(4) Probability and Uncertainty

1 Last Time

- Wavefunctions $\psi(x)$ and $\mathbb{P}(x) = |\psi(x)|^2$
- Superposition $\psi(x) = \sum_n c_n \, \psi_n(x)$
- from de Broglie's $p = h/\lambda = \hbar k$ to wave packets with Fourier

- Physical WFs are normalizable $\int \mathbb{P}(x) \, dx = 1$
- Any superposition of ok WFs is ok, but narrow spikes and plane-waves are easy to interpret classically, and we can make any WF from them

Superimpose waves with *definite momentum* to make localized WFs

Discrete vs. Continuous

$$\psi(x) \simeq \sum_n c_n e^{ik_n x}$$

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

Note: $\tilde{\psi}(k)$ plays the role of c_n telling you how much of each momentum you have. And you can go the other way to discover the momentum content in any WF

$$\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} \, dx \quad \text{and} \quad \mathbb{P}(k) = \left|\tilde{\psi}(k)\right|^2$$

The WF describes the position and momentum of our particle, just like x and p in classical mechanics!

2 This Time

- Randomness
- The momentum *operator*

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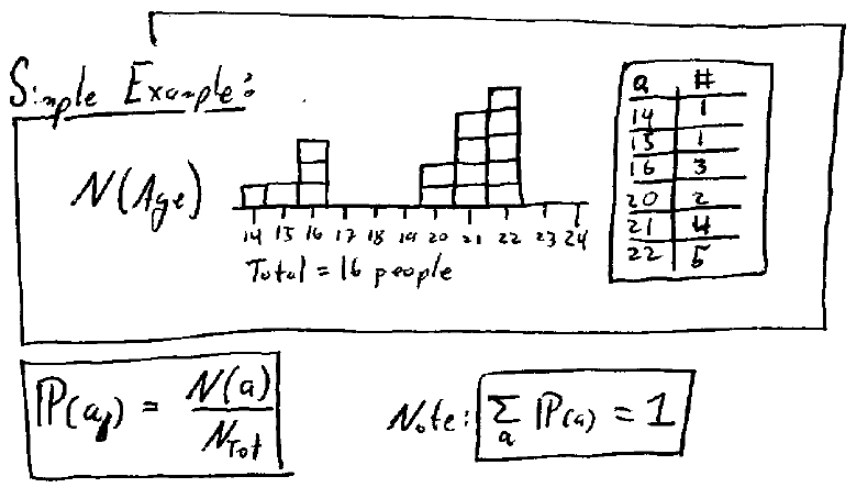
3 Probabilities and Statistics

- Gr. 1.3, Sc. 3.2

We have seen that randomness is critical to QM, and we have spent some time relating the WF to probability distributions in position and momentum (e.g., $\mathbb{P}(x)$ and $\mathbb{P}(k)$). Here we'll develop the tools necessary to make precise statements about the statistics which describe a particle with a given WF.

Let's start our exploration of statistics in the simple context of discrete probabilities. If we have a group of people each with an age in years (no fractions of a year, or months or whatever, just "Hi, I'm 22!') we can make a histogram which shows how many people we have of each age:

Age Histogram



Let's call the number of people with each age value $N(a)$. This means that the probability of finding someone with a given age, if you pick a member of the group at random, is

$$\mathbb{P}(a) = \frac{N(a)}{\sum_a N(a)} \quad \Rightarrow \quad \sum_a \mathbb{P}(a) = \sum_a \frac{N(a)}{\sum_b N(b)} = 1 \tag{1}$$

- Most likely a $\quad \text{Max}(\mathbb{P}(a)) = 22$
- Average a ? $\quad \langle a \rangle = \sum_a a\mathbb{P}(a) = 19.4$

Q: Does $\langle a \rangle$ have to be measureable? A: NO!

- Average a^2 ? $\quad \left\langle a^2 \right\rangle = \sum_a a^2\mathbb{P}(a) = 385.8$
- In general $\quad \langle f(a) \rangle = \sum_a f(a)\mathbb{P}(a)$

How do we characterize the "width" of the distribution, or the distance you are likely to end up form the average value?

- Distance from the mean: "deviation" $\quad a - \langle a \rangle$
- does avg deviation work? $\quad \langle (a - \langle a \rangle) \rangle$ NO!

$$\sum_a (a\mathbb{P}(a) - \langle a \rangle \mathbb{P}(a)) = \sum_a a\mathbb{P}(a) - \langle a \rangle \sum_a \mathbb{P}(a) = 0$$

- how about deviation squared? $\quad \left\langle (a - \langle a \rangle)^2 \right\rangle$

  ok, but the units are wrong. (like "variance")
- Use $\Delta a \equiv \sqrt{\langle (a - \langle a \rangle)^2 \rangle}$ (like "std deviation")

To hopefully avoid some common mistakes, let me point out a few things.

