The wave function $\psi(x)$ determines observables in quantum physics:

$$\psi^*(x) \psi(x) = |\psi(x)|^2 = P(x) = \text{Probability} \text{ of finding a particle at } x \quad (\int P(x) \, dx = 1)$$

$*$ = complex conjugate: $(x + iy) \rightarrow (x - iy)$  

$$i = j = \sqrt{-1}$$

Quantum-Mechanical Observables = Expectation Values = Averages:

$$\langle x \rangle = \psi^* (x) \cdot x \cdot \psi(x) \, d^3x$$  

Average position

$$\langle x^2 \rangle = \psi^* (x) \cdot x^2 \cdot \psi(x) \, d^3x$$  

Uncertainty (rms)

$$\Delta x = [(\langle (x - \langle x \rangle)^2 \rangle)^{1/2} = [(\langle x^2 \rangle - \langle x \rangle^2)^{1/2}$$

rms = root mean square

$$\langle p \rangle = \psi^* (x) \cdot -i\hbar \nabla \cdot \psi(x) \, d^3x$$  

Average momentum

$$\nabla = \frac{d}{dx}$$

$$\langle p^2 \rangle = \psi^* (x) \cdot -\hbar^2 \nabla^2 \cdot \psi(x) \, d^3x$$

Uncertainty (rms)

$$\Delta p = [(\langle (p - \langle p \rangle)^2 \rangle)^{1/2} = [(\langle p^2 \rangle - \langle p \rangle^2)^{1/2}$$

Uncertainty relation:

These definitions of $\Delta x, \Delta p$ give:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

$$\Delta x \cdot \Delta k \geq \frac{\hbar}{2}$$

with $p = \hbar k$

The equal sign is reached with a Gaussian wave function $\psi(x) = \exp[-\frac{1}{2}(x/\sigma)^2]$

Other wave functions have larger uncertainty products. For some of the examples below the integrals actually diverge and one has to resort to other definitions (labeled $\delta x, \delta p$).

Similarly for energy and time:

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

$$\Delta \omega \cdot \Delta t \geq \frac{\hbar}{2}$$

with $E = \hbar \omega$

$\Delta k, \Delta \omega$ are the widths of the $k, \omega$ distributions that are required to obtain a wave packet of length $\Delta x, \Delta t$. When $\Delta x, \Delta t$ become smaller, the distribution of frequencies $\Delta k, \Delta \omega$ in the wave packet becomes larger. This is a general property of waves, which can be quantified by taking a Fourier transform.
Fourier Transform

Real Space $x$:

Expansion of $f(x)$ into waves:

\[
f(x) = \frac{1}{(2\pi)^{1/2}} \int F(k) \exp(+i k x) \, dk
\]

\[
\exp(i z) = \cos(z) + i \sin(z)
\]

Small in $x$

Delta function: $f(x) = \delta(x)$

"Particle" limit: Position $x$ defined

Large in $x$

Plane wave: $f(x) = (2\pi)^{-1/2} \exp(i k_0 x)$

"Wave" limit: Position $x$ uncertain

Reciprocal Space $k$:

Define the Fourier transform $F(k)$:

\[
F(k) = \frac{1}{(2\pi)^{1/2}} \int f(x) \exp(-i k x) \, dx
\]

Large in $k$

Constant: $F(k) = (2\pi)^{-1/2}$

Momentum $hk$ defined

Small in $k$

Delta function: $F(k) = \delta(k-k_0)$

Momentum $hk$ uncertain

Examples

1. Gaussian (Ground state of the harmonic oscillator)

\[
f(x) = \exp\left[-\frac{1}{2}(x/\sigma_x)^2\right] \propto \psi(x)
\]

\[
f(x)^2 = \exp\left[-(x/\sigma_x)^2\right] \propto |\psi(x)|^2 = p(x)
\]

\[
F(k) = \sigma_x \cdot \exp\left[-\frac{1}{2}(k/\sigma_k)^2\right]
\]

\[
F(k)^2 = \sigma_x^2 \cdot \exp\left[-(k/\sigma_k)^2\right] \propto P(k)
\]

Standard deviation: $\sigma_x \cdot \sigma_k = 1$

Uncertainty relation: $\Delta x \cdot \Delta k = \frac{1}{2}$ ($\Delta x = \sigma_x/\sqrt{2}, \Delta k = \sigma_k/\sqrt{2}$)

2. Finite wave train (Resolution of a grating or crystal monochromator)

\[
f(x) = \exp(i k_0 x) \quad -a \leq x \leq +a
\]

\[
F(k) = (2/\pi)^{1/2} \sin[(k-k_0)a] / (k-k_0)
\]

\[
\delta x \cdot \delta k = \pi
\]
A wave of length $N \cdot \lambda$ produces a spectral resolution $\delta k/k_0 = 1/N = 1/(n \cdot m)$ where $n$ is the number of diffracting objects (grating lines, lattice planes) and $m$ the diffraction order (phase shift $m \cdot \lambda$ between adjacent lines or lattice planes).

3. Lorentzian  (Damped oscillator, finite mean free path)
This describes the spectral line width produced by a finite decay time. The spatial analog is the momentum broadening produced by a finite mean free path. For calculating the quantum mechanical uncertainty one has to take the square of the wave function in real and reciprocal space.

\[ f(t) = \exp[-i\omega_0 t - t/\tau'] \quad t \geq 0 \quad \tau' = 2\tau \quad F(\omega) = i (2\pi)^{-1/2} \cdot [\omega - \omega_0 + i/\tau']^{-1} \]
\[ |f(t)|^2 = \exp[-t/\tau] \quad |F(\omega)|^2 = (2\pi)^{-1} \cdot [(\omega - \omega_0)^2 + (\Gamma/2)^2]^{-1} \]

Defining $\delta \omega = \Gamma$, $\delta t = \tau$:
\[ \delta \omega \cdot \delta t = 1 \]

Linewidth $\delta E$ versus Lifetime $\tau$ : (multiply by $h$)
\[ \delta E = h / \tau \]

Momentum Broadening $\delta p$ vs. Pathlength $l$:
\[ \delta p = h / l \]

\[ \omega = 2\pi f \quad = \text{angular frequency} \]
\[ k = 2\pi / \lambda \quad = \text{wave vector} \]
\[ E = h \omega \quad = \text{energy (Planck)} \]
\[ p = h k \quad = \text{momentum (de Broglie)} \]