(5) Observables

1 Thus Far

- Configuration determined by wavefunction $\psi(x)$
  - continuous, normalizable, complex
  - Probability density given by $\mathbb{P}(x) = |\psi(x)|^2$
- Superposition $\psi(x) = \sum_n c_n \psi_n(x)$
  - given 2 or more WFs, an infinity of linear combinations are possible
- Curious relationship $\hat{p} = -i\hbar\frac{\partial}{\partial x}$
  - momentum is related to x derivative of $\psi(x)$

2 This Time

- What is an Operator?
- The relationship between operators and measurements
- and how measurement causes Wavefunction Collapse

3 Operators

In the last lecture we encountered the concept of an "operator", which was needed for the expression we asserted as being related to momentum: $\hat{p} = -i\hbar\frac{\partial}{\partial x}$. We needed it because this expression appears incomplete; the derivative needs something to *operate on*. While this sort of operator, a derivative waiting to happen, will be the most common in this course, the concept of an operator in QM is somewhat broader.

In general, an operator is a function on a function. That is, an operator is something which, given a function, produces another function. (A function, on the other hand, is something which given a value produces another value.)

Operators: Functions on Functions

$$\hat{\mathcal{O}} f(x) = g(x) \qquad \text{like} \qquad f(x) = y$$

for example

$$\begin{aligned}
\hat{\mathbf{1}} &= \text{identity} & \hat{\mathbf{1}}\, f(x) &= f(x) \\
\hat{D}_x &= \partial_x = \frac{\partial}{\partial x} & \hat{D}_x\, f(x) &= \partial_x f(x) \\
\hat{x} &= \text{multiply by } x & \hat{x}\, f(x) &= x f(x) \\
\hat{S} &= \text{squares } f(x) & \hat{S}\, f(x) &= f^2(x) \\
\hat{A}_3 &= \text{adds } 3 & \hat{A}_3\, f(x) &= f(x) + 3 \\
\hat{M}_4 &= \text{multiply by } 4 & \hat{M}_4\, f(x) &= 4 f(x) \\
\hat{R}_{42} &= \text{makes it } 42 & \hat{R}_{42}\, f(x) &= 42
\end{aligned}$$

Linear operators are a special kind of operators which are most useful in QM.

Linear Operators:

$$\hat{\mathcal{O}}\,(a\; f(x) + b\; g(x)) = a\; \hat{\mathcal{O}}\; f(x) + b\; \hat{\mathcal{O}}\; g(x) \qquad (1)$$

for example

$$\partial_x\,(a\; f(x) + b\; g(x)) = a\; \partial_x\; f(x) + b\; \partial_x\; g(x) \qquad (2)$$

All linear operators come with a set of special functions known as "eigenfunctions" on which their action is equivalent to multiplication by a constant (the "eigenvalue").

Eigenfunctions and Eigenvalues:

$$\hat{A}\; f_a(x) = a\; f_a(x) \qquad (3)$$

for example

$$\partial_x e^{ax} = a\; e^{ax} \quad \text{or} \quad \hat{x}\delta(x - x_0) = x_0 \delta(x - x_0) \qquad (4)$$

Note that for the operators we will encounter most functions are **not** eigenfunctions.

Non-Eigenfunctions:

$$\begin{aligned}
\hat{x}e^{ax} &= xe^{ax} \neq \alpha e^{ax} \\
\partial_x x^{42} &= 42\, x^{41} \neq \alpha x^{42} \\
\partial_x (e^{ax} + e^{bx}) &= ae^{ax} + be^{bx} \neq \alpha(e^{ax} + e^{bx})
\end{aligned}$$

Note: A sum of eigenfunctions is not likely to be an eigenfunction!

Another important property of operators is that the order in which they are applied can change the result.

Operator Order Matters:

$$\begin{aligned}
\partial_x \hat{x} e^{ax} &= \partial_x x e^{ax} = e^{ax} + axe^{ax} = (1 + ax)e^{ax} \\
&\neq \hat{x}\partial_x e^{ax} = x(ae^{ax})
\end{aligned}$$

Operator order is so important in QM that a special operator exists with which you can express *how much* changing the order of two operators changes the answer.

