Wave packet, group velocity

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1. Wave packet

If we consider a plane monochromatic wave travelling in the x direction, the wave amplitude *A* at time *t* and point *x* is

$$A(x,t) = A_0 \cos(kx - \omega t)$$

The wave number k is related to the wavelength l by

$$k = \frac{2\pi}{\lambda}$$

The angular frequency w is related to the frequency n by

$$\omega = 2\pi\nu$$

In many cases it is more useful to use complex notation, in which we express the cosine by exponential function according to the formula,

$$A(x,t) = \frac{A_0}{2}[e^{i(kx-\omega t)} + e^{-i(kx-\omega t)}]$$

Applying the relations; $\omega = \frac{E}{\hbar}$, and $k = \frac{p}{\hbar}$, we obtain the expression of the wave;

$$\exp[i(kx - \omega t)] = \exp[\frac{i}{\hbar}(px - Et)$$

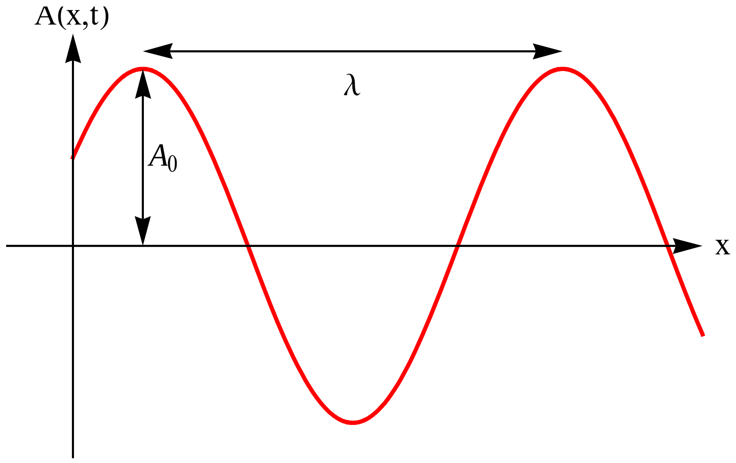


Fig. Instantaneous view of a wave with amplitude A_0 and wavelength λ.

This plane wave is an infinitely long wave train. On the other hand, we assume that particles are localized. We need to consider whether we can, by superposing a sufficient number of suitable wave trains, arrive at some spatially concentrated sort of wave. We are trying to form what are called wave packets, in which the amplitude is localized in a certain region of space.

We now consider a simple case of the superposition of two waves

$$
\begin{aligned}
A(x,t) &= A_0[\cos(k_1 x - \omega_1 t) + \cos(k_2 x - \omega_2 t)] \\
&= 2A_0 \cos[kx - \xi t] \cos[(\Delta k)x - (\Delta\omega)t]
\end{aligned}
$$

where

$$
k = \frac{k_1 + k_2}{2} \qquad \omega = \frac{\omega_1 + \omega_2}{2}
$$

$$
\Delta k = \frac{k_1 - k_2}{2}, \qquad \Delta\omega = \frac{\omega_1 - \omega_2}{2}
$$

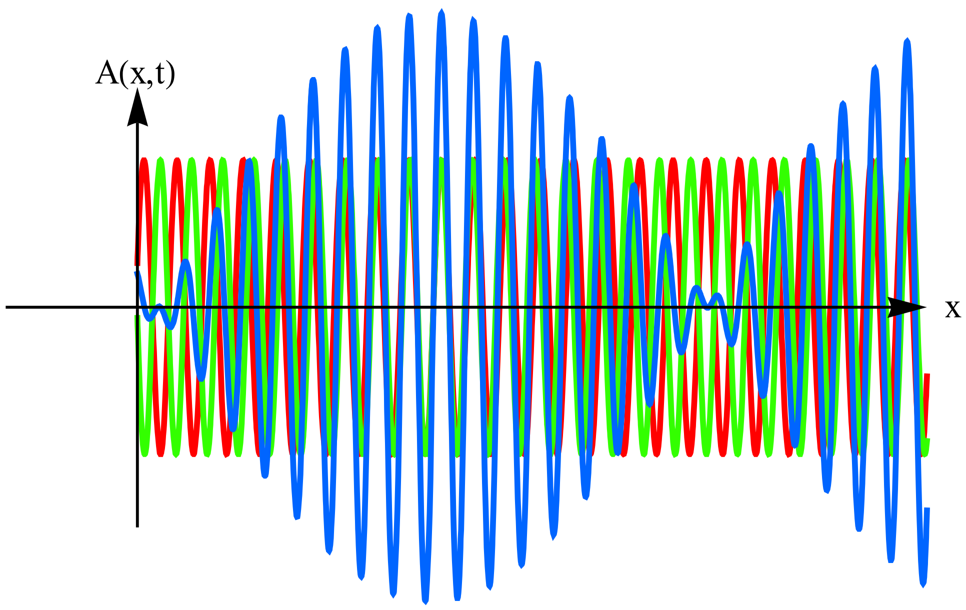


Fig. Superposition of two waves of the same amplitude. Fundamental wave 1 (red). Fundamental wave 2 (green). Resulting wave (blue). t = constant.

