Wave packet

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What is the wave packet?

In physics, a **wave packet** is a short "burst" or "envelope" of localized wave action that travels as a unit. A wave packet can be analyzed into, or can be synthesized from, an infinite set of component sinusoidal waves of different wavenumbers, with phases and amplitudes such that they interfere constructively only over a small region of space, and destructively elsewhere. Each component wave function, and hence the wave packet, are solutions of a wave equation. Depending on the wave equation, the wave packet's profile may remain constant (no dispersion) or it may change (dispersion) while propagating.
http://en.wikipedia.org/wiki/Wave_packet

1. Schrödinger equation (separation variable)

The state function for a system develops in time according to the equation

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle .$$

where $\hat{H}$ is the time-dependent Hamiltonian. The time dependent Schrödinger equation for the wavefunction $\langle \boldsymbol{r}|\psi(t)\rangle$ is given by

$$i\hbar\frac{\partial}{\partial t}\langle \boldsymbol{r}|\psi(t)\rangle = \langle \boldsymbol{r}|\hat{H}(\hat{\boldsymbol{r}})|\psi(t)\rangle = H(\boldsymbol{r})\langle \boldsymbol{r}|\psi(t)\rangle .$$

We assume that

$$\langle \mathbf{r}|\psi(t)\rangle = \varphi(\mathbf{r})T(t) , \qquad \text{(separation variable)}$$

$$i\hbar\varphi(\mathbf{r})\frac{\partial}{\partial t}T(t) = H(\mathbf{r})\varphi(\mathbf{r})T(t) ,$$

or

$$i\hbar\frac{\frac{\partial}{\partial t}T(t)}{T(t)} = \frac{H(\boldsymbol{r})\varphi(\boldsymbol{r})}{\varphi(\boldsymbol{r})} = E ,$$

where E is constant, independent of t and $\boldsymbol{r}$. Thus we get

$$i\hbar\frac{\partial}{\partial t}T(t) = E_n T(t) ,$$

$$H(\boldsymbol{r})\varphi_n(\boldsymbol{r}) = E_n\varphi_n(\boldsymbol{r}) .$$

Then we have

$$T(t) = \exp(-\frac{i}{\hbar}E_n t) ,$$

or

$$\psi_n(r,t) = \varphi_n(r)\exp(-\frac{i}{\hbar}E_n t) ,$$

where $\{\phi_n(\boldsymbol{r})\}$ (n = 1, 2, 3,…..): discrete set of eigenfunctions

2. One dimensional case

The Hamiltonian of the free particle with mass *m* is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} ,$$

The Schrödinger equation:

$$H\varphi_k = E_k\varphi_k ,$$

or

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi_k(x) = E_k\varphi_k(x) ,$$

where $\varphi_k(x)$ satisfies the second order differential equation,

$$\frac{\partial^2}{\partial x^2}\varphi_k(x) = -k^2\varphi_k(x) ,$$

where

$$E_k = \hbar\omega_k = \frac{\hbar^2 k^2}{2m} .$$

((**Plane wave solution**)):

$$\varphi_k(x) = Ae^{ikx} \qquad\qquad \psi_k(x) = Ae^{i(kx-\omega_k t)}$$

where A is constant. The phase velocity is defined as

$$v_p = \frac{E_k}{\hbar k} = \frac{\hbar k}{2m} = \frac{p}{2m}.$$

The group velocity is defined by

$$v_g = \frac{1}{\hbar}\frac{\partial E_k}{\partial k} = \frac{\partial \omega_k}{\partial k} = \frac{\hbar k}{m} = \frac{p}{m},$$

which is different from the phase velocity. Note that $|\psi_k(x,t)|^2 = |A|^2$, that is uniformly probable to find the particle anywhere along the x axis. The state function that better represents a classical (localized) particle is a wave packet.

3. Gaussian wave packet

A wave packet is a localized disturbance that results from the sum of many different wave forms. If the packet is strongly localized, more frequencies are needed to allow the constructive superposition in the region of localization and destructive superposition outside the region. From the basic solutions in one dimension, a general form of a wave packet can be expressed as some superposition of waves.

