Lecture 8

Relevant sections in text: §1.6, 1.7

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. Nonetheless, I shall not try to be rigorous in our discussion since that would take us too far afield. Instead I will try to give you a reasonably fool-proof – if somewhat formal – recipe for handling this class of observables. Later I will give you a hint or two 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 for any $a \in \mathbf{R}$

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

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

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

You can see that, given the operator A with continuous spectrum, the abstract state vector is completely characterized by the complex-valued function

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

$\psi(a)$ 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* (also the "probability amplitude") 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.

We also have

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

So the components of $A|\psi\rangle$ in the basis $|a\rangle$ are

$$\langle a|A|\psi\rangle = a\langle a|\psi\rangle,$$

we can view this as the action of A on the space of wave functions:

$$A\psi(a) \equiv \langle a|A|\psi\rangle = a\langle a|\psi\rangle = a\psi(a).$$

Again you have seen this before, *e.g.,* when letting A be the position operator for a particle. This is the continuous analog of using a matrix to transform the column vector representing components of a vector in the basis of eigenvectors of the matrix. Other operators are represented as

$$B\psi(a) \equiv \langle a|B|\psi\rangle,$$

but in general one cannot say any more without additional information about the relation of B to A.

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 "eigenvectors" $|a\rangle$ represent 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 $|\psi\rangle$. Alternatively, 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.

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

$$\phi(x) = Ne^{\kappa x},$$

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

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

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.

Even if the spectrum of an observable is not continuous, in an infinite dimensional Hilbert space it may be unbounded. For example, the energy spectrum of a harmonic oscillator is unbounded. 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. Here the domain refers to the set of vectors upon which the operator can actually be defined to act. 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",

* Since we don't have any eigenvectors, how do we *really* define the "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.

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 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.

Here is one last, important subtlety. Typically in applications we build operators and then try to deduce their spectrum. For some operators the spectrum turns out to be continuous (*e.g.,* position operator), sometimes it turns out to be discrete (*e.g.,* Hamiltonian for an oscillator), and sometimes it turns out to be *both*. Think of the Hamiltonian for an electron in an atom. The energy spectrum for the bound states is discrete. But it is possible to have an unbound electron moving in the Coulomb-type field of the nucleus (and remaining electrons, if any). This can happen in a scattering situation, or if the atom is ionized. The unbound electron has a continuously variable energy, so the energy spectrum corresponding to unbound states will be continuous. So, for example, if you solve for the spectrum of the usual hydrogen atom Hamiltonian it will consist of a discrete set ("bound

states") and a continuous set ("unbound" or "scattering" states). In general, then we have to be ready for operators A for which the eigenvalue/eigenvector relation is of the form

$$A|i\rangle = a_i|i\rangle, \quad A|a\rangle = a|a\rangle,$$

where a_i, $i = 1, 2, 3, \ldots$ is some discrete (usually infinite) set of eigenvalues, and $a \in U \subset \mathbf{R}$ is some continuous range of values. The ON basis condition is then

$$I = \sum_i |i\rangle\langle i| + \int_U da|a\rangle\langle a|,$$

with the normalization

$$\langle i|j\rangle = \delta_{ij}, \quad \langle a|a'\rangle = \delta(a, a').$$

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

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

In particular, the position operator maps functions to functions via

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

Here we have used

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

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 an idealized kind of "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. You can think of this wave function as a convenient mathematical representation of, say, a Gaussian wave function centered at x':

$$\psi_{x',\epsilon}(x) = \frac{1}{\sqrt{\pi}}\frac{1}{\epsilon}\exp\left\{-\frac{(x-x')^2}{\epsilon^2}\right\},$$

whose "width" ϵ is so small that it is physically negligible. Indeed, we have

$$\lim_{\epsilon\to 0}\psi_{x',\epsilon}(x) = \delta(x,x').$$

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!

Momentum

How shall we view momentum in quantum mechanics? Should it be "mass times velocity", or what? Our approach to the definition of momentum in quantum mechanics will rely on a rather fundamental understanding of what is "momentum". To motivate our definition, let me remind you that the principal utility of the quantity called "momentum" is due to its conservation for a closed system. One can then understand the motion of interacting systems via an "exchange of momentum". Next, recall the intimate connection between symmetries of laws of physics and corresponding conservation laws. In particular, symmetry under spatial translations corresponds to conservation of linear momentum. In the Hamiltonian formulation of the classical limit of mechanics this correspondence becomes especially transparent when it is seen that the momentum is the infinitesimal generator of translations, viewed as canonical transformations. In the Hamiltonian framework, the conservation of momentum is identified with the statement that the Hamiltonian is translationally invariant, that is, is unchanged by the canonical transformation generated by the momentum. We shall see that this same logic applies in quantum mechanics. Indeed, nowadays momentum is mathematically identified – by definition – as the generator of translations. Let us see how all this works.

Having defined the position (generalized) eigenvectors, which represent (idealized) states in which the position of the particle is known with certainty, we can define a *translation operator* T_a via

$$T_a|x\rangle = |x + a\rangle.$$

Since the $|x\rangle$ span the Hilbert space, this defines the operator. Note that (exercise)

$$T_a T_b = T_{a+b}, \quad T_0 = I.$$

Physically, we interpret this operator as taking the state of the particle and transforming it to the state in which the particle has been moved by an amount a in the positive x direction.