
Lecture 5

Operators and the Schrödinger Equation

Assigned Reading:

E&R	3 _{all} , 5 _{1,3,4,6}
Li.	2 ₅₋₈ , 3 ₁₋₃
Ga.	2 _{all≠4}
Sh.	3, 4

We have just seen that in quantum mechanics, momentum becomes associated with an operator proportional to the spatial derivative. But what exactly is an operator, and what is the relation of any other observable quantity to an operator? Let us take this moment to flesh out some mathematical definitions.

An *operator* is a rule for building one function from another.

Examples include the identity $\hat{1}$ such that $\hat{1}f(x) = f(x)$, the spatial derivative $\hat{D} = \frac{\partial}{\partial x}$ such that $\hat{D}f(x) = \frac{\partial f(x)}{\partial x}$, the position $\hat{x} = x$ such that $\hat{x}f(x) = xf(x)$, the square $\hat{2}$ such that $\hat{2}f(x) = f^2(x)$, the projection \hat{P}_y such that $\hat{P}_y f(x) = y$, and the addition \hat{A}_y such that $\hat{A}_y f(x) = f(x) + y$, among others. Notationally, operators will be distinguished by hats on top of symbols.

A *linear operator* is an operator that respects superposition:

$$\boxed{\hat{O}(af(x) + bg(x)) = a\hat{O}f(x) + b\hat{O}g(x)}. \quad (0.1)$$

From our previous examples, it can be shown that the first, second, and third operators are linear, while the fourth, fifth, and sixth operators are not linear.

All operators com with a small set of special functions of their own. For an operator \hat{A} , if

$$\hat{A}f(x; A) = A \cdot f(x; A)$$

for a given $A \in \mathbb{C}$, then $f(x)$ is an *eigenfunction* of the operator \hat{A} and A is the corresponding *eigenvalue*. Operators act on eigenfunctions in a way identical to multiplying the eigenfunction by a constant number. For instance, the aforementioned operator \hat{D} has as its eigenfunctions all exponentials $e^{\alpha x}$, with *any* $\alpha \in \mathbb{C}$ allowed.

In general, though, most functions are not eigenfunctions of a given operator. That is why eigenfunctions and eigenvalues of a given operator are particularly special!

Coming back to physics, **to every observable quantity is associated a corresponding operator**. For instance, the momentum operator is

$$\hat{p} = -i\hbar \frac{\partial}{\partial x},$$

the position operator is

$$\hat{x} = x,$$

the energy operator is

$$\hat{E} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x),$$

and so on. Given a state described by a wavefunction $\psi(x)$, we can calculate the expectation value of any observable quantity in that state by using the corresponding operator:

$$\langle A^n \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{A}^n \psi(x) dx,$$

and

$$\Delta A \equiv \sqrt{\langle A^2 \rangle - \langle A \rangle^2}.$$

Note that the operator order matters! For instance,

$$\hat{p}\hat{x}f(x) = \hat{p}(xf(x)) = -i\hbar \frac{\partial}{\partial x} (xf(x)) = -i\hbar \cdot \left(f(x) + x \frac{\partial f(x)}{\partial x} \right),$$

while

$$\hat{x}\hat{p}f(x) = \hat{x} \left(-i\hbar \frac{\partial f(x)}{\partial x} \right) = -i\hbar x \frac{\partial f(x)}{\partial x}.$$

To measure the importance of order, we define the *commutator* of two operators \hat{A} and \hat{B} as

$$\boxed{[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}}. \quad (0.2)$$

For example, we have just seen that

$$\hat{x}\hat{p}f(x) - \hat{p}\hat{x}f(x) = i\hbar f(x)$$

for all $f(x)$. Hence,

$$\boxed{[\hat{x}, \hat{p}] = i\hbar \hat{1}}. \quad (0.3)$$

This is a deep and profound result in quantum mechanics!

Upon measuring an observable A which has an associated operator \hat{A} , the measured value is one of the eigenvalues of \hat{A} . Then, immediately after the measurement occurs, the wavefunction corresponding to the system state changes to be the eigenfunction $\phi(x; A)$ of \hat{A} such that

$$\hat{A}\phi(x; A) = A \cdot \phi(x; A).$$

This immediate change in the wavefunction to be an eigenfunction of an operator corresponding to the measured quantity is called *wavefunction collapse*. It is a strange beast, but we will come back to it later.