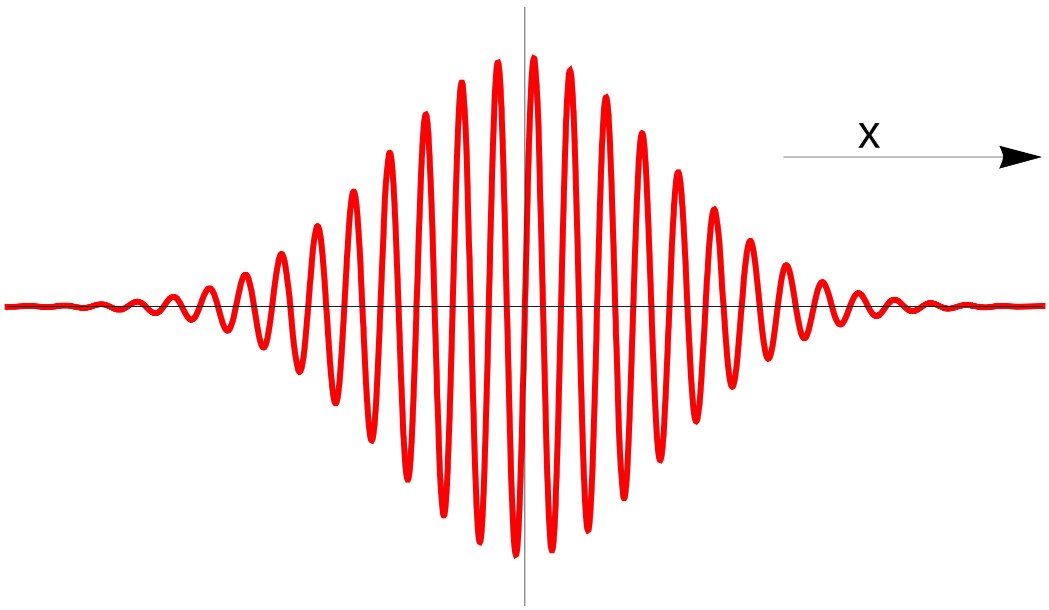


Fig. Gaussian wave packet propagating along the +x axis.

We consider the wave characterized by the wavenumber k,

$$E(k) = A\exp[ik(x - x_0) - i\omega(k)t]\, f(k).$$

where A is constant, and $f(k)$ is a Gaussian distribution function with a peak at $k = k_0$ and the width Δk,

$$f(k) = \exp[-\frac{(k-k_0)^2}{2(\Delta k)^2}].$$

If the Gaussian distribution $f(k)$ has a narrow enough peak at $k = k_0$, a good approximation is obtained by expanding $\omega(k)$ as a series of powers of $k - k_0$. This is because the main contributions to the integral come in a region of the order of the width of the peak in the Gauss distribution. Thus we obtain

$$\begin{aligned}\omega(k) &= \omega(k_0) + \frac{1}{1!}\left(\frac{\partial \omega}{\partial k}\right)_{k=k_0}(k-k_0) + \frac{1}{2!}\left(\frac{\partial^2 \omega}{\partial k^2}\right)_{k=k_0}(k-k_0)^2 + \ldots \\ &= \omega_0 + V_g(k-k_0) + \frac{1}{2!}\alpha(k-k_0)^2 + \ldots\end{aligned}$$

We set

$$\omega(k_0) = \omega_0, \qquad \left(\frac{\partial \omega}{\partial k}\right)_{k=k_0} = V_g, \qquad \left(\frac{\partial^2 \omega}{\partial k^2}\right)_{k=k_0} = \alpha .$$

For free electron with the energy dispersion $E_k = \hbar\omega_k = \frac{\hbar^2}{2m}k^2$, we have

$$V_g = \left(\frac{\partial \omega}{\partial k}\right)_{k=k_0} = \frac{\hbar k_0}{m}, \qquad \alpha = \left(\frac{\partial^2 \omega}{\partial k^2}\right)_{k=k_0} = \frac{\hbar}{m}.$$

So we get

$$\begin{aligned}E(k) &= A\exp[i(k-k_0)(x-x_0) + ik_0(x-x_0) - i\omega_0 t \\ &\quad - iV_g(k-k_0)t - \frac{i\alpha}{2}(k-k_0)^2 t - \frac{(k-k_0)^2}{2(\Delta k)^2}] \\ &= A\exp[ik_0(x-x_0) - i\omega_0 t + i(k-k_0)(x-x_0) \\ &\quad - iV_g(k-k_0)t - \frac{i\alpha}{2}(k-k_0)^2 t - \frac{(k-k_0)^2}{2(\Delta k)^2}] \\ &= A\exp[ik_0(x-x_0) - i\omega_0 t]\exp[i(k-k_0)(x-x_0-V_g t) - \frac{i\alpha}{2}(k-k_0)^2 t - \frac{(k-k_0)^2}{2(\Delta k)^2}]\end{aligned}$$

