Wave packets

Free Particle and Wave Packets

- Let's consider firstly a freely propagating particle not interacting with anything (and any potential)

- In classical mechanics we know that the particle is moving with constant velocity v and conserving the momentum p=mv and kinetic energy $K=mv^2/2$

- In quantum mechanics we know that the states of this particle must satisfy the S.E. with potential V=0

$$i\hbar \frac{\delta \Psi(\mathrm{r},t)}{dt} = -\frac{\hbar^2}{2m}\nabla^2 \Psi(\mathrm{r},t)$$

Free Particle and Wave Packets

$$i\hbar \frac{\delta\Psi(\mathrm{r},t)}{dt} = -\frac{\hbar^2}{2m}\nabla^2 \Psi(\mathrm{r},t)$$

- We have seen that stationary states of the S.E. and thus of this free particle are:

$$\Psi(\mathrm{r},t) = \mathrm{e}^{-\mathrm{i}\, E_p\, t/\hbar}\ \psi_p$$

Must be an eigenvector of he t.i.S.E.

Free Particle and Wave Packets

$$\Psi(\mathrm{r},t) = \mathrm{e}^{-\mathrm{i}\,E_p\,t/\hbar}\;\psi_p$$

It is evident that: $E_p = \dfrac{p^2}{2m}$ as in expected from classical mechanics

In 1D we can also write:

$$i\hbar\frac{\delta\Psi(\mathrm{x},t)}{dt} = \left[-\frac{\hbar^2}{2m}\frac{\delta}{dx}^2\right]\Psi(\mathrm{x},t)$$

With:

$$\psi(x,t) = \sqrt{\frac{1}{2\pi\hbar}}\,\mathrm{e}^{\mathrm{i}(kx - E_p\,t/\hbar)}$$

Free Particle and Wave Packets

According to de Broglie hypothesis, corresponds to motion of a free particle and is described by a plane-wave

$$\psi(x,t) = \psi_0 \, e^{i(kx-\omega t)}$$

$$p = \frac{h}{\lambda}$$

$$\lambda = 2\pi/k = \frac{h}{p}$$

$$p = \hbar k$$

$$k = p/\hbar$$

Free Particle and Wave Packets

We can also write the w.f.:

$$\psi(x,t) = \sqrt{\frac{1}{2\pi\hbar}}\, e^{\mathbf{i}(kx - E_p t/\hbar)}$$

with:

$$\psi(x,t) = \sqrt{\frac{1}{2\pi\hbar}}\, e^{i(\boldsymbol{p}\boldsymbol{x} - E_p t)/\hbar}$$

And, it is clear that by inserting the w.f. into the S.E. we get

$$E_p = \frac{p^2}{2m}$$

Free Particle and Wave Packets

According to de Broglie hypothesis, corresponds to motion of a free particle and is described by a plane-wave

$$\psi(x,t) = \psi_0 \, e^{i(kx-\omega t)}$$

$$p = \frac{h}{\lambda}$$

$$\lambda = 2\pi/k = \frac{h}{p}$$

$$p = \hbar k$$

$$k = p/\hbar$$

But, $E_p = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

and $E_p = \hbar\omega$

$$\omega = \frac{\hbar k^2}{2m}$$

Free Particle and Wave Packets

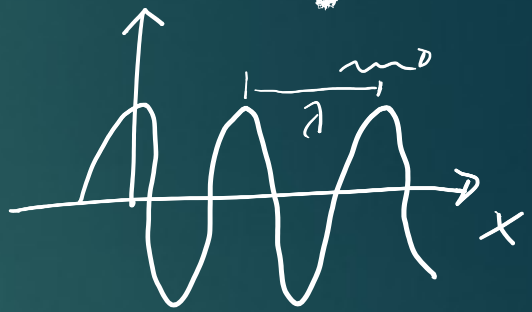
$$\psi(x,t) = \psi_0 \, e^{i(kx-\omega t)} \qquad \omega = \frac{\hbar k^2}{2m}$$

