_1|\bullet + a_2^*\langle\varphi_2|\bullet \tag{9.5}$$

i.e., dropping the '•' symbols, we have

$$\langle\psi| = a_1^*\langle\varphi_1| + a_2^*\langle\varphi_2| \tag{9.6}$$

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 $|\psi\rangle = a_1|\varphi_1\rangle + a_2|\varphi_2\rangle$ then the corresponding bra is $\langle\psi| = a_1^*\langle\varphi_1| + a_2^*\langle\varphi_2|$. 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 be of any concern here. 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. In fact, it has all 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 that act on ket vectors to produce other ket vectors. In mathematical texts a bra vector is usually referred to as a 'linear functional'. 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 talk of a system being in the state $\langle\psi|$.

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 $|\phi_1\rangle \to \langle\phi_1|$ and $|\phi_2\rangle \to \langle\phi_2|$ then
$$c_1|\phi_1\rangle + c_2|\phi_2\rangle \to c_1^*\langle\phi_1| + c_2^*\langle\phi_2|.$$