We now consider the superposition of waves defined by

$$
\begin{aligned}
E_1 &= \int_{-\infty}^{\infty} E(k)dk \\
&= A\exp[ik_0(x-x_0)-i\omega_0 t] \\
&\times \int_{-\infty}^{\infty} dk \exp[i(k-k_0)(x-x_0-V_g t)-\frac{i\alpha}{2}(k-k_0)^2 t-\frac{(k-k_0)^2}{2(\Delta k)^2}]]
\end{aligned}
$$

With $\kappa = k-k_0$, this becomes

$$
E_1 = A\exp[ik_0(x-x_0)-i\omega_0 t]\int_{-\infty}^{\infty} d\kappa \exp[i\kappa(x-x_0-V_g t)-\frac{\kappa^2}{2}(i\alpha t+\frac{1}{(\Delta k)^2})].
$$

If $\alpha = 0$, then the integral part is only a function of $x-x_0-V_g t$.
If $\alpha \neq 0$, we have

$$
\begin{aligned}
E_1 &= \int_{-\infty}^{\infty} d\kappa \exp[i\kappa(x-x_0-V_g t)-\frac{\kappa^2}{2}(i\alpha t+\frac{1}{(\Delta k)^2})] \\
&= A\exp[ik_0(x-x_0)-i\omega_0 t]\frac{\sqrt{2\pi}\exp[-\frac{(x-x_0-V_g t)(\Delta k)^2}{2(1-it\alpha(\Delta k)^2)}]}{\sqrt{\frac{1}{(\Delta k)^2}+it\alpha}}
\end{aligned}
$$

Note that we use the Mathematica to calculate the integral.

$E_1^* E_1$ is evaluated as

$$
\begin{aligned}
g_1 &= E_1^* E_{11} \\
&= \frac{2A^2\pi\exp[-\frac{1}{2}(x-x_0-V_g t)^2(\Delta k)^2\{\frac{1}{1+it\alpha(\Delta k)^2)}+\frac{1}{1-it\alpha(\Delta k)^2)}]}{\sqrt{\frac{1}{(\Delta k)^4}+t^2\alpha^2}} \\
&= \frac{2A^2\pi\exp[\frac{-(x-x_0-V_g t)^2(\Delta k)^2)}{1+t^2\alpha^2(\Delta k)^4}]}{\sqrt{\frac{1}{(\Delta k)^4}+t^2\alpha^2}}
\end{aligned}
$$

Normalization:

$$1 = \int_{-\infty}^{\infty} g_1 dx = \frac{2A^2\pi}{\sqrt{\frac{1}{\pi(\Delta k)^2}}},$$

or

$$A = \frac{1}{\sqrt{2}\pi^{3/4}\sqrt{\Delta k}}.$$

Thus we have

$$g_1 = \frac{1}{\sqrt{\pi}\Delta k}\frac{\exp[\frac{-(\Delta k)^2(x - x_0 - V_g t)^2}{1 + t^2\alpha^2(\Delta k)^4}]}{\sqrt{\frac{1}{(\Delta k)^4} + \alpha^2 t^2}}.$$

The final form of $E_1^* E_1$ is given by

$$\left|\psi(x,t)\right|^2 = E_1^* E_1 = \frac{\Delta k}{\sqrt{\pi}}\frac{\exp[\frac{-(\Delta k)^2(x - x_0 - V_g t)^2}{1 + t^2\alpha^2(\Delta k)^4}]}{\sqrt{1 + t^2\alpha^2(\Delta k)^4}},$$

which has the same form as the Gaussian distribution

$$\left|\psi(x,t)\right|^2 = \frac{1}{\sqrt{2\pi}\sigma}\exp[\frac{-(x - x_0 - V_g t)^2}{2\sigma^2}],$$

where the standard deviation σ is dependent on t and is given by

$$\sigma = \frac{1}{\sqrt{2}\Delta k}\sqrt{1 + t^2\alpha^2(\Delta k)^4}.$$

((**Mathematica**))

```
Clear["Global`*"];
f1 =
 Exp[ⅈ κ (x - x0 - Vg t) -
   κ^2/2 (ⅈ α t + 1/(Δk)^2)];

Integrate[f1, {κ, -∞, ∞}] //
 Simplify[#, Re[1/Δk^2] > Im[t α]] &
```

$$\frac{e^{\frac{i\,(t\,Vg-x+x0)^2\,\Delta k^2}{-2\,i+2\,t\,\alpha\,\Delta k^2}}\sqrt{2\,\pi}}{\sqrt{i\,t\,\alpha+\frac{1}{\Delta k^2}}}$$