The motion of the wave is characterized by phase velocity v_p

$$v_p = \frac{\omega}{k}$$

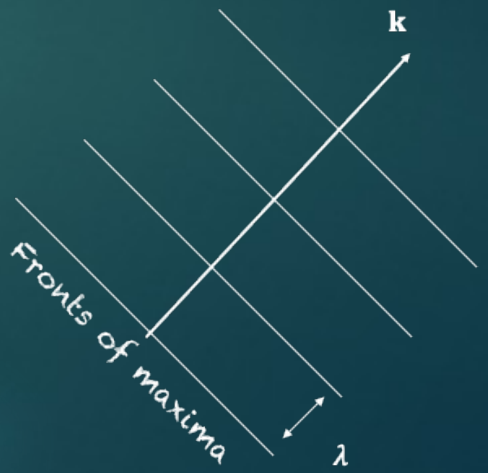
Why?

$$\Psi = A\cos(kx - \omega t)$$



After a time period T the Front will propagate for
$x = \lambda$
Thus, it's phase velocity is:

$$v_p = \frac{\lambda}{T} = \frac{2\pi/k}{2\pi/\omega} = \frac{\omega}{k}$$



Free Particle and Wave Packets

$$\psi(x,t) = \psi_0\, e^{i(kx-\omega t)}$$

$$\omega = \frac{\hbar k^2}{2m}$$

The motion of the wave is characterized by phase velocity v_p

$$v_p = \frac{\omega}{k} = \frac{\hbar k^2}{2mk} = \frac{\hbar k}{2m} = \frac{p}{2m}$$

Thus:

$$v_p = \frac{p}{2m}$$

What?

But classically the particle moves with velocity

$$v_c = \frac{p}{m}$$

Group Velocity

$$\psi(x,t) = \psi_0\, e^{i(kx-\omega t)}$$

$$v_p = \frac{p}{2m} \qquad v_c = \frac{p}{m}$$

To overcome this problem, it was suggested that the actual states of a particle are not represented by stationary states but by their superposition, so-called wave-packet.

The stationary states are uniform in space and time, thus it is not meaningful to discuss any movement associated with them.

But, the wave-packet is (quite) localized in space at any time.

To understand this, we have to introduce the concept of group velocity.

Group Velocity

The velocity of a wave packet or pulse is the "group velocity".

$$v_g = \frac{d\omega}{dk}$$

To understand this, let's consider a total wave made up out of a superposition of two waves:

$$\psi(x,t) = e^{i[(k+\partial k)x-(\omega+\partial\omega)t]} + e^{i[(k-\partial k)x-(\omega-\partial\omega)t]}$$

Both propagating to the right, *one at frequency* $\omega+\delta\omega$*, with a wavevector* $k+\delta k$*, and one at a frequency* $\omega-\delta\omega$ *and a wavevector* $k-\delta k$*.*

Group Velocity

To understand this, let's consider a total wave made up out of a superposition of two waves:

$$\psi(x,t) = e^{i[(k+\partial k)x-(\omega+\partial\omega)t]} + e^{i[(k-\partial k)x-(\omega-\partial\omega)t]}$$

We can rewrite it as:

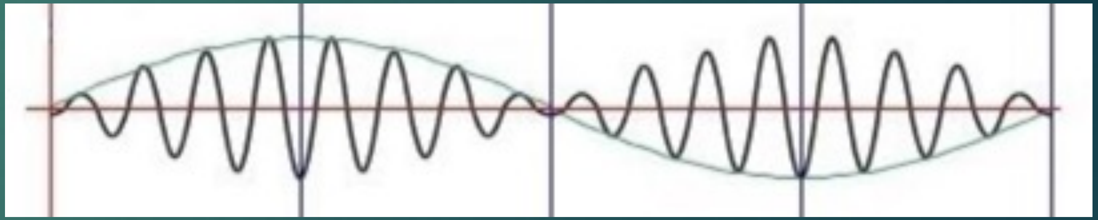
$$\psi(x,t) = 2\cos(\partial\omega\, t - \partial k\, x)\, e^{i(kx-\omega t)}$$

Which can be seen as a wave:

$e^{i(kx-\omega t)}$

Modulated by an envelope,

$\cos(\partial\omega\, t - \partial k\, x)$



Which is moving at a group velocity:

$v_g = \frac{\partial\omega}{\partial k}$ or in the limit of very small $\partial\omega$ and ∂k $v_g = \frac{d\omega}{dk}$

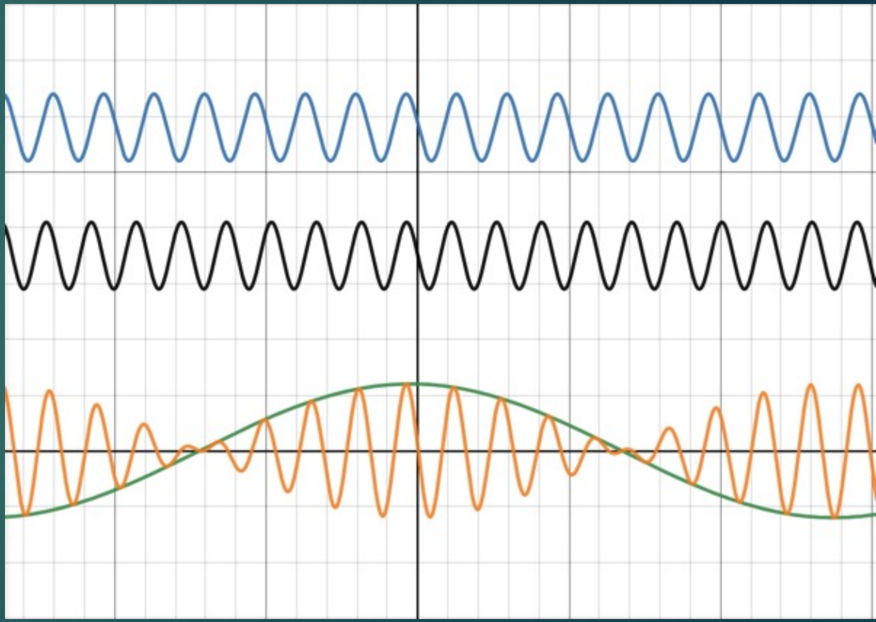
Group Velocity

To understand this, let's consider a total wave made up out of a superposition of two waves:

$$\psi(x,t) = e^{i[(k+\partial k)x-(\omega+\partial\omega)t]} + e^{i[(k-\partial k)x-(\omega-\partial\omega)t]}$$

We can rewrite it as:

$$\psi(x,t) = 2\cos(\partial\omega\, t - \partial k\, x)\, e^{i(kx-\omega t)}$$



Which can be seen as a wave:

$e^{i(kx-\omega t)}$

Modulated by an envelope,

$\cos(\partial\omega\, t - \partial k\, x)$

Which is moving at a group velocity:

$v_g = \frac{\partial\omega}{\partial k}$ or in the limit of very small $\partial\omega$ and ∂k $v_g = \frac{d\omega}{dk}$

Group Velocity and dispersion

For waves in free space, the velocity of the waves does not depend substantially on the frequency so

$d\omega / dk = \omega / k$

Thus, phase and group velocities are equal.

When ω is not proportional to k, we have "dispersion", e.g.,

Medium in which the refractive index changes quite rapidly with frequency

In waveguides, different modes propagate with different velocities, so there is dispersion from the geometry of the structure.

Group Velocity for free electrons

For a particle such as an electron,
phase velocity and group velocity of associated waves are almost never the same.

We have seen that from the t.i.S.E. we can derive:

$$\omega = \frac{\hbar k^2}{2m}$$

Thus: $\omega \propto k^2$
and..
the frequency ω is not proportional to the wavevector k
and..
the propagation of the electron wave is always highly dispersive.

Group Velocity for free electrons

For a particle such as an electron,
phase velocity and group velocity of associated waves are almost never the same.

We have seen that from the t.i.S.E. we can derive:

$$\omega = \frac{\hbar k^2}{2m}$$

In fact:

$$v_g = \frac{d\omega}{dk} = \frac{d}{dk}\frac{\hbar k^2}{2m} = \frac{\hbar k}{m} = \frac{p}{m}$$

or

$$E = \frac{1}{2} m {v_g}^2$$

As expected classically!