Q: Is $\langle a\rangle^2 = \left\langle a^2\right\rangle$? A: NO!

$$
\begin{aligned}
\Delta a^2 &= \left\langle (a - \langle a\rangle)^2 \right\rangle \\
&= \left\langle a^2 - 2a\langle a\rangle + \langle a\rangle^2 \right\rangle \\
&= \left\langle a^2\right\rangle - 2\langle a\rangle\langle a\rangle + \langle a\rangle^2 \\
&= \left\langle a^2\right\rangle - \langle a\rangle^2
\end{aligned}
$$

Note the similarities to center of mass and moment of inertial for a 1D collection of discrete particles:

$$
\begin{aligned}
\langle a\rangle = \sum_a a\mathbb{P}(a) = a\frac{N(a)}{\sum_a N(a)} \quad &\leftrightarrow \quad x_{CM} = \sum_n x_n \frac{m_n}{\sum_n m_n} \\
\left\langle a^2\right\rangle = \sum_a a^2\mathbb{P}(a) \quad &\leftrightarrow \quad \frac{I}{M} = \sum_n x_n^2 \frac{m_n}{\sum_n m_n} \\
\Delta a^2 = \sum_a (a - \langle a\rangle)^2\mathbb{P}(a) \quad &\leftrightarrow \quad \frac{I_{CM}}{M} = \sum_n (x_n - x_{CM})^2 \frac{m_n}{\sum_n m_n}
\end{aligned}
$$

The extension to continuous probability density function is straight forward.

$$
\begin{aligned}
&\text{Quantum} && \text{Classical} \\
&\text{for } \mathbb{P}(x) = |\psi(x)|^2 && \text{for mass density } \rho(x) \\
\langle x\rangle = \int x\,\mathbb{P}(x)\,dx \quad &\leftrightarrow && x_{CM} = \int x\,\frac{\rho(x)}{M} \\
\left\langle x^2\right\rangle = \int x^2\,\mathbb{P}(x)\,dx \quad &\leftrightarrow && \frac{I}{M} = \int x^2 \frac{\rho(x)}{M} \\
\Delta x^2 = \int (x - \langle x\rangle)^2\,\mathbb{P}(x)\,dx \quad &\leftrightarrow && \frac{I_{CM}}{M} = \int (x - x_{CM})^2 \frac{\rho(x)}{M}
\end{aligned}
$$

Note that we have assumed that $\psi(x)$ is normalized such that $\int \mathbb{P}(x) = 1$. Note also that $\langle x\rangle$ and Δx depend on $\psi(x)$. Expectation values can be written as

$$\langle x \rangle = \langle \psi | x | \psi \rangle \quad \text{or} \quad \left\langle x^2 \right\rangle = \langle \psi | x^2 | \psi \rangle$$

to make this clear.

I've just slipped in some Dirac notation, which goes deeper than just making expectation values, but more on that later.

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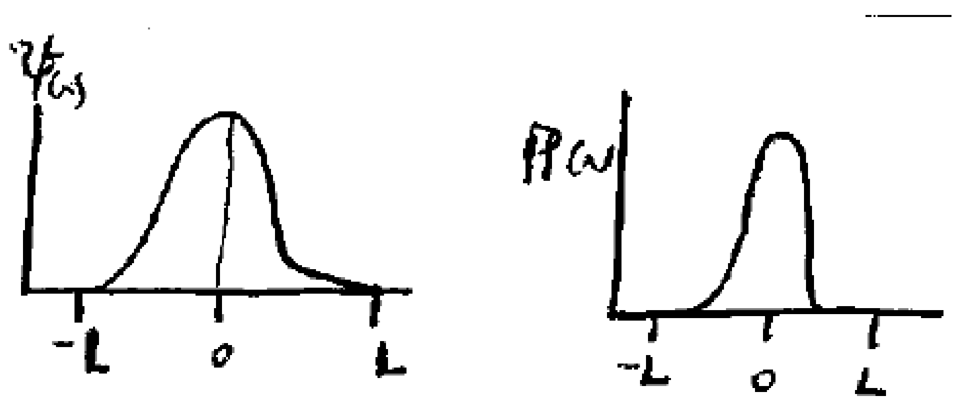
4 Position Expectation and Uncertainty: An Example

