

*Lecture 7**Relevant sections in text: §1.6***Observables with continuous and/or unbounded values**

We are now ready to turn to the quantum mechanical description of a (non-relativistic) particle. We shall define a (spinless) particle as a system that is completely characterized by the position and linear momentum, which are the basic observables in this model. This means that all observables are functions of position and momentum. While it is possible that the position and momentum variables take a discrete set of values (as angular momentum and – often – energy do), there is currently no experimental evidence of this. We therefore create a model in which these observables can take a continuous, unbounded set of values. Evidently, we need to define a Hilbert space that admits self-adjoint operators with a continuous, unbounded spectrum. Neither of these features are possible on finite-dimensional vector spaces, and so here we are forced into the infinite-dimensional setting (*i.e.*, spaces of functions). This leads to some mathematical subtleties that we need to be wary of. I shall not try to be perfectly rigorous in our discussion since that would take us too far afield. But I will try to give you a reasonably fool-proof – if somewhat formal – treatment. First, let me give you a recipe for dealing with the situation. Then let me give you a flavor of the underlying mathematics which makes the formal recipe work (and also which shows where it can become tricky).

Formal recipe

We want to define an observable A with a continuous, unbounded set of values $a \in \mathbf{R}$, say. We postulate the existence of a self-adjoint linear operator, again denoted A , and a continuous set of vectors $|a\rangle$ such that

$$A|a\rangle = a|a\rangle.$$

We say that A has a “continuous” spectrum. These vectors are to be “orthonormal in the delta-function sense”:

$$\langle a|a'\rangle = \delta(a, a').$$

You can think of this as a continuum generalization of the usual orthonormality expressed via the Kronecker delta. The vectors $|a\rangle$ are to form a basis, that is, they provide a continuous resolution of the identity:

$$I = \int_{-\infty}^{\infty} da |a\rangle\langle a|,$$

so that we can write

$$|\psi\rangle = \int_{-\infty}^{\infty} da |a\rangle \langle a|\psi\rangle.$$

Using quotation marks to indicate where the underlying mathematics is considerably more subtle than the words indicate, we can say the following. We interpret the “eigenvalues” a as the possible values of an outcome of the measurement of A , the vectors $|a\rangle$ are “states” in which A has the value a with certainty. The scalar $|\langle a|\psi\rangle|^2 da$ is the probability for finding A to have the value in the range $[a, a + da]$ in the state $|\psi\rangle$. In particular, the probability that the observable A is found to have a value in a region $[a_1, a_2]$ is given by

$$P(A \in [a_1, a_2]) = \int_{a_1}^{a_2} da |\langle a|\psi\rangle|^2.$$

Thus in this setting we call $|\langle a|\psi\rangle|^2$ the *probability density* for A in the state ψ . You can see that, given the operator A with continuous spectrum, the abstract state vector is completely characterized by the complex-valued function

$$\psi(a) = \langle a|\psi\rangle, \quad \int_{-\infty}^{\infty} da |\psi(a)|^2 = \langle \psi|\psi\rangle = 1.$$

$\psi(a)$ represents the “components” of the vector $|\psi\rangle$ along the “basis” provided by $|a\rangle$. It’s the continuous analog of the column vector representation! This function $\psi(a) = \langle a|\psi\rangle$ is called the *wave function* associated to the observable A . The Hilbert space can thus be identified with the set of all square-integrable functions $\psi(a)$. Of course, you have seen this before in the position and momentum representations for a particle.

Subtleties. A glimpse of the real story.

For the most part, using the above formalism you can treat operators with continuous spectra much the same as we did linear operators on finite-dimensional Hilbert spaces. It is worth warning you, however, that there are mathematical subtleties that can come into play.

To begin with, note that the “eigenvectors” $|a\rangle$ cannot really be elements of the Hilbert space since they do not have a norm — $\delta(a, a)$ is not defined! To see this concretely in a familiar example, consider the familiar momentum operator (to be justified soon), acting upon the Hilbert space of square-integrable functions of 1-variable:

$$p\psi(x) = \frac{\hbar}{i} \frac{d}{dx} \psi(x).$$

Its “eigenfunctions” are of the form

$$\phi(x) = N e^{i\kappa x},$$

with eigenvalues $\frac{\hbar\kappa}{i}$. No matter how you choose κ ,

$$\int_{-\infty}^{\infty} dx |\phi(x)|^2 \rightarrow \infty.$$

This means that $\phi(x)$ does not actually correspond to an element of the Hilbert space. This difficulty can be traced back to the fact that p has continuous spectrum.* Our formal prescription (delta-function normalization) *etc.* works if we pick $\kappa = ik$, where k is a real number.