Free propagating wave packet

For particles such as electrons we need a description in terms of propagation as a superposition of waves

Let's remember the Fourier Th.

$$\psi(x,t) = \int_{-\infty}^{\infty} \bar{\psi}(k)\, e^{i(kx-\omega t)}\, dk$$

If we consider the w.f. at t=0

$$\psi(x,0) = \int_{-\infty}^{\infty} \bar{\psi}(k)\, e^{ikx}\, dk$$

With

$$\bar{\psi}(\mathrm{k}) \propto \int_{-\infty}^{\infty} \psi(\mathrm{x},0)\, e^{-i\mathrm{kx}}\, \mathrm{dx}$$

Motion of a Gaussian wave packet

There are many form of linear superposition that could give a wavepacket.

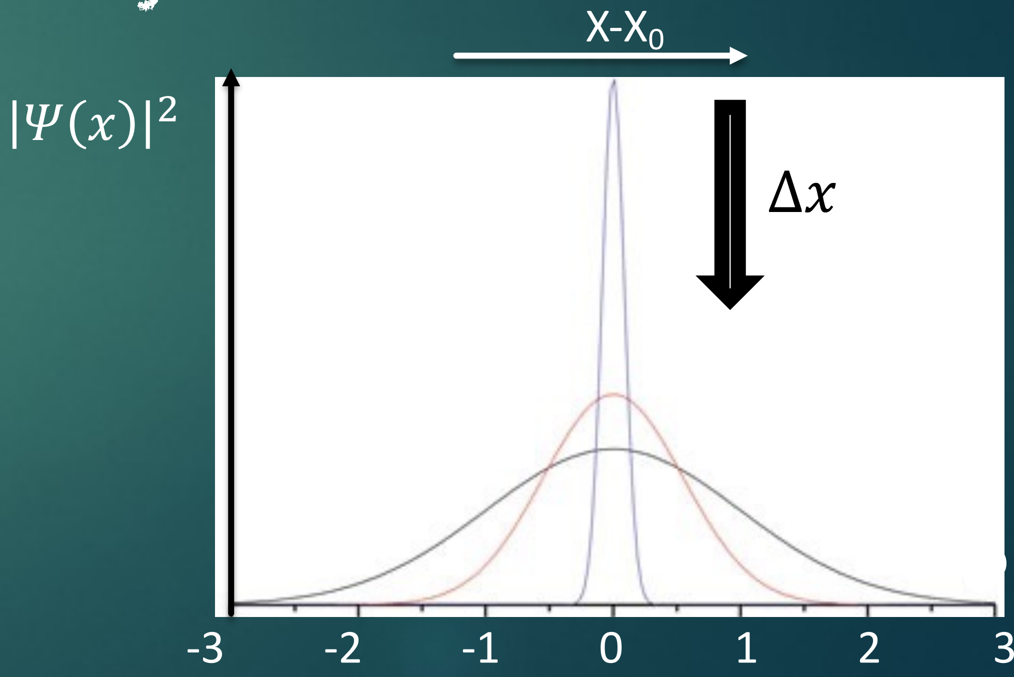
Let's introduce a particular w.f. with a probability distribution called Gaussian distribution

Then, the initial state is represented by the normalized wave function, where the amplitude of the plane wave is modulated by the Gaussian function, and it is called wave-packet:

$$\psi(x,0) = \frac{1}{\sqrt{\Delta x\sqrt{2\pi}}} e^{\left[i k_0 x - \frac{(x-x_0)^2}{4(\Delta x)^2}\right]}$$

With a probability density:

$$|\psi(x,0)|^2 \propto \exp\left[-\frac{(x-x_0)^2}{2(\Delta x)^2}\right]$$



Motion of a Gaussian wave packet

Then, the initial state is represented by the normalized wave function, where the amplitude of the plane wave is modulated by the Gaussian function:

$$\psi(x,0) = \frac{1}{\sqrt{\Delta x\sqrt{2\pi}}} e^{\left[\mathrm{i} k_0 x - \frac{(x-x_0)^2}{4(\Delta x)^2}\right]}$$