Let's run though an example of these calculations for a particular WF.

$$\psi(x) = \begin{cases} N(L^2 - x^2)^2 & -L < x < L \\ 0 & otherwise \end{cases} \tag{2}$$

Example WF



with which we can compute $\langle x \rangle$ and Δx. We start by determining the value of N which normalizes $\psi(x)$:

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} \mathbb{P}(x)\, dx = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx \\ &= \int_{-\infty}^{\infty} \psi^*(x)\psi(x)\, dx = \langle \psi | \psi \rangle \end{aligned}$$

Note conjugate! Recall $|\psi(x)|^2 = \psi^*(x)\,\psi(x)$

$$
\begin{aligned}
&= |N|^2 \int_{-L}^{L} (L^2 - x^2)^4 \, dx \\
&= |N|^2 \; L^9 \underbrace{\int_{-1}^{1} \left(1 - \left(\frac{x}{L}\right)^2\right)^4 \; \frac{dx}{L}}_{\text{unitless!}} \\
&= |N|^2 \; L^9 \; \frac{256}{315} \\
\Rightarrow N &= \underbrace{e^{i\phi}}_{\text{phase}} \sqrt{\frac{315}{256 \; L^9}}
\end{aligned}
$$

The expectation value of x is

$$
\begin{aligned}
\langle x \rangle = \langle \psi | x | \psi \rangle &= \int_{-\infty}^{\infty} \psi^*(x) \; x \; \psi(x) \; dx \\
&= |N|^2 \int_{-L}^{L} \underbrace{(L^2 - x^2)^4}_{\text{even}} \underbrace{x}_{\text{odd}} \; dx \\
&= 0
\end{aligned}
$$

Note conjugate! Think $\langle \psi(x)| \to \psi^*(x)$ *in the integral.*

Finally, to get Δx we compute $\langle x^2 \rangle$

$$
\begin{aligned}
\left\langle x^2 \right\rangle &= \langle \psi | x^2 | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x^2\, \psi(x)\, dx \\
&= |N|^2 \int_{-L}^{L} \left(L^2 - x^2\right)^4\, x^2\, dx \\
&= |N|^2\, L^{11}\, \underbrace{\int_{-1}^{1} \left(1 - \left(\frac{x}{L}\right)^2\right)^4\, \left(\frac{x}{L}\right)^2\, \frac{dx}{L}}_{\text{Unitless! Mathematica!}} \\
&= \frac{1}{11} L^2 \qquad \Rightarrow \Delta x = \frac{L}{\sqrt{11}} \quad \text{since} \quad \langle x \rangle = 0
\end{aligned}
$$

That's it for x, we know expectation value and uncertainty, but what about p?

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5 Momentum Expectation and Uncertainty

- Gr. 1.5, Sc. 3.2

To understand the momentum statistics like expectation value and uncertainty one might hope to apply the same approach as for position.

$$
\langle p \rangle \stackrel{?}{=} \int_{-\infty}^{\infty} \psi^*(x)\, p\, \psi(x)\, dx
$$

but what is p in this context?

We'll go about this first by seeing what hints our mathematical environment offers us. We know the momentum for a "plane wave" (e.g., $\psi(x) = e^{ikx}$, so called because in 3-D this would be a planar wave-front propagating in the $\vec{x}$ direction), and we know its expectation value.

Hint: Plane waves have definite momentum

$$\begin{aligned} \psi(x) = Ne^{ikx} & \qquad \text{has } \; p = \hbar k \\ \frac{\partial}{\partial x}\psi(x) = ikNe^{ikx} & \quad \Rightarrow \quad -i\hbar\,\partial_x\,\psi(x) = \hbar k\,\psi(x) \\ & \quad \Rightarrow \quad p \overset{?}{=} -i\hbar\,\partial_x \end{aligned}$$

But ∂_x needs to operate on something! Let's define an "operator"

Momentum Operator: $\hat{p} = -i\hbar\,\partial_x$

and then see how this plays in our computation of the expectation value.

$$\begin{aligned} \langle p \rangle &= \langle \psi|\hat{p}|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\,\hat{p}\,\psi(x)\,dx \\ &= \int_{-\infty}^{\infty} \psi^*(x)\,(-i\hbar\,\partial_x)\,\psi(x)\,dx \\ &= -i\hbar \int_{-\infty}^{\infty} \psi^*(x)\,\partial_x\psi(x)\,dx \end{aligned}$$