Commutator:

$$\left[\hat{A}, \hat{B}\right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \tag{5}$$

for example

$$\begin{aligned}
\left[\hat{M}_4, \partial_x\right] f(x) &= (4\partial_x - \partial_x 4) f(x) \\
&= 4\,\partial_x f(x) - \partial_x(4f(x)) = 0 \\
\Rightarrow \left[\hat{M}_4, \partial_x\right] = 0 & \qquad \hat{M}_4 \text{ and } \partial_x \text{ "commute"}
\end{aligned}$$

or

$$\begin{aligned}
[\hat{x}, \partial_x] f(x) &= (x\partial_x - \partial_x x) f(x) \\
&= x\partial_x f(x) - (f(x) + x\partial_x f(x)) \\
&= -f(x) \\
\Rightarrow [\hat{x}, \partial_x] = -1 & \qquad \hat{x} \text{ and } \partial_x \text{ don't commute}
\end{aligned}$$

We will see more operators, and hear more about the importance of commutation, as the course goes on. For now, let's investigate the role of operators in measurement.

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4 Measurement and Wavefunction Collapse

Let's take a step back and look at how we got here. We were trying to compute momentum statistics from a wavefunction, e.g. $\langle p \rangle$ from $\psi(x)$. We did this by sandwiching the momentum operator $\hat{p}$ in between $\langle\psi|$ and $|\psi\rangle$, Operators and Observables:

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, \hat{A}\, \psi(x)\, dx \tag{6}$$

as in

$$\langle x \rangle = \langle \psi | \hat{x} | \psi \rangle \text{ or } \left\langle p^2 \right\rangle = \langle \psi | \hat{p}^2 | \psi \rangle \tag{7}$$

Every observable has a corresponding operator, but not every operator corresponds to an observable.

And the relationship between measurement and operators goes deeper.

Expectation values are statistical statements which answer the question "if I were to measure this observable many times, what would the average be?" What if, instead of asking about averages, we want to measure the *value of an observable in a particular system* (e.g., "where IS that particle?")? Unfortunately, to make a measurement we must inevitably allow our QM system to interact with some large, messy system which we cannot really write the WF of. Take, for example, the photon which encounters a screen in a 2-slit experiment. We can write the WF of the propagating photon without trouble, but what about the screen? We can't know the WF of every molecule in the screen! So, how do we proceed?

The inventors of QM discovered a way out of this nasty problem, but it came at a great price. Werner Heisenberg and John von Neumann, back around 1930, solved this problem by a dramatic assertion which happens to work very well:

Measurement causes the WF to "collapse" to an eigenstate of the observable.

To which you must ask, *which eigenstate*? And therein lies the rub. The result of WF collapse is selected at random!

If we write our WF as a superposition of eigenstate of our observable, the probability of wavefunction collapse resulting in any particular eigenstate is simply the coefficient of that eigenstate squared.

$$\text{Given} \quad \psi(x) = \sum_n c_n \psi_{A,n}(x) \tag{8}$$

$$\text{where} \quad \hat{A}\, \psi_{A,n}(x) = \alpha_n\, \psi_{A,n}(x) \tag{9}$$

Measuring A gives α_n, and results in state $\psi_{A,n}$, with probability $\mathbb{P}_n = |c_n|^2$

Operating with an operator is NOT the same as making a measurement of the associated observable!

Let me stress here and now that wavefunction collapse is an approximation, and an idealization, which as far as I can tell nobody likes. That said, the alternative is too complicated to be useful, so we will go with it, but I wouldn't let the philosophical implications of wavefunction collapse keep me up and night.

As an example, we can use our favorite observable: momentum. Plane-waves are eigenfunctions of the momentum operator, since

Momentum EFs: $\psi_p(x) = Ne^{ikx}$ where $p = \hbar k$

$$\hat{p}\, \psi_p(x) = (-i\hbar\partial_x)\, Ne^{ikx} = \hbar k N e^{ikx} = p\, \psi_p(x) \tag{10}$$

where N is a normalization constant.[1] Thus, if we measure momentum of a particle represented by a sum of momentum states

Example:

$$\psi(x) = c_1 N e^{ik_1 x} + c_2 N e^{ik_2 x}$$

measure p to get $\hbar k_1$ with probability $|c_1|^2$ OR $\hbar k_2$ with probability $|c_2|^2 = 1 - |c_1|^2$.