By exploiting the Fourier Th:

$$\bar{\psi}(k) \propto \mathrm{e}^{-\mathrm{i}(k-k_0)x_0} \int_{-\infty}^{\infty} exp\left[-\mathrm{i}(k-k_0)(x-x_0) - \frac{(x-x_0)^2}{4(\Delta x)^2}\right] dx$$

Fourier Theorem

$$\psi(x,0) = \int_{-\infty}^{\infty} \bar{\psi}(k)\, \mathrm{e}^{\mathrm{i}kx}\, dk$$

$$\bar{\psi}(\mathrm{k}) \propto \int_{-\infty}^{\infty} \psi(\mathrm{x},0)\, \mathrm{e}^{-\mathrm{i}kx}\, \mathrm{dx}$$

Wich can be reduced to:

$$\bar{\psi}(k) \propto \mathrm{e}^{-\mathrm{i}kx_0} \int_{-\infty}^{\infty} \exp(-\mathrm{i}\beta y - y^2)\, dy$$

With $y = \frac{x-x_0}{2\Delta x}$

and $\beta = 2(k-k_0)\Delta x$

Motion of a Gaussian wave packet

Then, the initial state is represented by the normalized wave function, where the amplitude of the plane wave is modulated by the Gaussian function:

$$\psi(x,0) = \frac{1}{\sqrt{\Delta x\sqrt{2\pi}}} e^{\left[i k_0 x - \frac{(x-x_0)^2}{4(\Delta x)^2}\right]}$$

By exploiting the Fourier Th:

$$\bar{\psi}(k) \propto e^{-i k x_0} \int_{-\infty}^{\infty} \exp(-i\beta y - y^2)\, dy$$

Introducing: $y_0 = -i\beta/2$

$$\exp(2yy_o - y^2) = \exp(y_o{}^2)\exp[-(y_o - y)^2]$$

$$-y_0^2 - y^2 + 2yy_o$$

Motion of a Gaussian wave packet

Then, the initial state is represented by the normalized wave function, where the amplitude of the plane wave is modulated by the Gaussian function:

$$\psi(x,0) = \frac{1}{\sqrt{\Delta x\sqrt{2\pi}}} e^{\left[i k_0 x - \frac{(x-x_0)^2}{4(\Delta x)^2}\right]}$$

Thus:

$$\rightarrow \bar{\psi}(k) \propto e^{-i k x_0} \; e^{y_0^2} \int_{-\infty}^{\infty} e^{-(y-y_0)^2} dy$$

With:

$$y - y_0 = z$$

$$\bar{\psi}(k) \propto e^{-i k x_0} \; e^{y_0^2} \int_{-\infty}^{\infty} e^{-z^2} dz$$

$$= \sqrt{\pi}$$

Motion of a Gaussian wave packet

Then, the initial state is represented by the normalized wave function, where the amplitude of the plane wave is modulated by the Gaussian function:

$$\psi(x,0) = \frac{1}{\sqrt{\Delta x\sqrt{2\pi}}} e^{\left[i k_0 x - \frac{(x-x_0)^2}{4(\Delta x)^2}\right]}$$

Thus:

$$\bar{\psi}(k) \propto e^{-i k x_0} \; e^{y_0^2} \int_{-\infty}^{\infty} e^{-z^2} dz$$

$$\bar{\psi}(k) \propto e^{-i k x_0 - (k-k_0)^2 (\Delta x)^2}$$

$$y_0 = -i\frac{\beta}{2} = -i(k-k_0)\Delta x$$

Finally

$$\bar{\psi}(k) \propto e^{\left[i k x_0 - \frac{(k-k_0)^2}{4(\Delta k)^2}\right]}$$