For a plane wave we have

$$
\begin{aligned}
\langle p \rangle &= -i\hbar \int_{-\infty}^{\infty} N^* e^{-ikx}\, \partial_x N e^{ikx}\, dx \\
&= -i\hbar \int_{-\infty}^{\infty} N^* e^{-ikx}\, (ik) N e^{ikx}\, dx \\
&= \hbar k \int_{-\infty}^{\infty} N^* e^{-ikx}\, N e^{ikx}\, dx \\
&= \hbar k \underbrace{\int_{-\infty}^{\infty} \underbrace{\psi^*(x)\, \psi(x)}_{=|\psi(x)|^2 = \mathbb{P}(x)}\, dx}_{=\langle \psi | \psi \rangle = 1} = p
\end{aligned}
$$

which is good, since the momentum is *exactly* p. This should also mean that Δp is zero for a plane wave. Let's check:

$$
\begin{aligned}
\left\langle p^2 \right\rangle &= \int_{-\infty}^{\infty} \psi^*(x)\, \left(-i\hbar\, \partial_x\right)^2 \psi(x)\, dx \\
&= -\hbar^2 \int_{-\infty}^{\infty} N^* e^{-ikx}\, \partial_x^2 N e^{ikx}\, dx \\
&= -\hbar^2 \int_{-\infty}^{\infty} N^* e^{-ikx}\, (ik)^2 N e^{ikx}\, dx \\
&= (\hbar k)^2 \langle \psi | \psi \rangle = p^2 \\
\Rightarrow\ & \Delta p^2 = \left\langle p^2 \right\rangle - \langle p \rangle^2 = 0
\end{aligned}
$$

And back to our example WF, let's find $\langle p \rangle$ and Δp.

$$\begin{aligned}\langle p\rangle &= -i\hbar\,|N|^2\int_{-L}^{L}\left(L^2-x^2\right)^2\;\partial_x\left(L^2-x^2\right)^2\;dx\\ &= i\hbar\,|N|^2\int_{-L}^{L}\underbrace{\left(L^2-x^2\right)^2}_{\text{even}}\left(\underbrace{2\left(L^2-x^2\right)}_{\text{even}}\underbrace{2x}_{\text{odd}}\right)\;dx\\ &= 0\end{aligned}$$

which should not be surprising, since there is nothing like e^{ikx} there.

$$\begin{aligned}\left\langle p^2\right\rangle &= -\hbar^2\,|N|^2\int_{-L}^{L}\left(L^2-x^2\right)^2\;\partial_x^2\left(L^2-x^2\right)^2\;dx\\ &= -\hbar^2\,|N|^2\int_{-L}^{L}\left(L^2-x^2\right)^2\left(12x^2-4L^2\right)\;dx\\ &= \frac{3\hbar^2}{L^2}\qquad\Rightarrow\Delta p=\sqrt{3}\frac{\hbar}{L}\\ &\quad\text{units?}\;\left[\frac{\text{J s}}{\text{m}}\right]=\left[\frac{\text{kg m}^2\text{ s}}{\text{s}^2\text{ m}}\right]=\left[\frac{\text{kg m}}{\text{s}}\right]\end{aligned}$$

On the pset you will prove

$$\begin{aligned}\langle p\rangle &= \int_{-\infty}^{\infty}(\hbar\,k)\mathbb{P}(k)\;dk\\ \left\langle p^2\right\rangle &= \int_{-\infty}^{\infty}(\hbar\,k)^2\mathbb{P}(k)\;dk\end{aligned}$$

as expected from our discussion of the FT.

In this class we have hinted at the relationship between uncertainty in x and p, and you should have read about it in your texts. We have also seen in the example wave packets that when Δx is small Δp is large and vice versa. Now that we have clear definitions of Δx and Δp, I can make a clear statement about how they are related.

Uncertainty Principle: $\Delta x \, \Delta p \geq \hbar/2$

We can check this for our example WF

Example:

$$\Delta x \, \Delta p = \frac{L}{\sqrt{11}} \cdot \sqrt{3}\frac{\hbar}{L} = \sqrt{\frac{3}{11}}\hbar \simeq 1.0445 \, \frac{\hbar}{2} \tag{3}$$

very close!

On the pset you will show that a Gaussian wavepacket, unlike our example wavepacket, has minimal uncertainty.

Concept question time!

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6 Next Time

- The truth about Operators
- their relationship to Measurements
- and the disaster of Wavefunction Collapse!

7 Momentum Aside

<u>Aside</u>: What does $\hat{p}$ have to do with having momentum $p = \hbar k$?