4. Physical meaning of the equation for the wave packet

The position of center:

$$\langle x\rangle = x_0 + V_g t\,.$$

The velocity of center, which is called as the group velocity

$$\frac{d\langle x\rangle}{dt} = V_g = \left(\frac{\partial\omega}{\partial k}\right)_{k=k_0}.$$

The spreading of the wave packet:

$$\Delta x = \sigma = \frac{1}{\sqrt{2}\Delta k}\sqrt{1+t^2\alpha^2(\Delta k)^4}\,.$$

For times so short that $t^2\alpha^2(\Delta k)^4 << 1$, we have

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

The amplitude of $|\psi(x,t)|^2$:

$$\frac{\Delta k}{\sqrt{\pi}}\frac{1}{\sqrt{1+t^2\alpha^2(\Delta k)^4}}.$$

The evolution of the wave packet is not confined to a simple displacement at a velocity v_0. The wave packet also undergoes a deformation. The amplitude decreases with increasing t, while the width Δx increases with increasing time. Note that the peak position moves at the constant velocity along the $+x$ direction.

The Heisenberg's principle of uncertainty:

$$(\Delta x)(\Delta k) = \frac{1}{\sqrt{2}}\sqrt{1+\frac{t^2\hbar^2}{m^2}(\Delta k)^4} > \frac{1}{\sqrt{2}},$$

or

$$(\Delta x)(\Delta p) > \frac{\hbar}{\sqrt{2}} > \frac{\hbar}{2}.$$

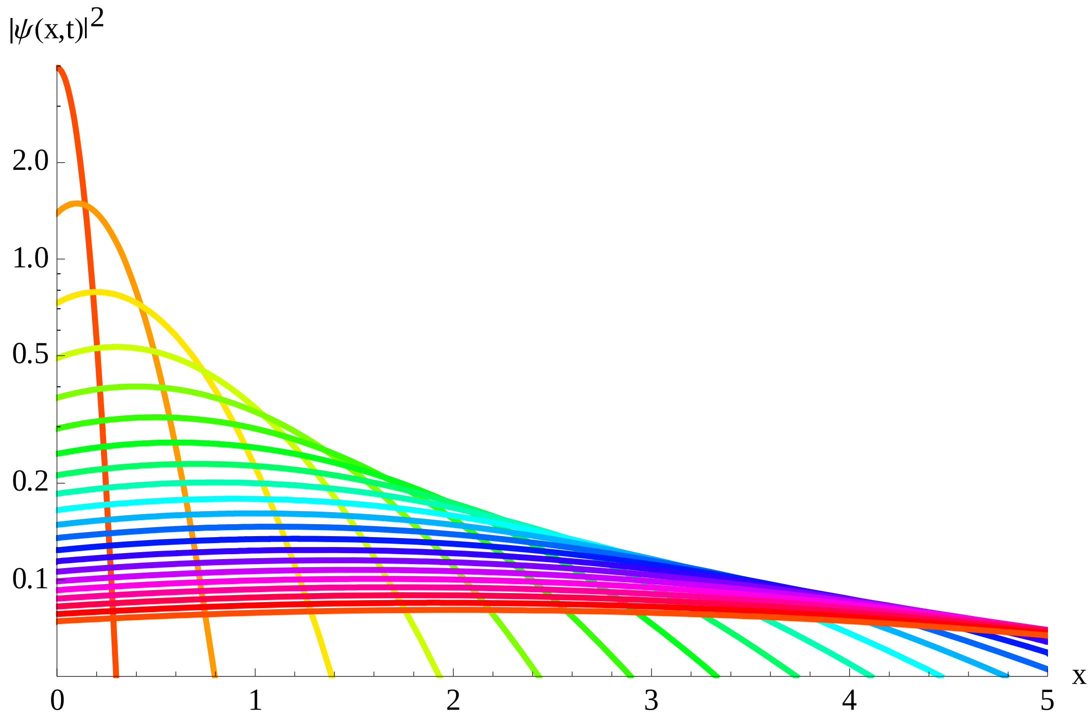


Fig. Propagation of Gaussian wave packet. Plot of $|\psi(x,t)|^2$ as a function of x. The time t is changed as a parameter; t = 0 - 1 with Δt = 0.05. m = 1. $\hbar = 1$. k_0 = 2. Δk = 7. x_0 = 0.

