Chapter 10

State Spaces of Infinite Dimension

So far we have limited the discussion to state spaces of finite dimensions, but it turns out that, in practice, state spaces of infinite dimension are fundamental to a quantum description of almost all physical systems. The simple fact that a particle moving in space requires for its quantum mechanical description a state space of infinite dimension shows the importance of being able to work with such state spaces. This would not be of any concern if doing so merely required transferring over the concepts already introduced in the finite case, but infinite dimensional state spaces have mathematical peculiarities and associated physical interpretations that are not found in the case of finite dimension state spaces. Some of these issues are addressed in this Chapter, while other features of infinite dimensional state spaces are discussed as the need arises in later Chapters.

10.1 Examples of state spaces of infinite dimension

All the examples given in Chapter 8 yield state spaces of finite dimension. Much the same argument can be applied to construct state spaces of infinite dimension. A couple of examples follow.

The Tight-Binding Model of a Crystalline Metal The examples given above of an electron being positioned on one of a (finite) number of atoms can be readily generalized to a situation in which there are an infinite number of such atoms. This is not a contrived model in any sense, as it is a good first approximation to modelling the properties of the conduction electrons in a crystalline solid. In the free electron model of a conducting solid, the conduction electrons are assumed to be able to move freely (and without mutual interaction) 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 $\{|n\rangle, n = 0, \pm1, \pm2, \dots\}$ where na is the position of the n^{th} atom, and a is the separation between neighbouring atoms, then any state of the system can then be written as

$$|\psi\rangle = \sum_{n=-\infty}^{+\infty} c_n|n\rangle. \tag{10.1}$$

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.

Free Particle We can generalize the preceding model by supposing that the spacing between the neighbouring atoms is allowed to go to zero, so that the positions at which the electron can be found become continuous. This then acts as a model for the description of a particle free to move anywhere in one dimension, and is considered in greater detail later in Section 10.2.2. In setting up this model, we find that as well as there being an infinite number of basis states — something we have already encountered — we see that these basis states are not discrete, i.e. a particle at position x will be in the basis state $|x\rangle$, and as x can vary continuously over the range $-\infty < x < \infty$, there will be a non-denumerably infinite, that is, a continuous range of such basis states. As a consequence, the completeness relation ought to be written as an integral:

$$|\psi\rangle = \int_{-\infty}^{+\infty} |x\rangle\langle x|\psi\rangle\, dx. \tag{10.2}$$

The states $|x\rangle$ and $|x'\rangle$ will be orthonormal if $x \neq x'$, but in order to be able to retain the completeness relation in the form of an integral, it turns out that these basis states have to have an infinite norm. However, there is a sense in which we can continue to work with such states, as will be discussed in Section 10.2.2.

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 ψ_n, i.e.

$$\begin{aligned}\psi_n(x) = \langle x|n\rangle &= \sqrt{\frac{2}{L}}\sin(n\pi x/L) \qquad 0 < x < L\\ &= 0 \qquad\qquad\qquad\qquad x < 0, \quad x > L.\end{aligned} \tag{10.3}$$

The state space is obviously of infinite dimension.

It has been pointed out before that a state space can have any number of sets of basis states, i.e. the states $|n\rangle$ introduced here do not form the sole possible set of basis states for the state space of this system. In this particular case, it is worthwhile noting that we could have used as the base states the states labelled by the position of the particle in the well, i.e. the states $|x\rangle$.

As we have seen, there are an infinite number of such states which is to be expected as we have already seen that the state space is of infinite dimension. But the difference between this set of states and the set of states $|n\rangle$ is that in the latter case, these states are discrete, i.e. they can be labelled by the integers, while the states $|x\rangle$ are continuous, they are labelled by the continuous variable x. Thus, something new emerges from this example: for state spaces of infinite dimension, it is possible to have a denumerably infinite number of basis states (i.e. the discrete states $|n\rangle$) or non-denumerably infinite number of basis states (i.e. the states $|x\rangle$.) This feature of state spaces of infinite dimension, plus others, are discussed separately below in Section 10.2.

