Wave Packets: An Example

Consider the following function

\[ f(x) = \left( \frac{2a}{\pi} \right)^{1/4} e^{-ax^2} \]

This is a normalized Gaussian function (please verify!)

Note that the function value becomes less than \( 1/e = 0.368 \) of its peak value for \( x < -1/\sqrt{a} \) and \( x > 1/\sqrt{a} \).
Example

This function can be used to represent a particle. In principle, the particle can be anywhere between $-\infty$ and $\infty$ and the probability for the particle to appear at $x$ is given by the square of the above function,

$$|\psi(x)|^2 = \sqrt{\frac{2a}{\pi}} e^{-2ax^2}$$

Note again that $|\psi(x)|^2 < (1/e)^2 \approx 13.6\%$ of its peak value for $|x| > 1/\sqrt{a}$. 
Example

The total probability for the particle to be in region $[-1/\sqrt{a}, 1/\sqrt{a}]$ is given by

$$p_1 = \int_{-1/\sqrt{a}}^{1/\sqrt{a}} |\psi(x)|^2 \, dx = \sqrt{\frac{2a}{\pi}} \int_{-1/\sqrt{a}}^{1/\sqrt{a}} e^{-2ax^2} \, dx$$

while the particle has the following chance of $1 - p_1$ to be outside this region.

It can be shown by direct evaluation of the above integral that the particle will have probability of about 95% to be in the region bounded by $[-1/\sqrt{a}$ and $1/\sqrt{a}]$.

The probability for the particle to be in the region $[-1/\sqrt{a}, 1/\sqrt{a}]$ is also given by the area under the curve of $|\psi(x)|^2$, bounded by $[-1/\sqrt{a}$ and $1/\sqrt{a}]$. It is obvious from the graph that the particle will be in this region most of the time. Therefore, $1/\sqrt{a}$ can be used to represent the size of the particle.
Example

The Fourier transform of the function is defined by

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

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

We now evaluate $\bar{\psi}(k)$.

$$\bar{\psi}(k) = \frac{1}{\sqrt{2\pi}} \left( \frac{2a}{\pi} \right)^{1/4} \int_{-\infty}^{\infty} e^{-ax^2 - ikx} \, dx$$

Write the exponent in a complete square

$$-ax^2 - ikx = -a \left( x + \frac{ik}{2a} \right)^2 - \frac{k^2}{4a}$$

$$\bar{\psi}(k) = \frac{1}{\sqrt{2\pi}} \left( \frac{2a}{\pi} \right)^{1/4} e^{-k^2/(4a)} \int_{-\infty}^{\infty} e^{-a[x+ik/(2a)]^2} \, dx$$
Example

To evaluate this integral, you can then make a variable substitution such as \( q = x + \frac{ik}{2a} \). The final integral involves complex variable. You will learn in mathematical methods (complex variable and function), if you have not encountered before, that this particular integral actually can be done along the real axis. The result of the integral is the same as what you get when you just ignore the imaginary part in the exponent.

\[
\int_{-\infty}^{\infty} e^{-a[x+ik/(2a)]^2} \, dx = \sqrt{\frac{\pi}{a}}
\]

Therefore

\[
\bar{\psi}(k) = \left( \frac{1}{2\pi a} \right)^{1/4} e^{-k^2/(4a)}
\]
Example

\[ \tilde{\psi}(k) = \left( \frac{1}{2\pi a} \right)^{1/4} e^{-k^2/(4a)} \]

\( \tilde{\psi} \) is a Gaussian function of \( k \) and its width is given by \( 4\sqrt{a} \).
Conclusion

- $e^{ikx}$ is a plane wave with wave vector $k$. The function $\psi(x) = e^{-ax^2}$ (and any function) can be obtained by superposition of plane waves.

- Because $\psi(x)$ is non-periodic, an infinite number of plane waves are required in order to represent the function exactly.

- The contribution of the plane wave $e^{ikx}$ is given by $|\psi|^2$ (spectrum).

- If $\psi(x)$ is wave packet representing a particle, the characteristic size of the particle is $1/\sqrt{a}$.

- $p = \hbar k$ represents possible values of the momentum of the particle. The probability for the particle to have a momentum of $\hbar k$ is given by $|\tilde{\psi}(k)|^2$. 
Conclusion

Another very important observation from this example is that the spreading of the particle in real space is given by

\[ \Delta x = \frac{2}{\sqrt{a}} \]

while in the momentum space, the particle spreads over a range of

\[ \Delta p = \hbar \Delta k = 4\hbar \sqrt{a} \]

The product of \( \Delta x \) and \( \Delta p \) is a constat of order \( \hbar \)

\[ \Delta x \Delta p = \frac{2}{\sqrt{a}} \frac{4\hbar \sqrt{a}}{2\pi} \sim \hbar \]

\( \implies \text{Uncertainty Principle} \)
Uncertainty Principle

\[ f(x) = \left( \frac{2a}{\pi} \right)^{1/4} e^{-ax^2} \]

\[ \tilde{\psi}(k) = \left( \frac{1}{2\pi a} \right)^{1/4} e^{-k^2/(4a)} \]

The \( a \) value of the red curve is 4 times the \( a \) value of the blue curve.
Combination of Quantum States

Sound waves and light waves in classical physics obey the combination principle: linear combination of two waves $\phi_1$ and $\phi_2$, $c_1\phi_1 + c_2\phi_2$ is also a wave.