If the spectrum of an observable is unbounded, then another difficulty arises: not all elements of the Hilbert space are in the *domain* of the operator. This difficulty – which can only occur if the Hilbert space is infinite-dimensional – arises whenever the spectrum is unbounded, irrespective of whether the spectrum is discrete or continuous. To illustrate this, return to the momentum operator. It is clear that, say, a square wave pulse defines a normalizable wave function, that is, an element of the Hilbert space of a particle.** However, the derivative of a square wave is not defined at “the corners”, so one doesn’t get a function after applying the operator – let alone a square-integrable function. We say that the square wave function is not in the domain of the momentum operator. Likewise, it is easy to construct wave functions that are not in the domain of the position operator. For example, you can easily check that

$$\psi(x) = \frac{x}{x^2 + 1}$$

is a square integrable (normalizable) function of x . However, the position operator X acts on such functions via

$$X\psi(x) = x\psi(x),$$

so that, in our example,

$$X\psi(x) = \frac{x^2}{x^2 + 1},$$

which is not square-integrable, *i.e.*, not an element of the Hilbert space for a particle.

In a more rigorous treatment of observables with continuous and/or unbounded spectrum, one handles these issues as follows. One accepts the limited domain of unbounded operators. One adds to the definition of self-adjoint operators the requirement that the operator and its adjoint have the same domain. The domain of an observable with unbounded

* Since we don’t have any eigenvectors, how do we define “spectrum”? Roughly, the spectrum of an operator A is the set of scalars λ such that the linear operator $A - \lambda I$ has no inverse.

** Physically, such a wave function describes a particle that is known with certainty to be somewhere in the region in which the square wave function is non-vanishing. For example, this would be the state of a particle after it has passed into a particle detector of finite size.

spectrum forms a “dense” subset of the Hilbert space. This means that every vector can be arbitrarily well approximated (relative to the Hilbert space norm) by elements in the domain. If the spectrum is discrete (if unbounded), an orthonormal basis of eigenvectors for the Hilbert space can be found inside this dense domain. If the spectrum is continuous, the eigenvectors are not in the Hilbert space, but are “generalized eigenvectors”. They live in the vector space of *distributions*, which are linear functions on a dense subspace of the Hilbert space. Thus the generalized eigenvectors have a well-defined “scalar product” with elements from a dense subset of the Hilbert space, but not with the whole Hilbert space or among themselves. It can be shown that a self-adjoint operator with continuous spectrum admits a delta-function normalized set of generalized eigenvectors which can be used to define a generalized basis much as indicated in our formal treatment above.

If all this mathematical detail leaves you a little dazed, don’t feel bad. I only gave you vague hints as to how the story goes. I did not attempt to give a complete, coherent description. Still, now you at least know where some of the subtleties lie. In what follows all of our formal manipulations will have a justification within the more complete mathematical formulation that I hinted at above.

Position Operator

We have already mentioned that a particle is defined as a system in which the only relevant observables are position and momentum. How do we implement this idea in quantum mechanics? We need to define self-adjoint operators representing position and momentum. As mentioned earlier, we do this so that the spectrum is continuous and unbounded, ranging over all real numbers. We begin with the position operator, which can be constructed formally as we did the generic operator A above. We will denote by X the position operator and the spectral values will be denoted x , so that we have the generalized eigenvectors $|x\rangle$.

$$X|x\rangle = x|x\rangle.$$

We have (on a suitable dense domain) $X = X^\dagger$. The position wave function is defined by

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

A vector is completely specified by its position wave function and vice versa. The position wave function is a continuous version of a column vector! A linear operator maps vectors to vectors and so defines – and is defined by – a linear mapping from wave functions to wave functions. This mapping can be computed via

$$\psi(x) \rightarrow A\psi(x) \equiv \langle x|A|\psi\rangle.$$

In particular, the position operator maps functions to functions via

$$\psi(x) \rightarrow X\psi(x) = \langle x|X|\psi\rangle = x\langle x|\psi\rangle = x\psi(x).$$

Here we have used

$$X|x\rangle = x|x\rangle \implies \langle x|X = x\langle x|.$$

The wave function $\psi(x)$ is the *probability amplitude* for position. This means that $|\psi(x)|^2$ is the probability density for position. This means that

$$Prob(X \in [a, b]) = \int_a^b dx |\psi(x)|^2.$$

Note the unit vector condition implies normalization of the wave functions:

$$1 = \langle \psi|\psi\rangle = \int_{-\infty}^{\infty} dx \langle \psi|x\rangle \langle x|\psi\rangle = \int_{-\infty}^{\infty} dx |\psi(x)|^2.$$

Finally we note that the generalized eigenvector $|x'\rangle$ represents a “state” in which the particle has definite position. Formally, the wave function for this state is then

$$\psi(x) = \langle x|x'\rangle = \delta(x, x').$$

Of course this wave function is not normalizable – except in the delta function sense. (Try it!)

Remarks: Note that all the foregoing results are in fact valid for any observable with continuous spectrum. We simply select one and use it to represent position and adapt our notation accordingly. Also note that, as is the tradition when presenting material at this level, we have been completely cavalier with domains. The idea is that the formal manipulations given above will make sense provided the domains are sufficiently restricted. These restrictions are usually not explicitly made since we are only trying to understand the formal structure of things. When performing concrete computations one must usually pay more attention to such things. But it’s amazing how far one can get without doing so!