Note that all eigenvalues of operators corresponding to an observable quantity must be real. Operators with only real eigenvalues have many special properties that we will explore later.

For example, the eigenvalues of \hat{p} are real momenta

$$p = \hbar k,$$

and for a given k , these are the momenta that can be measured. This means that the eigenfunctions must be

$$\phi(x; k) = N e^{ikx}$$

for some normalization N . That said, the eigenfunctions $\phi(x; k)$ are not strictly normalizable, because they do not approach 0 as $x \rightarrow \pm\infty$. Non-normalizable wavefunctions like this one are not valid as physical single-particle states, but are useful for building normalizable wavepackets that do represent physical single-particle states. This also means that we can never measure quantities like momentum or position with full precision, either, because like momentum, position is a continuous variable so its eigenfunctions are not normalizable.

As another example, let us suppose a particle is found at position x_0 . What is its wavefunction immediately after this measurement occurs? It must be an eigenfunction of the position operator \hat{x} , and it must vanish for $x \neq x_0$. This implies that

$$\phi(x; x_0) = N \delta(x - x_0)$$

is the desired wavefunction with some normalization coefficient N , because by the properties of the Dirac delta function,

$$\hat{x} \delta(x - x_0) = x_0 \cdot \delta(x - x_0).$$

As with momentum eigenfunctions, position eigenfunctions are not normalizable, but they can be used in superpositions to form normalizable wavepackets corresponding to physical single-particle states.

As yet another example, let us say that a quantum object is in a state given by the wavefunction $\psi(x)$. Measuring the position to be x_0 changes the wavefunction to $\delta(x - x_0)$, which is not a superposition. Measuring the momentum to be p_0 would instead change the wavefunction to $e^{\frac{ip_0x}{\hbar}}$, which is also not a superposition. Hence, measurement of a particular eigenvalue collapses the wavefunction into the corresponding eigenfunction.

Let us say that we know the state given by a wavefunction $\psi(x)$ and we want to measure the position. The probability density, given that position is continuous, of measuring x_0 is $\mathbf{p}(x_0) = |\psi(x_0)|^2$. What does this look like for a more general observable A ?

Given an operator \hat{A} with observable eigenvalues A and corresponding eigenfunctions $\phi(x; A)$ fulfilling

$$\hat{A}\phi(x; A) = A \cdot \phi(x; A),$$

we can expand any wavefunction $\psi(x)$ as a superposition of eigenfunctions of \hat{A} . If A is discrete, then

$$\psi(x) = \sum_A c_A \phi(x; A) \quad (0.4)$$

while if A is continuous, then

$$\psi(x) = \int c(A) \phi(x; A) dA. \quad (0.5)$$

The probability of measuring an eigenvalue A_0 in the state ψ is, if A is discrete,

$$\mathbb{P}(A_0) = |c_{A_0}|^2 \quad (0.6)$$

or if A is continuous, then the probability density is

$$\mathbf{p}(A_0) = |c(A_0)|^2. \quad (0.7)$$

For example, for position,

$$\psi(x) = \int c(x_0) \phi(x; x_0) dx_0.$$

In this case,

$$c(x_0) = \psi(x_0)$$

as

$$\phi(x; x_0) = N\delta(x - x_0).$$

The probability density of measuring a position is then

$$\mathbf{p}(x_0) = |\psi(x_0)|^2.$$

For momentum,

$$\psi(x) = \int c(k) \phi(x; k) dk.$$

In this case,

$$c(k) = \tilde{\psi}(k)$$

as

$$\phi(x; k) = N e^{ikx}.$$

The probability density of measuring a momentum is then

$$\mathbf{p}(k) = |\tilde{\psi}(k)|^2.$$

For energy, which typically takes just discrete values,

$$\psi(x) = \sum_n c_n \phi(x; E_n).$$

Generally, the eigenfunctions $\phi(x; E_n)$ depend on the particular system, so a general form cannot be given for them, and thus neither can a general form be given for c_n . Still, though, the probability (not a density for discrete energies) of measuring an energy is

$$\mathbb{P}(E_n) = |c_n|^2.$$

When the wavefunction representing a state is expanded as a superposition of eigenfunctions of an operator \hat{A} corresponding to an observable A , it is useful to find the expansion coefficients. Whether or not A is continuous, the following is true (though notationally, c_A would be used in the discrete case, while $c(A)$ would be used in the continuous case, so the notation should be chosen based on context):

$$c(A) = \int \phi^*(x; A) \psi(x) dx \equiv \langle \phi(A) | \psi \rangle. \quad (0.8)$$

