Learning Objectives

- Expand on the introduction of Heisenberg's Uncertainty Principle by calculating the $\Delta x$ or $\Delta p$ directly from the wavefunction.

As will be discussed in Section 4.6, the operators $\langle \hat{\text{x}} \rangle$ and $\langle \hat{\text{p}} \rangle$ are not compatible and there is no measurement that can precisely determine the corresponding observables ($\langle x \rangle$ and $\langle p \rangle$) simultaneously. Hence, there must be an uncertainty relation between them that specifies how uncertain we are about one quantity given a definite precision in the measurement of the other. Presumably, if one can be determined with infinite precision, then there will be an infinite uncertainty in the other. The uncertainty in a general quantity $\langle A \rangle$ is

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2} \tag{3.8.1}$$

where $\langle A^2 \rangle$ and $\langle A \rangle$ are the expectation values of $\langle \hat{A^2} \rangle$ and $\langle \hat{A} \rangle$ operators for a specific wavefunction. Extending Equation \ref{3.8.1} to $\langle x \rangle$ and $\langle p \rangle$ results in the following uncertainties

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \tag{3.8.2a}$$
$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \tag{3.8.2b}$$

These quantities can be expressed explicitly in terms of the (time-dependent) wavefunction $\langle \Psi(x, t) \rangle$ using the fact that

$$\langle x \rangle = \langle \Psi(t) | \hat{x} | \Psi(t) \rangle \tag{3.8.3}$$
$$= \int \Psi^*(x,t) x \Psi(x,t) \, dx \nonumber$$

and

$$\langle x^2 \rangle = \langle \Psi(t) | \hat{x}^2 | \Psi(t) \rangle \tag{3.8.4}$$
$$= \int \Psi^*(x,t) x^2 \Psi(x,t) \, dx \nonumber$$

The middle terms in both Equations \ref{3.8.3} and \ref{3.8.4} are the integrals expressed in Dirac's Bra-ket notation. Similarly using the definition of the linear momentum operator:

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

So

$$\langle p \rangle = \langle \Psi(t) | \hat{p} | \Psi(t) \rangle \tag{3.8.5}$$
$$= \int \Psi^*(x,t) - i \hbar \frac{\partial}{\partial x} \Psi(x,t) \, dx \nonumber$$

and

$$\langle p^2 \rangle = \langle \Psi(t) | \hat{p}^2 | \Psi(t) \rangle \tag{3.8.6}$$
$$= \int \Psi^*(x,t) \left(-\hbar^2 \frac{\partial^2}{\partial x^2}\right) \Psi(x,t) \, dx \nonumber$$

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**Time-dependent vs. time-independent wavefunction**

The expectation values above are formulated with the total time-dependence wavefunction $\psi(x,t)$ that are functions of $x$ and $t$. However, it is easy to show that the same expectation value would be obtained if the time-independent wavefunction $\psi(x)$ that are functions of only $x$ are used. If $V(x)$ in $\hat{H}$ is time independent, then the wavefunctions are stationary and the expectation value are time-independent. You can easily confirm that by comparing the expectation values using the general formula for a stationary wavefunction

$$\langle \psi(x) \rangle = \psi(x) e^{-iEt / \hbar}$$

and for $\langle \psi(x) \rangle$.

The Heisenberg uncertainty principle can be quantitatively connected to the properties of a wavefunction, i.e., calculated via the expectation values outlined above:

$$\Delta p \Delta x \geq \frac{\hbar}{2} \label{3.8.8}$$

This essentially states that the greater certainty that a measurement of $\langle x \rangle$ or $\langle p \rangle$ can be made, the greater will be the uncertainty in the other. Hence, as $\langle \Delta p \rangle$ approaches 0, $\langle \Delta x \rangle$ must approach $\langle \infty \rangle$, which is the case of the free particle (e.g., with $V(x)=0$) where the momentum of a particle can be determined precisely.

**Example 3.8.1 : Uncertainty with a Gaussian wavefunction**

A particle is in a state described by the wavefunction

$$\psi(x) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-ax^2} \label{Ex1eq1}$$

where $a$ is a constant and $-\infty \leq x \leq \infty$. Verify that the value of the product $\langle \Delta p \Delta x \rangle$ is consistent with the predictions from the uncertainty principle (Equation \ref{3.8.8}).

**Solution**

Let's calculate the average of $\langle x \rangle$:

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx$$

since the integrand is an odd function (an even function times an odd function is an odd function). This makes sense given that the gaussian wavefunction is symmetric around $x=0$.

Let's calculate the average of $\langle x^2 \rangle$:

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* x^2 \psi \, dx$$
Let's calculate the average in $\langle p \rangle$:

\[
\begin{align*}
\langle p \rangle &= \int_{-\infty}^{\infty} \psi^{*} p \psi \, dx \\
&= \int_{-\infty}^{\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2} - i\hbar \frac{d}{dx} \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2} \, dx \\
&= \int_{-\infty}^{\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2} (-i\hbar) \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2} (-2ax) \, dx \\
&= 0
\end{align*}
\]

since the integrand is an odd function.

Let's calculate the average of $\langle p^2 \rangle$:

\[
\begin{align*}
\langle p^2 \rangle &= \int_{-\infty}^{\infty} \psi^{*} p^2 \psi \, dx \\
&= -\hbar^2 \left(\frac{2a}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} 2a(ax^2 - 1) e^{-2ax^2} \, dx \\
&= -4\hbar^2 a^2 \left(\frac{2a}{\pi}\right)^{1/2} \int_{0}^{\infty} x^2 e^{-2ax^2} \, dx + 4\hbar^2 a \left(\frac{2a}{\pi}\right)^{1/2} \int_{0}^{\infty} e^{-2ax^2} \, dx \\
&= a\hbar^2
\end{align*}
\]

We use Equation \ref{3.8.1} to check on the uncertainty

\[
\begin{align*}
\Delta{x^2} &= \langle x^2 \rangle - \langle x \rangle^2 = \frac{1}{4a} - 0 \\
\Delta{x} &= \sqrt{\Delta{x^2}} = \frac{1}{2\sqrt{a}} \\
\Delta{p^2} &= \langle p^2 \rangle - \langle p \rangle^2 = a\hbar^2 - 0 \\
\Delta{p} &= \sqrt{\Delta{p^2}} = \hbar \sqrt{a}
\end{align*}
\]

Finally we have

\[
\Delta{p}\Delta{x} = \left(\frac{1}{2\sqrt{a}}\right) (\hbar \sqrt{a}) = \frac{\hbar}{2}
\]

Not only does the Heisenburg uncertainly principle hold (Equation \ref{3.8.8}), but the equality is established for this wavefunction. This is because the Gaussian wavefunction (Equation \ref{Ex1eq1}) is special as discussed later.

**Exercise 3.8.1**

A particle is in a state described by the ground state wavefunction of a particle in a box

\[
\psi = \sqrt{\frac{2}{L}} \sin \left(\frac{\pi x}{L}\right)
\]

where $L$ is the length of the box and $0 \leq x \leq L$. Verify that the value of the product $\langle \Delta p \Delta x \rangle$ is consistent with the predictions from the uncertainty principle (Equation \ref{3.8.8}).

The uncertainty principle is a consequence of the wave property of matter. A wave has some finite extent in space and generally is not localized at a point. Consequently there usually is significant uncertainty in the position of a quantum particle in space.

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**Contributors and Attributions**

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