A System of Identical Photons Many other features of a quantum system not related to the position or energy of the system can be used as a means by which a set of basis states can be set up. An important example is one in which the system consists of a possibly variable number of identical particles. One example is a 'gas' of photons, all of the same frequency and polarization. Such a situation is routinely achieved in the laboratory using suitably constructed hollow superconducting metallic cavities designed to support just one mode (i.e. a single frequency and polarization) of the electromagnetic field. The state of the electromagnetic field can then be characterized by the number n of photons in the field which can range from zero to positive infinity, so that the states of the field (known as number states) can be written $|n\rangle$ with $n = 0, 1, 2, \ldots$. The state $|0\rangle$ is often referred to as the vacuum state. These states will then constitute a complete, orthonormal set of basis states (called Fock or number states), i.e.

$$\langle n|m\rangle = \delta_{nm} \tag{10.4}$$

and as n can range up to infinity, the state space for the system will be infinite dimensional. An arbitrary state of the cavity field can be then be written

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n|n\rangle \tag{10.5}$$

so that $|c_n|^2$ will be the probability of finding n photons in the field. In terms of these basis states, it is possible to describe the processes in which particles are created or destroyed. For instance if there is a single atom in an excited energy state in the cavity, and the cavity is in the vacuum state $|0\rangle$, then the state of the combined atom field system can be written $|e, 0\rangle$, where the e indicates that the atom is in an excited state. The atom can later lose this energy by emitting it as a photon, so that at some later time the state of the system will be $a|e, 0\rangle + b|g, 1\rangle$, where now there is the possibility, with probability $|b|^2$, of the atom being found in its ground state, and a photon having been created.

10.2 Some Mathematical Issues

Some examples of physical systems with state spaces of infinite dimension were provided in the previous Section. In these examples, we were able to proceed, at least as far as constructing the state space was concerned, largely as was done in the case of finite dimensional state spaces. However, further investigation shows that there are features of the mathematics, and the corresponding physical interpretation in the infinite dimensional case that do not arise for systems with finite dimensional state spaces. Firstly, it is possible to construct state vectors that cannot represent a state of the system and secondly, the possibility arises of the basis states being continuously infinite. This latter state of affairs is not at all a rare and special case — it is just the situation needed to describe the motion of a particle in space, and hence gives rise to the wave function, and wave mechanics.

10.2.1 States of Infinite Norm

To illustrate the first of the difficulties mentioned above, consider the example of a system of identical photons in the state $|\psi\rangle$ defined by Eq. (10.5). As the basis states are orthonormal we have for $\langle\psi|\psi\rangle$

$$\langle\psi|\psi\rangle = \sum_{n=0}^{\infty} |c_n|^2 \tag{10.6}$$

If the probabilities $|c_n|^2$ form a convergent infinite series, then the state $|\psi\rangle$ has a finite norm, i.e. it can be normalized to unity. However, if this series does not converge, then it is not possible to supply a probability interpretation to the state vector as it is not normalizable to unity. For instance, if $c_0 = 0$ and $c_n = 1/\sqrt{n}, n = 1, 2, \ldots$, then

$$\langle\psi|\psi\rangle = \sum_{n=1}^{\infty} \frac{1}{n} \tag{10.7}$$

which is a divergent series, i.e. this state cannot be normalized to unity. In contrast, if $c_n = 1/n, n = 1, 2, \ldots$, then

$$\langle\psi|\psi\rangle = \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \tag{10.8}$$

which means we can normalize this state to unity by defining

$$|\tilde{\psi}\rangle = \frac{\sqrt{6}}{\pi}|\psi\rangle. \tag{10.9}$$

This shows that there are some linear combination of states that do not represent possible physical states of the system. Such states 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. (10.6) [1]. This is a new feature: the possibility of constructing vectors that do not represent possible physical states of the system. It turns out that some very useful basis states have this apparently undesirable property, as we will now consider.

10.2.2 Continuous Basis States

In Section 10.1 an infinite one-dimensional model of a crystal was used as an illustrative model for a state space of infinite dimension. We can now consider what happens if we suppose that the separation between the neighbouring atoms in the crystal goes to zero, so that the electron can be found anywhere over a range extending from $-\infty$ to ∞. This, in effect, is the continuous limit of the infinite crystal model just presented, and represents the possible positions that a particle free to move anywhere in one dimension, the X axis say, can have.

In this case, we could label the possible states of the particle by its X position, i.e. $|x\rangle$, where now, instead of having the discrete values of the crystal model, the position can now assume any of a continuous range of values, $-\infty < x < \infty$. It would seem that we could then proceed in the same way as we have done with the discrete states above, but it turns out that such states cannot be normalized to unity and hence do not represent (except in an idealised sense) physically allowable states of the system.