The reason why doing this is useful is because an observable A with a corresponding operator \hat{A} has real eigenvalues and orthonormal eigenvectors. What this means is that

$$\langle \phi_a | \phi_b \rangle = \delta_{ab}.$$

This is exactly like expanding a physical 3-dimensional vector in an orthonormal basis $\mathbf{v} = \sum_j v_j \mathbf{e}_j$ with $\mathbf{e}_j \cdot \mathbf{e}_l = \delta_{jl}$, and the expansion coefficients would be $v_j = \mathbf{e}_j \cdot \mathbf{v}$. That is also why the term $c(A) = \langle \phi(A) | \psi \rangle$ is known as an *inner product*.

Thus far, we have seen that the configuration of the system is given by a wavefunction corresponding to a quantum state. Expectation values of observables are found through the actions of corresponding operators on quantum states. Measuring a particular value for a quantity is probabilistic, but once the measurement is made, the wavefunction collapses into the eigenfunction corresponding to that measured eigenvalue. Given the wavefunction, these are all the predictions that can be made about the system at a given moment in time. So what happens at a later time? We have seen that translations are tied to time derivatives, so the real question is, what is $\frac{\partial \psi(x,t)}{\partial t}$?

We know from de Broglie that plane waves

$$\psi(x, t; k) = e^{i(kx - \omega t)}$$

have energy

$$E = \hbar\omega.$$

In fact, this is true of any wavefunction like

$$\psi(x, t) = e^{-i\omega t} \phi(x)$$

regardless of $\phi(x)$. We can also see that

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hbar\omega \psi(x, t)$$

in such a case. This seems to suggest that the energy operator \hat{E} is tied to the operator $i\hbar \frac{\partial}{\partial t}$. Along with this, we need that translation in time respect superposition and that the total probability

$$\int_{-\infty}^{\infty} \psi^*(x, t) \psi(x, t) dx = 1$$

be conserved. This means that the time derivative, which is linear, acting on a wavefunction should be equal to a linear operator acting on the wavefunction.

Indeed, the *Schrödinger equation* is

$$\boxed{\hat{E}\psi(x, t) = i\hbar \frac{\partial \psi(x, t)}{\partial t}}. \quad (0.9)$$

This equation describing the time evolution of a quantum state is analogous to the equation of motion $\mathbf{F} = \dot{\mathbf{p}}$. Take care to note that \hat{E} is not defined as the operator $i\hbar \frac{\partial}{\partial t}$ any more than \mathbf{F} is defined to be $\dot{\mathbf{p}}$. Like \mathbf{F} , the definition of \hat{E} depends on the details of the system. In this class, the general form for \hat{E} comes from turning the classical equation

$$E = \frac{p^2}{2m} + V(x)$$

into an operator definition

$$\hat{E} = \frac{\hat{p}^2}{2m} + V(\hat{x}).$$

Finally, this is not a derivation per se of the Schrödinger equation, but has been motivated by our finding of the momentum operator as a generator of spatial translations.

There are a few key features of the Schrödinger equation:

1. It is linear, so it respects superposition. If $\psi(x, t; n) = i\hbar \frac{\partial \psi(x, t; n)}{\partial t}$, then

$$\hat{E} \left(\sum_n c_n \psi(x, t; n) \right) = i\hbar \frac{\partial}{\partial t} \left(\sum_n c_n \psi(x, t; n) \right).$$

2. It is unitary, so it conserves probability. This will be explained later.
3. It is deterministic! It is first-order in t , so if $\psi(x, 0)$ is known, then the Schrödinger equation determines $\psi(x, t)$ for all t . However, note that wavefunction collapse upon measurement is *not* deterministic!

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