2. Example

2.1 Example-1: Problem 5-31 (Thornton, Modern Physics)

Use equation

$$\psi(x,t) = \int \widetilde{A}(k)\cos(kx - \omega t)dk$$

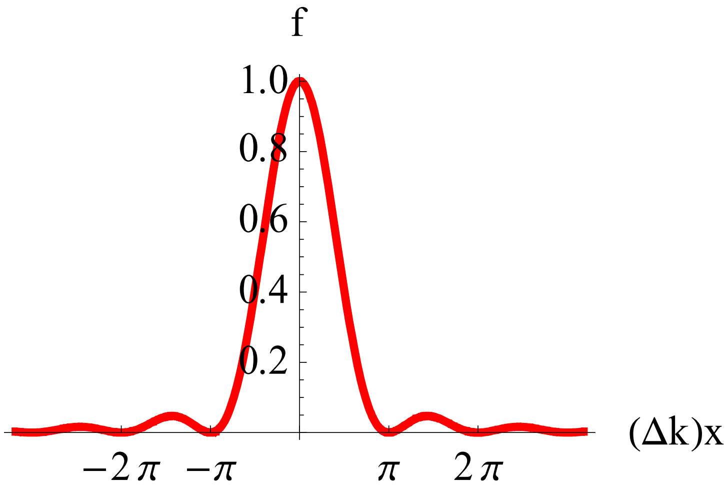
with $\widetilde{A}(k) = A_0$ for the range of $k_0 - \dfrac{\Delta k}{2}$ and $k_0 + \dfrac{\Delta k}{2}$, and $\widetilde{A}(k) = 0$ elsewhere to determine $\psi(x,t=0)$, that is at t = 0. Sketch the envelope term, the oscillation term, and $|\psi(x,t=0)|^2$. Approximately, what is the width Δx over the full-width at half-maximum part of $|\psi(x,t=0)|^2$? What is the value of $\Delta k \Delta x$?

((**Solution**))

$$\psi(x,t=0) = \int_{k_0-\frac{1}{2}\Delta k}^{k_0+\frac{1}{2}\Delta k} \widetilde{A}(k)\cos(kx)dk = A_0 \int_{k_0-\frac{1}{2}\Delta k}^{k_0+\frac{1}{2}\Delta k} \cos(kx)dk$$

$$= \frac{2\cos(k_0 x)}{x}\sin(\frac{x\Delta k}{2})$$

$$= \Delta k\cos(k_0 x)\frac{\sin(\frac{x\Delta k}{2})}{\frac{x\Delta k}{2}}$$



We make a plot of

$$f(y) = \frac{\sin^2(\frac{y}{2})}{\left(\frac{y}{2}\right)^2}$$

where

$$y = (\Delta k)x$$

f(*y*) is equal to 1/2 when $(\Delta k)x$ = 1.39156. Then the full-width at half-maximum is

$$\Delta k\Delta x = 2.78312 = 0.88589\ \pi \approx \pi.$$

((**Mathematica**))

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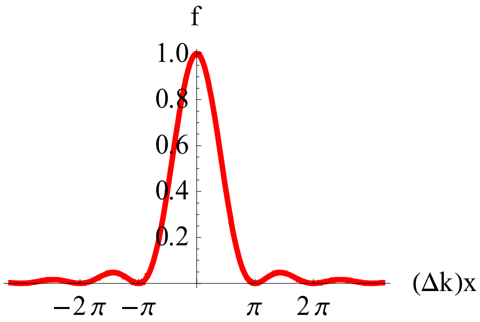
$$\int_{k0-\frac{\Delta k}{2}}^{k0+\frac{\Delta k}{2}} \text{Cos}[k\, x]\, dk \; // \; \text{Simplify}$$

$$\frac{2\,\text{Cos}[k0\, x]\,\text{Sin}\left[\frac{x\,\Delta k}{2}\right]}{x}$$

$$f[y\_] := \left(\frac{\text{Sin}[y]}{y}\right)^2;$$

```
Plot[f[y], {y, -10, 10},
 AxesLabel →
  {"(Δk)x", "f"},
 PlotStyle →
  {Thick, Red},
 Ticks →
  {Range[-2 π, 2 π, π]}]
```



$$\text{FindRoot}\left[\text{Sin}[y]^2 - \frac{1}{2}\, y^2 == 0, \{y, 1, 5\}\right]$$

$$\{y \to 1.39156\}$$

2.2 Example-2

Problem 5-63 (Thornton, Modern Physics)