The aim here is to try to develop a description of the possible basis states for a particle that is not limited to being found only at discrete positions on the X axis. After all, in principle, we would expect that a particle in free space could be found at any position x in the range $-\infty < x < \infty$. We will get at this description by a limiting procedure which is not at all mathematically rigorous, but nevertheless yields results that turn out to be valid. Suppose we return to the completeness relation for the states $|na\rangle$ for the one dimensional crystal

$$|\psi\rangle = \sum_{n=-\infty}^{+\infty} |na\rangle\langle na|\psi\rangle. \tag{10.10}$$

If we now put $a = \Delta x$ and $na = x_n$, and write $|na\rangle = \sqrt{a}|x_n\rangle$, this becomes

$$|\psi\rangle = \sum_{n=-\infty}^{+\infty} |x_n\rangle\langle x_n|\psi\rangle\Delta x \tag{10.11}$$

where now

$$\langle x_n|x_m\rangle = \frac{\delta_{nm}}{a} \tag{10.12}$$

[1] Note however, that we can still construct a bra vector

$$\langle\psi| = \sum_{n=0}^{n=\infty} c_n^*\langle n|$$

without placing any restrictions on the convergence of the c_n's such as the one in Eq. (10.6). 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.

i.e. each of the states $|x_n\rangle$ is not normalized to unity, but we can nevertheless identify such a state as being that state for which the particle is at position x_n – recall if a state vector is multiplied by a constant, it still represents the same physical state of the system.

If we put to one side any concerns about the mathematical legitimacy of what follows, we can now take the limit $\Delta x \to 0$, i.e. $a \to 0$, then Eq. (10.11) can be written as an integral, i.e.

$$|\psi\rangle = \int_{-\infty}^{+\infty} |x\rangle\langle x|\psi\rangle\, dx \tag{10.13}$$

We can identify the state $|x\rangle$ with the physical state of affairs in which the particle is at the position x, and the expression Eq. (10.13) is consistent with the completeness requirement i.e. that the states $\{|x\rangle, -\infty < x < \infty\}$ form a complete set of basis states, so that any state of the one particle system can be written as a superposition of the states $|x\rangle$, though the fact that the label x is continuous has forced us to write the completeness relation as an integral. The difficulty with this procedure is that the states $|x\rangle$ are no longer normalized to unity. This we can see from Eq. (10.12) which tells us that $\langle x|x'\rangle$ will vanish if $x \neq x'$, but for $x = x'$ we see that

$$\langle x|x\rangle = \lim_{a\to 0} \frac{1}{a} = \infty \tag{10.14}$$

i.e. the state $|x\rangle$ has infinite norm! This means that there is a price to pay for trying to set up the mathematics in such a manner as to produce the completeness expression Eq. (10.13), which is that we are forced to introduce basis states which have infinite norm, and hence cannot represent a possible physical state of the particle! Nevertheless, provided care is taken, it is still possible to work with these states as if they represent the state in which the particle is at a definite position. To see this, we need to look at the orthonormality properties of these states, and in doing so we are lead to introduce a new kind of function, the Dirac delta function.

10.2.3 The Dirac Delta Function

We have just seen that the inner product $\langle x|x'\rangle$ vanishes if $x \neq x'$, but appears to be infinite if $x = x'$. In order to give some mathematical sense to this result, we return to Eq. (10.13) and look more closely at the properties that $\langle x|x'\rangle$ must have in order for the completeness relation also to make sense.

The probability amplitude $\langle x|\psi\rangle$ appearing in Eq. (10.13) are functions of the continuous variable x, and is often written $\langle x|\psi\rangle = \psi(x)$, which we identify as the wave function of the particle. If we now consider the inner product

$$\langle x'|\psi\rangle = \int_{-\infty}^{+\infty} \langle x'|x\rangle\langle x|\psi\rangle dx \tag{10.15}$$

or

$$\psi(x') = \int_{-\infty}^{+\infty} \langle x'|x\rangle\psi(x) dx \tag{10.16}$$

we now see that we have an interesting difficulty. We know that $\langle x'|x\rangle = 0$ if $x' \neq x$, so if $\langle x|x\rangle$ is assigned a finite value, the integral on the right hand side will vanish, so that $\psi(x) = 0$ for all x!! But if $\psi(x)$ is to be a non-trivial quantity, i.e. if it is not to be zero for all x, then it cannot be the case that $\langle x|x\rangle$ is finite. In other words, $\langle x'|x\rangle$ must be infinite for $x = x'$ in some sense in order to guarantee a non-zero integral. The way in which this can be done involves introducing a new 'function', the Dirac delta function, which has some rather unusual properties.