[1] I admit that you will have trouble assigning a value to N since the integral of $\mathbb{P}(x) = \left|Ne^{ikx}\right|^2 = |N|^2$ over all space diverges for all values of N. If you must, you can assume that $N \to N(x)$ is a very wide Gaussian, which changes so slowly that $\partial_x N(x) \simeq 0$, but none of this is important for the result.

Say we get $p = \hbar k_1$. The new state is

$$\psi'(x) = Ne^{ik_1 x}$$

Wavefunction Collapse!

An interesting tidbit: if you make a measurement which cannot distinguish between multiple states due to degeneracy (same eigenvalue), the WF can collapse to a superposition of degenerate states.

So here is the executive summary:

- Observables (like momentum)
- correspond to operators ($\hat{p} = -i\hbar\frac{\partial}{\partial x}$)
- which have eigenfunctions ($\psi_p(x) = Ne^{ikx}$)
- with eigenvalues ($p = \hbar k$)
- which correspond to measurable values of the observable (momentum)
- for which the probability is $\mathbb{P}_p = |\langle\psi_p(x)|\psi(x)\rangle|^2$
- and should you make such a measurement on the state $\psi(x)$
- and get eigenvalue $p = \hbar k_1$
- the state will collapse to the eigenfunction $\psi_{p_1}(x) = Ne^{ik_1 x}$.

Questions?

SKIP THIS in lecture

A similar situation holds for position measurements. (Imagine the photon in a 2-slit experiment as it hits the screen and excites some electron, with which we eventually measure its location.)

Position EFs: $\psi_{x_0}(x) = N\delta(x - x_0)$

$$\hat{x}\,\psi_{x_0}(x) = x\,N\delta(x - x_0) = x_0\,N\delta(x - x_0) = x_0\,\psi_{x_0}(x)$$

where N is a normalization constant.[2] Note that x_0 is a continuous parameter which result in a continuous set of eigenfunctions!

Unlike the previous example, we will use a continuous superposition of position eigenfunctions to describe our particle.

Example:

$$\psi(x) = \int_{-\infty}^{\infty} f(x')\delta(x' - x)\,dx' = f(x) \tag{11}$$

measure x to get a value between x_0 and $x_0 + \epsilon$ with probability $\epsilon\mathbb{P}(x_0)$ for small ϵ.

Having measured $x \simeq x_0$, the new state is

$$\psi(x) = \frac{1}{\sqrt[4]{\pi\,\epsilon^2}} e^{-(x-x_0)^2/2\epsilon^2} \simeq N\delta(x - x_0)$$

[2]Again, you will have trouble assigning a value to N. If you must, you can approximate the delta function as a very narrow Gaussian.

5 Hermitian Operators and Observables

Operators which can be associated with observables, known as Hermitian operators, are defined as

Hermitian Operators: for Observables

$$\hat{A} = \hat{A}^\dagger \leftrightarrow \hat{A} = \hat{A}^* \tag{12}$$

where † means "Hermitian adjoint", which is defined by

$$\begin{aligned} \langle \hat{A}\,\psi|\psi\rangle &= \int_{-\infty}^{\infty} (\hat{A}\psi)^*\psi\,dx \\ &\equiv \int_{-\infty}^{\infty} \psi^*\hat{A}^\dagger\psi\,dx \\ &= \langle\psi|\hat{A}^\dagger|\psi\rangle \end{aligned}$$

which for our purposes is just a complex conjugate for operators and wavefunctions.

In fact, the adjoint of a complex number is its conjugate.

Moving Numbers

$$\begin{aligned} \langle a\,\psi|\psi\rangle &= \langle\psi|a^\dagger|\psi\rangle = \langle\psi|a^*|\psi\rangle \text{ for } a \in \mathbb{C} \\ \Rightarrow \langle \hat{x}\,\psi|\psi\rangle &= \langle\psi|\hat{x}|\psi\rangle \text{ since } \hat{x}^\dagger = x^* = x = \hat{x} \end{aligned}$$

The adjoint of an operator can, however, but more complicated. The derivative ∂_x is a fundamental operator of this course, so let's look at how this works for $\hat{p}$.

