Wave packet

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(Date: August, 12, 2011)

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

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

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

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

2. One dimensional case

The Hamiltonian of the free particle 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

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

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

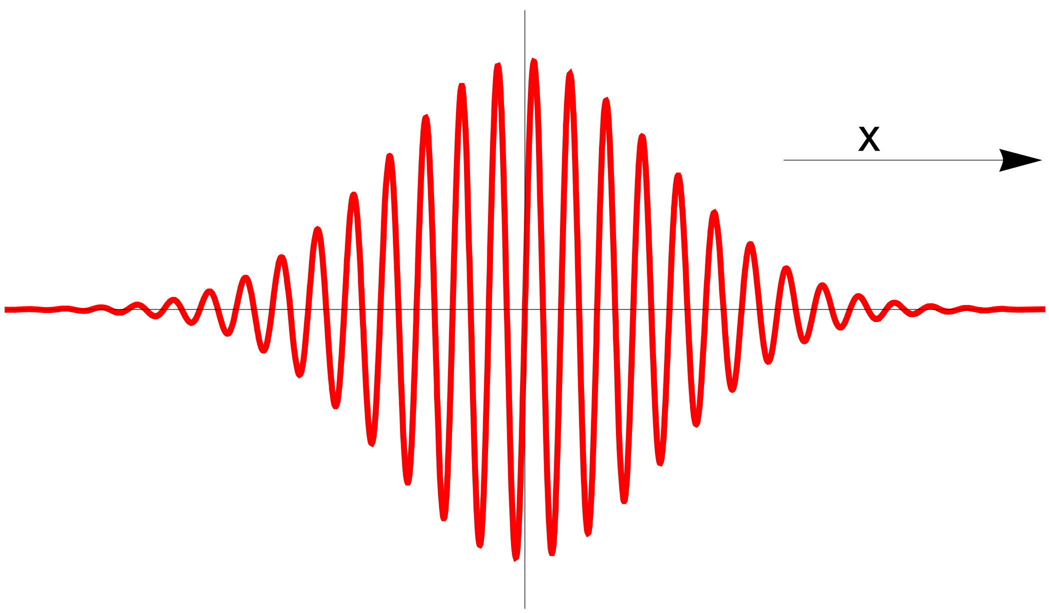


Fig. Gaussian wave packet propagating along the $+x$ axis.

We now consider the Gaussian wave packet.

$$f = A\exp[ik(x-x_0) - i\frac{\hbar^2 k^2}{2m}t]\exp[-\frac{(k-k_0)^2}{2(\Delta k)^2}].$$

The superposition of f over k leads to

$$
\begin{aligned}
f_1 &= \int_{-\infty}^{\infty} f dk \\
&= \int_{-\infty}^{\infty} A\exp[ik(x-x_0) - i\frac{\hbar^2 k^2}{2m}t]\exp[-\frac{(k-k_0)^2}{2(\Delta k)^2}]dk \\
&= \frac{A\sqrt{2\pi}\exp[\dfrac{m(x-x_0)(2ik_0-(x-x_0)(\Delta k)^2)-ik_0{}^2 t\hbar}{2(m+it(\Delta k)^2\hbar)}]}{\sqrt{\dfrac{1}{(\Delta k)^2}+\dfrac{it\hbar}{m}}}
\end{aligned}
$$

$f_1^* f_1$ is evaluated as

$$
g_1 = f_1^* f_1 = \frac{2A^2\pi\exp[\dfrac{-(\Delta k)^2(x-x_0-\dfrac{k_0 t\hbar}{m})^2}{1+\dfrac{t^2(\Delta k)^4\hbar^2}{m^2}}]}{\sqrt{\dfrac{1}{(\Delta k)^4}+\dfrac{t^2\hbar^2}{m^2}}}
$$

Normalization:

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

or

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

Thus we have

$$
g_1 = f_1^* f_1 = \frac{2A^2\pi}{\sqrt{\pi}\Delta k}\exp[\frac{-(\Delta k)^2(x-x_0-\dfrac{k_0 t\hbar}{m})^2}{1+\dfrac{t^2(\Delta k)^4\hbar^2}{m^2}}
$$

or

$$g_1 = \frac{1}{\sqrt{\pi}\Delta k}\frac{\exp[\frac{-(\Delta k)^2(x-x_0-\frac{k_0 t\hbar}{m})^2}{1+\frac{t^2(\Delta k)^4\hbar^2}{m^2}}]}{\sqrt{\frac{1}{(\Delta k)^4}+\frac{t^2\hbar^2}{m^2}}}$$

The final form of $f_1^* f_1$ is given by

$$|\psi(x,t)|^2 = f_1^* f_1 = \frac{\Delta k}{\sqrt{\pi}}\frac{\exp[\frac{-(\Delta k)^2(x-x_0-\frac{k_0 t\hbar}{m})^2}{1+\frac{t^2(\Delta k)^4\hbar^2}{m^2}}]}{\sqrt{1+\frac{t^2\hbar^2}{m^2}(\Delta k)^4}}$$

which has the same form as the Gaussian distribution

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi}\sigma}\exp[\frac{-(x-x_0-\frac{k_0 t\hbar}{m})^2}{2\sigma^2}]$$

where the standard deviation σ is given by

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

((Note)) The final form of the normalized wave function is given as

$$\psi(x,t) = \frac{(\Delta k)^{1/2}}{\pi^{1/4}}\frac{\exp[\frac{\{ik_0(x-x_0)-\frac{1}{2}(x-x_0)^2(\Delta k)^2-\frac{ik_0^{\ 2}}{2m}t\hbar\}(1-\frac{it\hbar}{m}(\Delta k)^2)}{(1+\frac{(\Delta k)^4\hbar^2}{m^2})}]}{\sqrt{1+\frac{it\hbar(\Delta k)^2}{m}}}\ .$$

((**Mathematica**))

```
Clear["Global`"];
SuperStar /: expr_* :=
 expr /. {Complex[a_, b_] :> Complex[a, -b]}
```

```
f = Exp[ⅈ k (x - x0) - ⅈ (ℏ k^2)/(2 m) t] Exp[-(k - k0)^2/(2 (Δk)^2)];
f1 =
 Integrate[f, {k, -∞, ∞},
   Assumptions → {Im[(t ℏ)/m] < Re[1/Δk^2]}] //
  Simplify
```

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

```
g1 = f1* f1 // FullSimplify
```

$$\frac{2\,e^{-\frac{\Delta k^2\,(m\,(-x+x0)+k0\,t\,\hbar)^2}{m^2+t^2\,\Delta k^4\,\hbar^2}}\,\pi}{\sqrt{\frac{1}{\Delta k^2}-\frac{i\,t\,\hbar}{m}}\,\sqrt{\frac{1}{\Delta k^2}+\frac{i\,t\,\hbar}{m}}}$$

4. Physical meaning of the equation for the wave packet

The position of center:

$$\langle x\rangle = x_0 + \frac{k_0 t\hbar}{m}.$$

The velocity of center:

$$\frac{d\langle x\rangle}{dt} = \frac{\hbar k_0}{m} = v_0 \, .$$

The spreading of the wave packet:

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

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

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

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 A 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