What we are after is a ‘function’ $\delta(x - x_0)$ with the property that

$$f(x_0) = \int_{-\infty}^{+\infty} \delta(x - x_0) f(x) dx \tag{10.17}$$

for all (reasonable) functions $f(x)$.

So what is $\delta(x - x_0)$? Perhaps the simplest way to get at what this function looks like is to examine beforehand a sequence of functions defined by

$$\begin{aligned} D(x, \epsilon) &= \epsilon^{-1} \qquad -\epsilon/2 < x < \epsilon/2 \\ &= 0 \qquad x < -\epsilon/2, x > \epsilon/2. \end{aligned} \tag{10.18}$$

What we first notice about this function is that it defines a rectangle whose area is always unity for any (non-zero) value of ϵ, i.e.

$$\int_{-\infty}^{+\infty} D(x, \epsilon) dx = 1. \tag{10.19}$$

Secondly, we note that as ϵ is made smaller, the rectangle becomes taller and narrower. Thus, if we look at an integral

$$\int_{-\infty}^{+\infty} D(x, \epsilon) f(x) dx = \epsilon^{-1} \int_{-\epsilon/2}^{\epsilon/2} f(x) dx \tag{10.20}$$

where $f(x)$ is a reasonably well behaved function (i.e. it is continuous in the neighbourhood of $x = 0$), we see that as $\epsilon \to 0$, this tends to the limit $f(0)$. We can summarize this by the equation

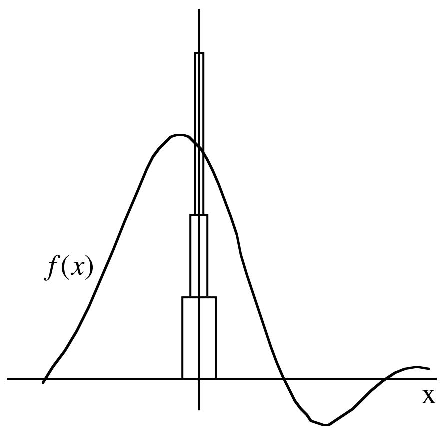

Figure 10.1: A sequence of rectangles of decreasing width but increasing height, maintaining a constant area of unity approaches an infinitely high ‘spike’ at $x = 0$..

$$\lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} D(x, \epsilon) f(x) dx = f(0). \tag{10.21}$$

Taking the limit inside the integral sign (an illegal mathematical operation, by the way), we can write this as

$$\int_{-\infty}^{+\infty} \lim_{\epsilon \to 0} D(x, \epsilon) f(x) dx = \int_{-\infty}^{+\infty} \delta(x) f(x) dx = f(0) \tag{10.22}$$

where we have introduced the ‘Dirac delta function’ $\delta(x)$ defined as the limit

$$\delta(x) = \lim_{\epsilon \to 0} D(x, \epsilon), \tag{10.23}$$

a function with the unusual property that it is zero everywhere except for $x = 0$, where it is infinite.

The above defined function $D(x, \epsilon)$ is but one ‘representation’ of the Dirac delta function. There are in effect an infinite number of different functions that in an appropriate limit behave as the rectangular function here. Some examples are

$$\begin{aligned} \delta(x - x_0) &= \lim_{L \to \infty} \frac{1}{\pi} \frac{\sin L(x - x_0)}{x - x_0} \\ &= \lim_{\epsilon \to 0} \frac{1}{\pi} \frac{\epsilon}{(x - x_0)^2 + \epsilon^2} \\ &= \lim_{\lambda \to \infty} \tfrac{1}{2} \lambda e^{-\lambda |x - x_0|}. \end{aligned} \tag{10.24}$$

In all cases, the function on the right hand side becomes narrower and taller as the limit is taken, while the area under the various curves remains the same, that is, unity.