Moving ∂_x

$$\begin{aligned}
\langle \hat{p}\,\psi|\psi\rangle &= \int_{-\infty}^{\infty} (-i\hbar\partial_x\psi)^*\psi = i\hbar \int_{-\infty}^{\infty} \partial_x\psi^*\psi \\
\text{integration by parts} &\quad \int_{-\infty}^{\infty} \partial_x u\; v\; dx = [uv]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} u\;\partial_x v\; dx \\
\text{identify} &\quad u = \psi^* \text{ and } v = \psi \\
\text{assume} &\quad [\psi^*\psi]_{-\infty}^{\infty} = 0 \text{ since WF is normalizable} \\
\Rightarrow \langle \hat{p}\,\psi|\psi\rangle &= -i\hbar \int_{-\infty}^{\infty} \psi^*\partial_x\psi \\
&= \langle\psi|\hat{p}|\psi\rangle
\end{aligned}$$

Note: i and ∂_x are anti-Hermitian (e.g., $\partial_x^\dagger = -\partial_x$)

Hermitian operators have several important properties. (The first of these tells us why observables are associated with Hermitian operators.)

Hermitian Operator Properties:

- eigenvalues are always real (observable!)
  $\hat{A}\,\psi_{A,n} = a_n\psi_{A,n}$ with $a_n \in \mathbb{R}$
- eigenfunctions are orthogonal
  $\langle\psi_{A,n}|\psi_{A,m}\rangle = \delta_{n,m}$ or $\langle\psi_{A,n}|\psi_{A,m}\rangle = \delta(n-m)$
- eigenfunctions from complete basis
  $\psi(x) = \sum_n c_n\,\psi_{A,n}(x)$ or $\psi(x) = \int c(n)\psi_{A,n}(x)\,dn$

*Yes, $\langle\psi_{A,n}|\psi_{A,m}\rangle = \delta(n-m)$ is right for **continuous** n and m. You will see why below.*

Now, let's see what happens when we put these things together:

$$
\begin{aligned}
\langle \psi_{A,n} | \psi \rangle &= \int_{-\infty}^{\infty} \psi^*_{A,n}(x) \psi(x)\, dx \\
&= \int_{-\infty}^{\infty} \psi^*_{A,n}(x) \sum_m c_m\, \psi_{A,m}(x)\, dx \\
&= \sum_m c_m \int_{-\infty}^{\infty} \psi^*_{A,n}(x)\, \psi_{A,m}(x)\, dx \\
&= \sum_m c_m\, \langle \psi_{A,n} | \psi_{A,m} \rangle \\
&= \sum_n c_m\, \delta_{n,m} \\
&= c_n
\end{aligned}
$$

which gives

$$
\mathbb{P}_n = \left| \langle \psi_{A,n} | \psi \rangle \right|^2 = \left| c_n \right|^2 \tag{13}
$$

if $\psi(x)$ is written as the sum of a discrete set of eigenfunctions of $\hat{A}$ each with coefficients c_n, as shown above.

What about the case of an operator with a continuous set of eigenfunctions? To make a superposition, we have to exchange the sum for an integral:

Continuous Superposition:

$$
\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx}\, dk
$$

And finally we can evaluate the “overlap integral” we started with. For momentum, we have

$$
\begin{aligned}
\langle\psi_p|\psi\rangle &= \int_{-\infty}^{\infty}\psi_p^*(x)\psi(x)\,dx \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty}(e^{ikx})^*\left(\int_{-\infty}^{\infty}\tilde{\psi}(k')e^{ik'x}\,dk'\right)\,dx \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{\psi}(k')\underbrace{\left(\int_{-\infty}^{\infty}e^{i(k'-k)x}\,dx\right)}_{=2\pi\delta(k'-k)}\,dk' \\
&= \int_{-\infty}^{\infty}\tilde{\psi}(k')\,\langle\psi_{p'}|\psi_p\rangle\,dk' \\
&= \tilde{\psi}(k)
\end{aligned}
$$

And, as we have seen in lecture and on the pset, the probability density around some value of momentum is

$$
\mathbb{P}_p = \mathbb{P}(k) = \left|\tilde{\psi}(k)\right|^2 = |\langle\psi_p|\psi\rangle|^2 \tag{14}
$$

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6 Next Time

- So we have some wavefunction, what happens next?
- What happened to our beloved $F = ma$?
- Next time: the Schrödinger Equationand how to tell the FUTURE!