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

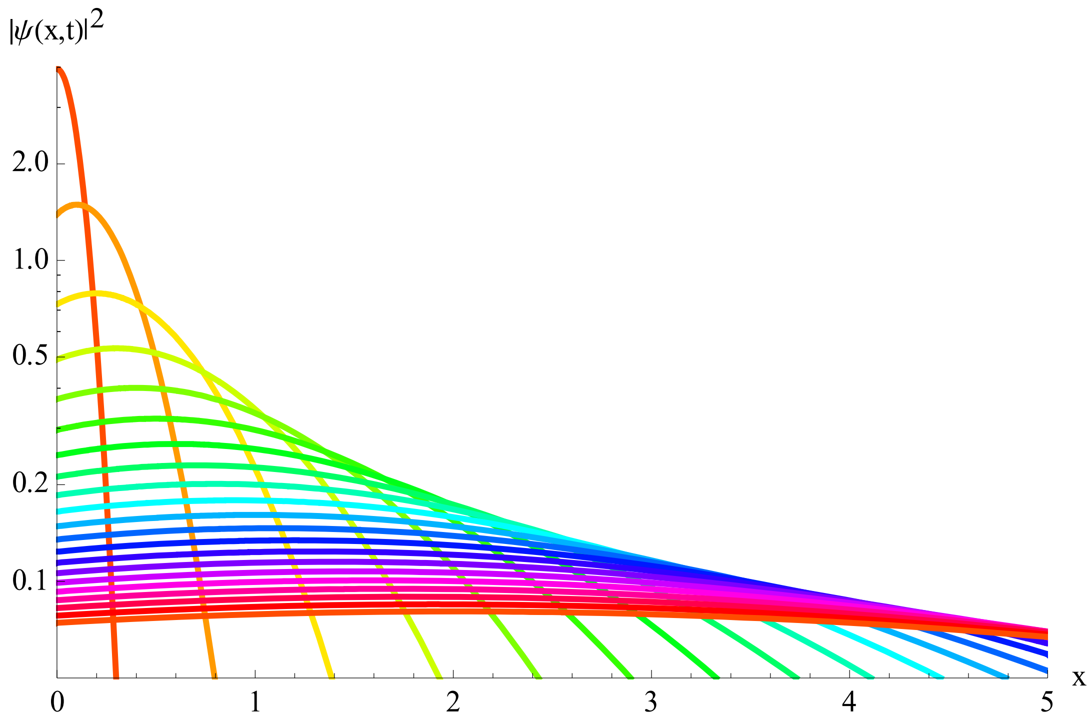


Fig. Propagation of Gaussian wave packet. Plot of $|\psi(x,t)|^2$ as a function of x. The time t is changed as a parameter; $t = 0$ - 1 with $\Delta t = 0.05$. $m = 1$. $\hbar = 1$. $k_0 = 2$. $\Delta k = 7$. $x_0 = 0$.

((**Mathematica**)) QM wavepacket

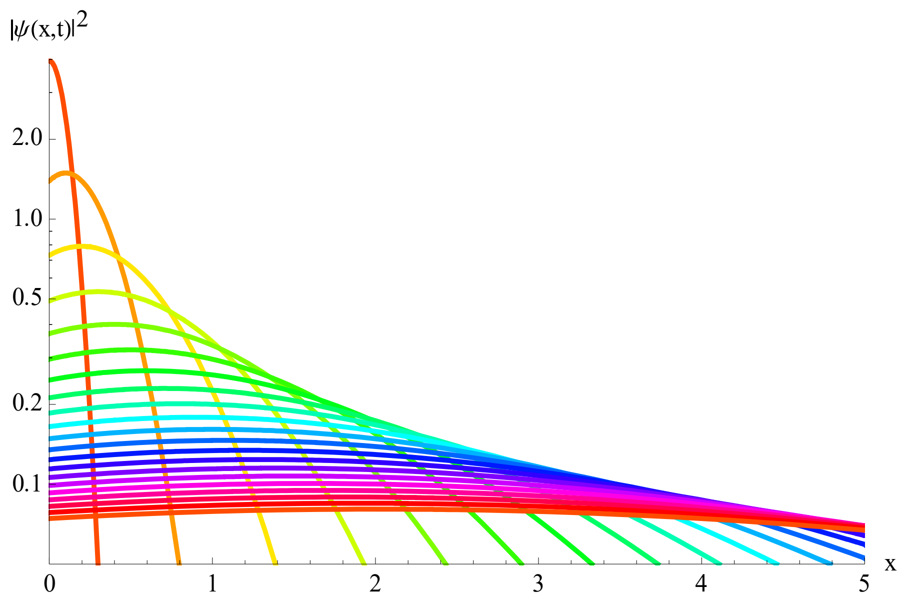
Evolution of Gaussian Wave packet Gaussian

```
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"}]
```



$$\text{Avex1} = \text{Integrate}\left[x\, P\psi,\ \{x, -\infty, \infty\},\ \text{Assumptions} \to \left\{\text{Re}\left[\frac{m^2\, \Delta k^2}{m^2 + t^2\, \Delta k^4\, \hbar^2}\right] > 0\right\}\right]$$

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

REFERENCES

D. Bohm, Quantum Theory (Dover, 1989).