The first representation above is of particular importance. It arises by via the following integral:

$$\frac{1}{2\pi}\int_{-L}^{+L} e^{ik(x-x_0)}dk = \frac{e^{iL(x-x_0)} - e^{iL(x-x_0)}}{2\pi i(x-x_0)} = \frac{1}{\pi}\frac{\sin L(x-x_0)}{x-x_0} \tag{10.25}$$

In the limit of $L \to \infty$, this then becomes

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ik(x-x_0)}dk = \delta(x-x_0). \tag{10.26}$$

The delta function is not to be thought of as a function as it is usually defined in pure mathematics, but rather it is to be understood that a limit of the kind outlined above is implied whenever the delta function appears in an integral[2]. However, such mathematical niceties do not normally need to be a source of concern in most instances. It is usually sufficient to be aware of the basic property Eq. (10.17) and a few other rules that can be proven using the limiting process, such as

$$\begin{aligned}
\delta(x) &= \delta(-x) \\
\delta(ax) &= \frac{1}{|a|}\delta(x) \\
x\delta(x) &= 0 \\
\int_{-\infty}^{+\infty} \delta(x-x_0)\delta(x-x_1) &= \delta(x_0-x_1) \\
\int_{-\infty}^{+\infty} f(x)\delta'(x-x_0)dx &= -f'(x_0).
\end{aligned}$$

The limiting process should be employed if there is some doubt about any result obtained. For instance, it can be shown that the square of a delta function cannot be given a satisfactory meaning.

Delta Function Normalization

Returning to the result

$$\psi(x') = \int_{-\infty}^{+\infty} \langle x'|x\rangle\psi(x)dx \tag{10.27}$$

we see that the inner product $\langle x'|x\rangle$, must be interpreted as a delta function:

$$\langle x'|x\rangle = \delta(x-x'). \tag{10.28}$$

The states $|x\rangle$ are said to be delta function normalized, in contrast to the orthonormal property of discrete basis states. One result of this, as has been pointed out earlier, is that states such as $|x\rangle$ are of infinite norm and so cannot be normalized to unity. Such states cannot represent possible physical states of a system, though it is often convenient, with caution, to speak of such states as if they were physically realizable. Mathematical (and physical) paradoxes can arise if care is not taken. However, linear combinations of these states can be normalized to unity, as this following example illustrates. If we consider a state $|\psi\rangle$ given by

$$|\psi\rangle = \int_{-\infty}^{+\infty} |x\rangle\langle x|\psi\rangle dx, \tag{10.29}$$

[2]This raises the question as to whether or not it would matter what representation of the delta function is used. Provided the function $f(x)$ is bounded over $(-\infty, +\infty)$ there should be no problem, but if the function $f(x)$ is unbounded over this interval, e.g. $f(x) = \exp(x^2)$, then only the rectangular representation of the delta function will give a sensible answer.

then

$$\langle\psi|\psi\rangle = \int_{-\infty}^{+\infty} \langle\psi|x\rangle\langle x|\psi\rangle dx. \tag{10.30}$$

But $\langle x|\psi\rangle = \psi(x)$ and $\langle\psi|x\rangle = \psi(x)^*$, so that

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 dx. \tag{10.31}$$

Provided $|\psi(x)|^2$ is a well behaved function, in particular that it vanish as $x \to \pm\infty$, this integral will converge to a finite result, so that the state $|\psi\rangle$ can indeed be normalized to unity, and if so, then we can interpret $|\psi(x)|^2 dx$ as the probability of finding the particle in the region $(x, x + dx)$, which is just the standard Born interpretation of the wave function.

10.2.4 Separable State Spaces

We have seen that state spaces of infinite dimension can be set up with either a denumerably infinite number of basis states, i.e. the basis states are discrete but infinite in number, or else a non-denumerably infinite number of basis states, i.e. the basis states are labelled by a continuous parameter. Since a state space can be spanned by more than one set of basis states, it is worthwhile investigating whether or not a space of infinite dimension can be spanned by a set of denumerable basis states, as well as a set of non-denumerable basis states. An example of where this is the case was given earlier, that of a particle in an infinitely deep potential well, see p 113. It transpires that not all vector spaces of infinite dimension have this property, i.e. that they can have both a denumerable and a non-denumerable set of basis states. Vector spaces which can have both kinds of basis states are said to be separable, and in quantum mechanics it is assumed that state spaces are separable.