With:

$$\Delta k = \frac{1}{2\Delta x}$$

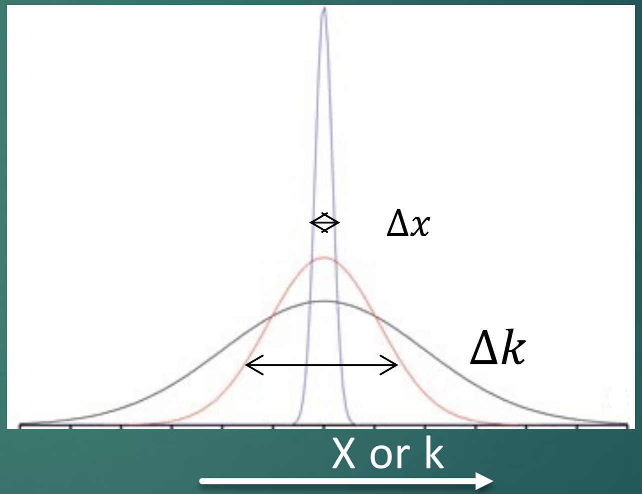
Motion of a Gaussian wave packet

Then, the initial state is represented by the wave-packet:

$$\psi(x,0) = \frac{1}{\sqrt{\Delta x\sqrt{2\pi}}} e^{\left[\mathrm{i}\, k_0\, x - \frac{(x-x_0)^2}{4\,(\Delta x)^2}\right]}$$

Its Fourier Transform is $\bar{\psi}(k) = \frac{1}{\sqrt{\Delta k\sqrt{2\pi}}} e^{\left[\mathrm{i}\, k\, x_0 - \frac{(k-k_0)^2}{4\,(\Delta k)^2}\right]}$

With $\Delta x\, \Delta k = \frac{1}{2}$



This illustrates an important property of wave-packets:
if we wish to construct a packet that is very localized in x-space (i.e., if Δx is small) then we need to combine plane-waves with a very wide range of different k-values (i.e., Δk will be large), and the way around is also true.

Motion of a Gaussian wave packet

So far, we have considered the wave-packet at t=0.
Let's consider now the time evolution of the wavefunction:

$\psi(x,t) = \int_{-\infty}^{\infty} \bar{\psi}(k)\, e^{i\phi(k)}\, dk,$ with $\phi(k) = k\,x - \omega(k)\,t$

$|\bar{\psi}(k)|$ is strongly peaked around $k=k_0$, thus, it is reasonable to Taylor expand $\phi(k)$ about k_0, and by doing so one can show that:

$$\psi(x,t) \propto \frac{\exp\left[i\,(k_0\,x - \omega_0\,t) - \left(x - x_0 - v_g\,t\right)^2 \{1 - i\,2\,\alpha\,(\Delta k)^2\,t\}/(4\,\sigma^2)\right]}{[1 + i\,2\,\alpha\,(\Delta k)^2\,t]^{1/2}}$$

With:

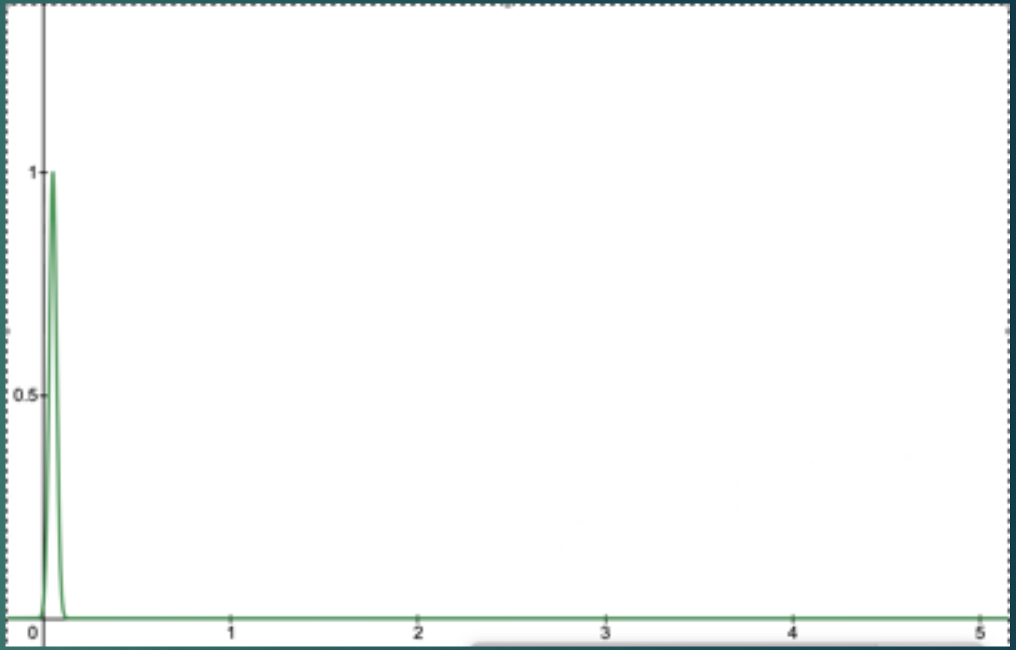
$$\omega_0 = \omega(k_0), \quad v_g = \frac{d\omega(k_0)}{dk}, \quad \alpha = \frac{d^2\omega(k_0)}{dk^2}, \quad \sigma(t) = \sqrt{(\Delta x)^2 + \frac{\alpha^2\,t^2}{4\,(\Delta x)^2}}$$