Use a computer program to produce a wave packet using the function

$$\psi_n = A_n \cos(2\pi n x)$$

where the integer n ranges from 9 to 15. Let the amplitude A_{12} = 1 with the amplitudes A_n decreasing symmetrically by 1/2, 1/3, 1/4 on either side of A_{12} = 1/3 and A_{15} = 1/4). (a) Plot the wave packet

$$\psi = \sum_{n=9}^{15} A_n \cos(2\pi n x)$$

versus x to see repeatable behavior for the wave packet. (b) Where is the wave packet centered? Over what value of x is the wave packet repeated?

((**Mathematica**))

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

ψ = 1/4 Cos[18 π x] + 1/3 Cos[20 π x] + 1/2 Cos[22 π x] +
    Cos[24 π x] + 1/2 Cos[26 π x] + 1/3 Cos[28 π x] +
    1/4 Cos[30 π x] ;

Plot[ψ, {x, -1, 1}, PlotStyle → {Red, Thick},
 Background → LightGray, AxesLabel → {"x", "ψ(x)"}]
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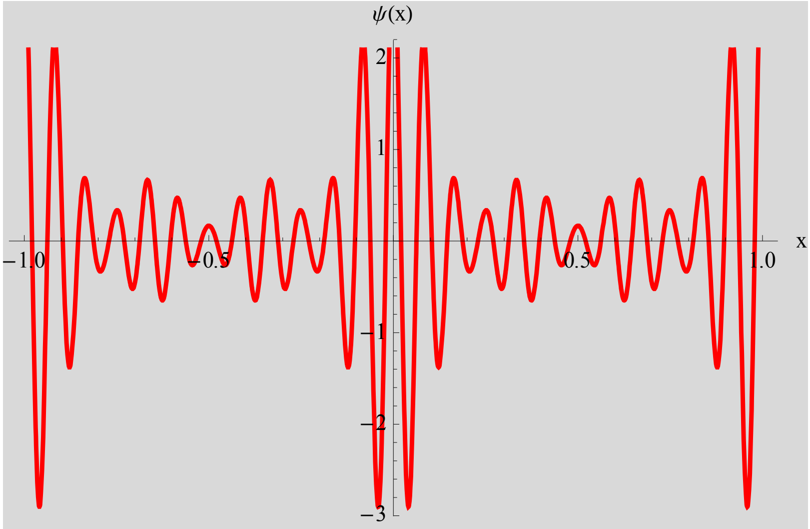