- Consider two states:

$$\underbrace{\Psi_k = e^{ikx}}_{\text{state with def momentum } p=\hbar k} \qquad \underbrace{\Psi_s = e^{ikx} + e^{iqx}}_{\text{Does not have def momentum! Rather, a superposition of } \hbar k \text{ and } \hbar q}$$

- Watch what happens when we <u>act</u> with $\hat{p}$!

$$\hat{p}\,\Psi_k = \frac{\hbar}{i}\partial_x e^{ikx} = \frac{\hbar}{i}(ik)e^{ikx} = \hbar k\, e^{ikx}$$

$$\boxed{\hat{p}\,\Psi_k = \hbar k\,\Psi_k}$$

$$\hat{p}\,\Psi_s = \frac{\hbar}{i}\partial_x\left(e^{ikx} + e^{iqx}\right) = \frac{\hbar}{i}\left(ike^{ikx} + iqe^{iqx}\right) = \hbar\left(ke^{ikx} + qe^{iqx}\right)$$

$$\boxed{\hat{p}\,\Psi_s \neq \Psi_s}$$

- $\hat{p}$ is an operator which acts simply on WF's corresponding to states with definite momenta, but not on superpositions of momentum states.

- $\hat{p}$ is the operator whose eigenstates are states with definite momenta

The eigenvalues of $\hat{p}$ are the momenta of the corresponding states

8 Uncertainty Proof: for the doubtful and masochistic

Start with some ingredients which we will need. In this ψ is always $\psi(x)$, so I will drop the (x). All integrals go from $-\infty$ to ∞ on x.

We start by showing how a Hermitian operator like $\hat{p}$ can be moved around ψ

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

Next we show that the commutator of $\hat{x}$ and $\hat{p}$ is $i\hbar$. (Note that $\hat{x} = x$.)

$$\begin{aligned}
[\hat{x},\hat{p}] &\equiv \hat{x}\,\hat{p} - \hat{p}\,\hat{x} = -i\hbar(x\,\partial_x - \partial_x\,x) \\
\text{use product rule} & \quad \partial_x\,x\,f(x) = f(x) + x\,\partial_x\,f(x) = f(x)(1 + x\,\partial_x) \\
& \quad \Rightarrow \partial_x\,x = 1 + x\,\partial_x \\
\Rightarrow\ [\hat{x},\hat{p}] &= -i\hbar(x\,\partial_x - (1 + x\,\partial_x)) = i\hbar
\end{aligned}$$

Lastly we define the function $\phi(x)$ as

$$\phi = (x + i\lambda\hat{p})\psi \tag{4}$$

and require $\langle\phi|\phi\rangle \geq 0$ (which is just saying that $|\phi|^2$ is non-negative).

$$\begin{aligned}
\langle\phi|\phi\rangle &= \langle (x + i\lambda\hat{p})\psi|(x + i\lambda\hat{p})\psi\rangle \\
&= \langle\psi|(x - i\lambda\hat{p})(x + i\lambda\hat{p})|\psi\rangle \\
&= \langle\psi|x^2|\psi\rangle + \lambda^2\langle\psi|\hat{p}^2|\psi\rangle + i\lambda\left(\langle\psi|x\,\hat{p}|\psi\rangle - \langle\psi|\hat{p}\,x|\psi\rangle\right) \\
&= \left\langle x^2\right\rangle + \lambda^2\left\langle p^2\right\rangle + i\lambda\langle\psi|\,[x,\hat{p}]\,|\psi\rangle \\
&= \Delta x^2 + \lambda^2\Delta p^2 - \lambda\hbar \geq 0
\end{aligned}$$

where in the last step we assume that $\langle x\rangle = \langle p\rangle = 0$ since any WF can be shifted or boosted to make this true without changing Δx or Δp.

Since this quantity must be positive, let's find its minimum

$$\partial_\lambda \left(\lambda^2 \Delta p^2 - \lambda \hbar + \Delta x^2 \right) = 2\Delta p^2 \lambda - \hbar \; \Rightarrow \; \lambda_{min} = \frac{\hbar}{2\Delta p^2}$$

inserting this into the above gives

$$\begin{aligned} \Delta x^2 + \frac{\hbar^2}{4\Delta p^2} - \frac{\hbar^2}{2\Delta p^2} &\geq 0 \\ \Rightarrow \Delta x^2 \, \Delta p^2 &\geq \frac{\hbar^2}{4} \\ \Rightarrow \Delta x \, \Delta p &\geq \frac{\hbar}{2} \end{aligned}$$

QED