Motion of a Gaussian wave packet

In fact, the probability distribution is still a Gaussian with characteristic width $\sigma(t)$:

$$|\psi(x,t)|^2 \propto \sigma^{-1}(t)\exp\left[-\frac{(x-x_0-v_g\,t)^2}{2\,\sigma^2(t)}\right]$$

$$\sigma(t) = \sqrt{(\Delta x)^2 + \frac{\alpha^2 t^2}{4\,(\Delta x)^2}}$$



You may notice the time dependence of the characteristic width;
thus, the width of our wave-packet grows as time progresses

Motion of a Gaussian wave packet

In fact, the probability distribution is still a Gaussian with characteristic width σ(t) :

$$|\psi(x,t)|^2 \propto \sigma^{-1}(t)\exp\left[-\frac{(x-x_0-v_g t)^2}{2\sigma^2(t)}\right]$$

$$\sigma(t) = \sqrt{(\Delta x)^2 + \frac{\alpha^2 t^2}{4(\Delta x)^2}} \qquad \alpha = \frac{d^2\omega(k_0)}{dk^2}$$

Note that the rate of spreading of a wave-packet depends on the second derivative of $\omega(k)$ with respect to k

This explains why a functional relationship between ω and k is generally known as a dispersion relation: it determines how fast wave-packets grows with time.

Free Particle and Wave Packets

In fact, the probability distribution is still a Gaussian with characteristic width σ(t) :

$$|\psi(x,t)|^2 \propto \sigma^{-1}(t)\exp\left[-\frac{(x-x_0-v_g\,t)^2}{2\,\sigma^2(t)}\right]$$

$$\sigma(t) = \sqrt{(\Delta x)^2 + \frac{\alpha^2 t^2}{4\,(\Delta x)^2}}$$

However, when ω is a linear function of k there is no dispersion of wave-packets: wave-packets propagate without spreading.

This is the case of light waves: light propagate through a vacuum without spreading.

In fact, according to classical electromagnetism, the freq. of light is: $\omega = kc$

Free Particle and Wave Packets

In fact, the probability distribution is still a Gaussian with characteristic width σ(t) :

$$|\psi(x,t)|^2 \propto \sigma^{-1}(t)\exp\left[-\frac{(x-x_0-v_g\,t)^2}{2\,\sigma^2(t)}\right]$$

$$v_g = \frac{d\omega}{dk}$$

is known as the group-velocity.

While a plane-wave travels at the phase-velocity, $v_p = \omega/k$

a wave-packet travels at the group-velocity, $v_g = d\omega/dk$,

which is the effective uniform velocity of the particle

$$v_g = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{\mathrm{d}}{\mathrm{d}k}\frac{\hbar k^2}{2m} = \frac{\hbar k}{m} = \frac{p}{m}$$

As expected classically!

In case of linear dispersion relations, the phase-velocity and the group-velocity are identical.