5. Group velocity and phase velocity

(a) Photon

The dispersion relation of photon is given by

$$E_k = \hbar\omega(k) = \hbar ck .$$

The group velocity is given by

$$V_g = \left(\frac{\partial\omega(k)}{\partial k}\right)_{k=k_0} = c ,$$

which is the same as the phase velocity,

$$V_p = \left(\frac{\omega(k)}{k}\right)_{k=k_0} = c .$$

The parameter α is given by

$$\alpha = \left(\frac{\partial^2\omega(k)}{\partial k^2}\right)_{k=k_0} = 0 .$$

(b) Free electron with mass *m*

The dispersion relation of electron is given by

$$E_k = \hbar\omega_k = \frac{\hbar^2}{2m}k^2 .$$

The group velocity is given by

$$V_g = \left(\frac{\partial\omega}{\partial k}\right)_{k=k_0} = \frac{\hbar k_0}{m} .$$

which is not the same as the phase velocity

$$V_p = \left(\frac{\omega(k)}{k}\right)_{k=k_0} = \frac{\hbar k_0}{2m}$$

The parameter α is given by

$$\alpha = \left(\frac{\partial^2 \omega}{\partial k^2}\right)_{k=k_0} = \frac{\hbar}{m}.$$

6. Simulation

Using the Mathematica, we make a plot of $|\psi(x,t)|^2$

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi}\sigma}\exp[\frac{-(x-x_0-V_g t)^2}{2\sigma^2}],$$

as a function of *t*, where the standard deviation σ is given by

$$\sigma = \frac{1}{\sqrt{2}\Delta k}\sqrt{1+t^2\alpha^2(\Delta k)^4}.$$

((**Mathematica**))

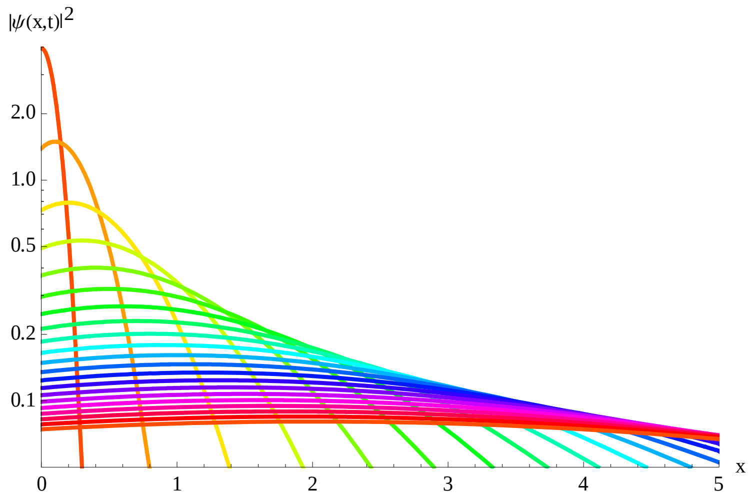
Evolution of Gaussian Wave packet Gaussian

```
Clear["Global`"];
```

$$P\psi = \frac{e^{-\frac{\Delta k^2 \left(x - x0 - \frac{k0\, t\, \hbar}{m}\right)^2}{1 + \frac{t^2 \Delta k^4 \hbar^2}{m^2}}}}{\sqrt{\pi}\, \Delta k \sqrt{\frac{1}{\Delta k^4} + \frac{t^2 \hbar^2}{m^2}}};$$

```
rule1 = {m → 1, ℏ → 1, k0 → 2, Δk → 7, x0 → 0};
seq1 = Pψ /. rule1;

p1 = LogPlot[Evaluate[Table[seq1, {t, 0, 1, 0.05}]], {x, 0, 5},
  PlotStyle → Table[{Thick, Hue[0.05 i]}, {i, 1, 20}],
  PlotRange → {{0, 5}, {0.05, 4}}, AxesLabel → {"x", "|ψ(x,t)|²"}]
```




```
Avex1 = Integrate[x Pψ, {x, -∞, ∞},
  Assumptions → {Re[m² Δk² / (m² + t² Δk⁴ ℏ²)] > 0}]
```

$$\frac{m\, x0 + k0\, t\, \hbar}{m\, \Delta k \sqrt{\frac{1}{\Delta k^4} + \frac{t^2 \hbar^2}{m^2}} \sqrt{\frac{m^2 \Delta k^2}{m^2 + t^2 \Delta k^4 \hbar^2}}}$$

REFERENCES

D. Bohm, *Quantum Theory* (Dover, 1989).
G. Auletta, M. Fortunato, and G. Parisi, *Quantum Mechanics* (Cambridge, 2009).