Quantum states can be combined similarly. For example, in a double slit experiment, if $\Psi_1$ represents the wave passing through the upper slit, $\Psi_2$ represents the wave passing through the lower slit, and $\Psi$ represents the quantum state at a point on the detecting screen, then $\Psi = c_1\Psi_1 + c_2\Psi_2$, where $c_1$ and $c_2$ are complex numbers.

In general, if $\Psi_1$ and $\Psi_2$ are two possible states of a system, then their linear combination

$$c_1\Psi_1 + c_2\Psi_2$$

($c_1, c_2$ are complex)

is also a possible state of the system.
Combination of Quantum States

The linear combination of quantum states implies that when a particle is in a state given by
\[ \Psi = c_1 \Psi_1 + c_2 \Psi_2, \]
the particle is in both state \( \Psi_1 \) and \( \Psi_2 \).

For example, the probability at a point on the detecting screen in a double slit experiment is given by

\[
|\Psi|^2 = |c_1 \Psi_1 + c_2 \Psi_2|^2 = (c_1^* \Psi^*_1 + c_2^* \Psi^*_2)(c_1 \Psi_1 + c_2 \Psi_2) = |c_1 \Psi_1|^2 + |c_2 \Psi_2|^2 + c_1^* c_2 \Psi^*_1 \Psi_2 + c_1 c_2^* \Psi_1 \Psi^*_2
\]

In the above, \( c_1 |\Psi_1|^2 \) is the probability for particle to reach the point on the screen by going through the upper slit, \( c_2 |\Psi_2|^2 \) is the probability for particle to reach the point on the screen by going through the lower slit, \( c_1^* c_2 \Psi^*_1 \Psi_2 \) and \( c_1 c_2^* \Psi_1 \Psi^*_2 \) are due to their interference which produces the diffraction pattern. Note that \( |\Psi|^2 \neq c_1 |\Psi_1|^2 + c_2 |\Psi_2|^2 \).
Combination of Quantum States

In general, a quantum state $\Psi$ may be a linear combination of many other states, $\Psi_1, \Psi_2, \cdots, \Psi_n, \cdots$, i.e.

$$\Psi = c_1 \Psi_1 + c_2 \Psi_2 + \cdots + c_n \Psi_n + \cdots = \sum_n c_n \Psi_n$$

Here $c_1, c_2, \cdots, c_n, \cdots$ are complex numbers.

If $\Psi_1, \Psi_2, \cdots, \Psi_n, \cdots$ are states of a given system, their linear combination $\Psi$ is also a state of the system. If the system is in the state $\Psi$, it is partially in states $\Psi_1, \Psi_2, \cdots, \Psi_n, \cdots$. 
Electron Diffraction

After reflection from the crystal surface, an electron can travel with any momentum \( \vec{p} \). The wave function for a given \( \vec{p} \) is a plane wave,

\[
\Psi_p(\vec{r}, t) = Ae^{i(\vec{p} \cdot \vec{r} - Et)/\hbar}
\]

The wave function describing the entire system is then a linear combination of states with different momenta

\[
\Psi(\vec{r}, t) = \sum_{\vec{p}} c(\vec{p}) \Psi_p(\vec{r}, t)
\]

The interference of these waves produces the observed diffraction pattern.
General Wave Function

The above can be generalized to any wave function \( \Psi(\mathbf{r}, t) \). Any wave function \( \Psi(\mathbf{r}, t) \) can be considered as a linear combination of plane waves of different momenta, \( i.e. \)

\[
\Psi(\mathbf{r}, t) = \frac{1}{(2\pi \hbar)^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{\Psi}(\mathbf{p}, t)e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} d\mathbf{p}_x d\mathbf{p}_y d\mathbf{p}_z
\]

\[
\tilde{\Psi}(\mathbf{p}, t) = \frac{1}{(2\pi \hbar)^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi(\mathbf{r}, t)e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} d\mathbf{x} d\mathbf{y} d\mathbf{z}
\]

\( \Psi(\mathbf{r}, t) \) and \( \tilde{\Psi}(\mathbf{p}, t) \) are Fourier transform of each other. Once we know \( \Psi(\mathbf{r}, t) \), \( \tilde{\Psi}(\mathbf{p}, t) \) can be calculated using the Fourier transform and vice versa.

\( \Psi(\mathbf{r}, t) \) and \( \tilde{\Psi}(\mathbf{p}, t) \) are two different representations of the same quantum state. \( \Psi(\mathbf{r}, t) \) describes the particle using real space variables while \( \tilde{\Psi}(\mathbf{p}, t) \) does the same in terms of momentum.