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Plot[ψ, {x, -3, 3}, PlotStyle → {Red, Thick},
 Background → LightGray, AxesLabel → {"x", "ψ(x)"}]
```

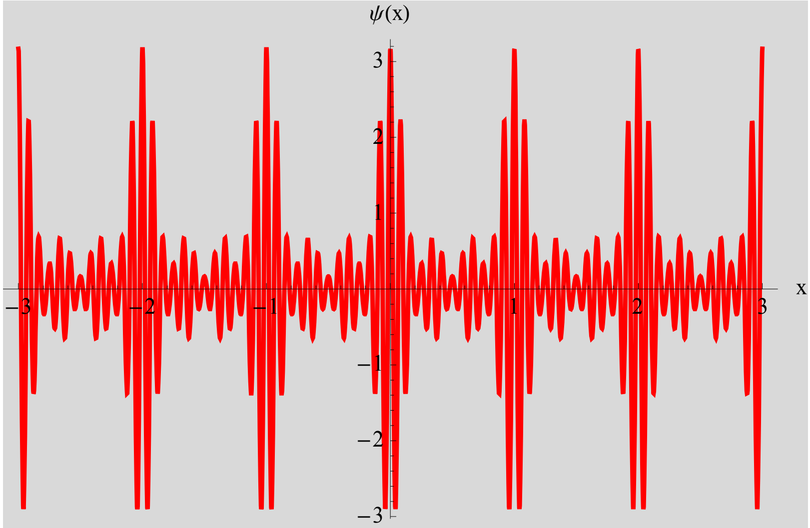

3. Group velocity

We assume that the energy dispersion relation is given by

$$\omega = \omega(k) \qquad \text{(energy dispersion relation)}$$

In evaluation the integral

we set

$$k = k_0 + (k - k_0)$$

and expand ω about the value k_0 using a Taylor series in (k - k_0), which we terminate after the second term:

$$\omega = \omega_0 + v_g(k - k_0) + ...$$

where v_g is called the *group velocity*,

$$v_g = \frac{\partial \omega}{\partial k}|_{k=k_0}$$

Then we get

$$\begin{aligned}\psi(x,t) &= A\int_{k0-\Delta k}^{k0+\Delta k} \exp[i(kx - \omega_k t)]dk \\ &= A\exp[i(k_0x - \omega_0 t)]\int_{k0-\Delta k}^{k0+\Delta k} \exp[i((k-k_0)x - v_g(k-k_0)t)]dk \\ &= A\exp[i(k_0x - \omega_0 t)]\int_{-\Delta k}^{\Delta k} \exp[i\xi(x - v_g t)]dk\end{aligned}$$

where we have set $(k - k_0) = \xi$. Finally, this integral; takes the form

$$\psi(x,t) = A\exp[i(k_0x - \omega_0 t)][\frac{2\Delta k \sin(x - v_g t)\Delta k}{(x - v_g t)\Delta k}]$$

We make a plot of $\{\mathrm{Re}[\psi(x, \mathrm{t})]\}^2$ as a function of x with t varied as a parameter.

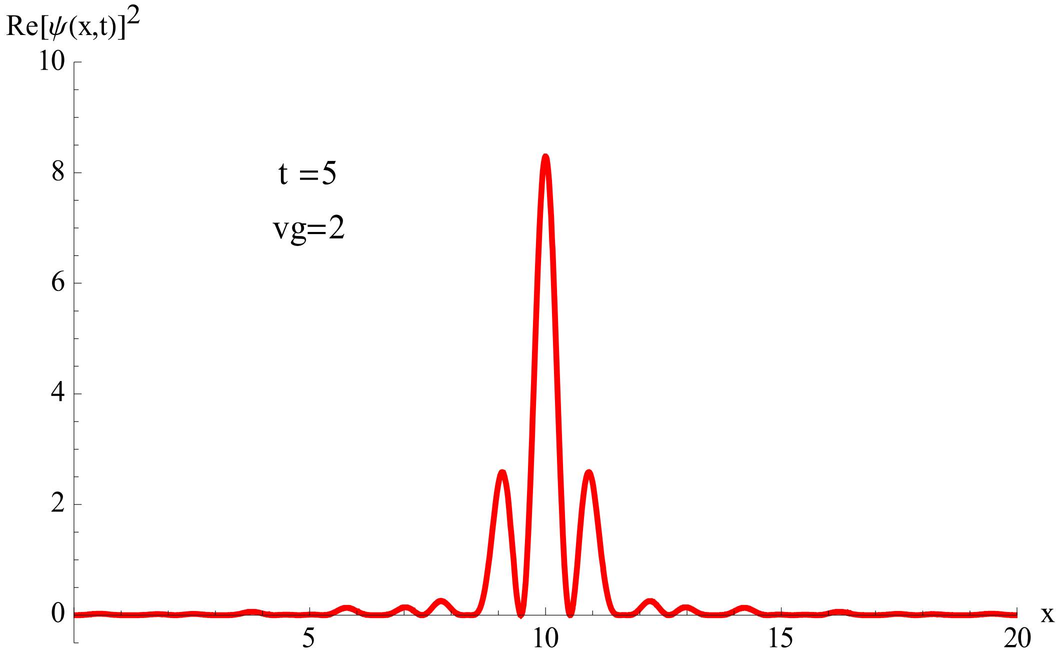

Fig. Typical example for the plot of $\{\mathrm{Re}[\psi(x, \mathrm{t})]\}^2$ vs x with $t = 5$. $v_g = 2.0$. $t = 5$.

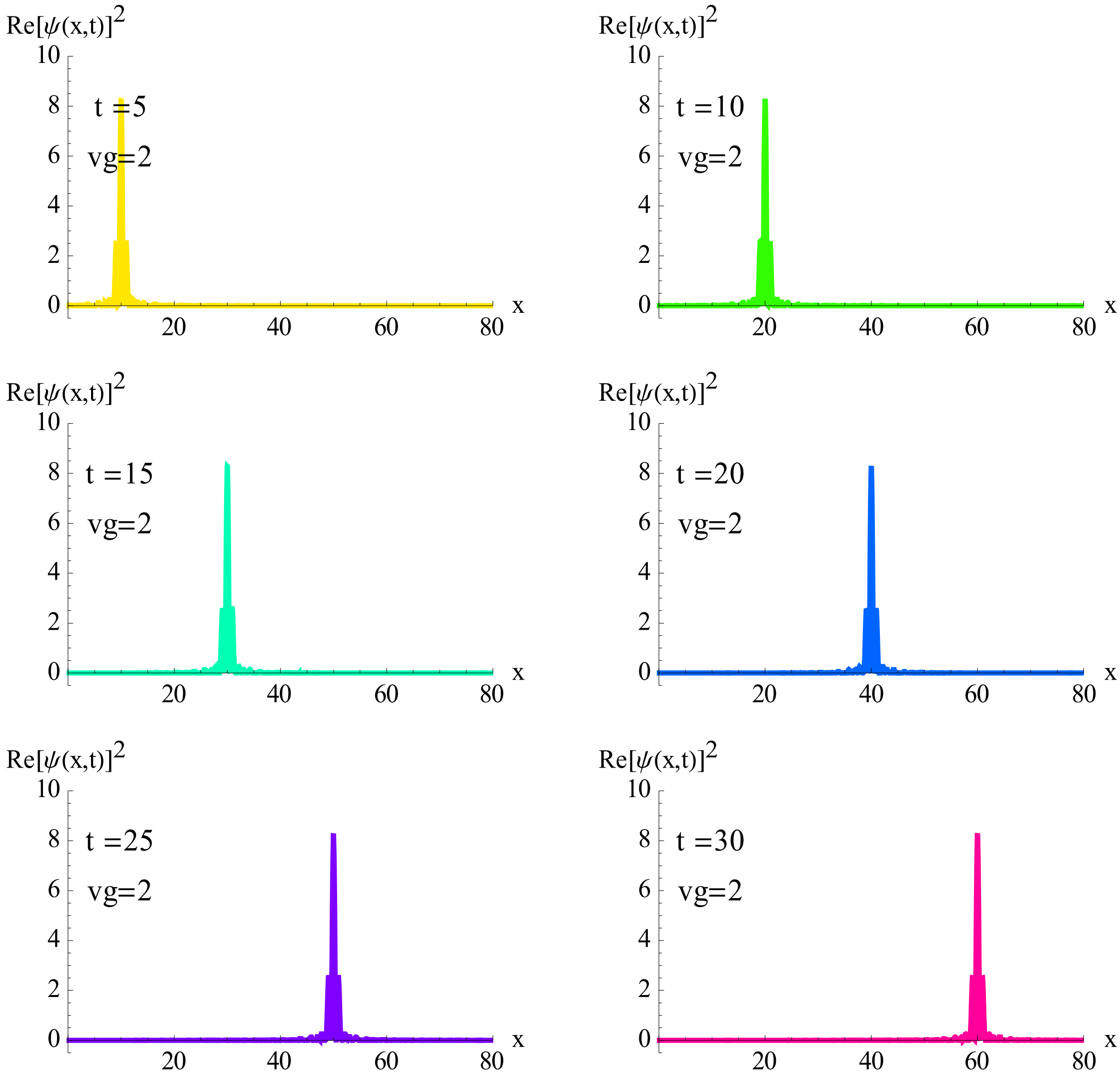

Fig. The plot of $\{\mathrm{Re}[\psi(x, t)]\}^2$ vs x with t varied as a parameter.t = 5, 10, 15, 20, 25, and 30. $v_g = 2.0$. $t = 5$.

((**Conclusion**))

We can draw two important conclusions from the above Fig.

(1) The wave packet represented by $\psi(x,t)$ is strongly localized in the region of $x = v_g t$. The maximum amplitude moves with a group velocity v_g.

$$v_g = \frac{\partial \omega}{\partial k} = \frac{1}{\hbar}\frac{\partial E}{\partial p}$$

(2) The width of a wave packet is roughly the distance between the first two zero points to the left and right of the maximum. The width of the wave packet would be

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

or

$$\Delta k \Delta x = 2\pi \qquad \text{(The principle of uncertainty).}$$

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4. Gaussian wave packet

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

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

$f_1^* f_1$ is evaluated as

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

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

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

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

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

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

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

((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:

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

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

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

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 Heisenberg's principle of uncertainty:

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

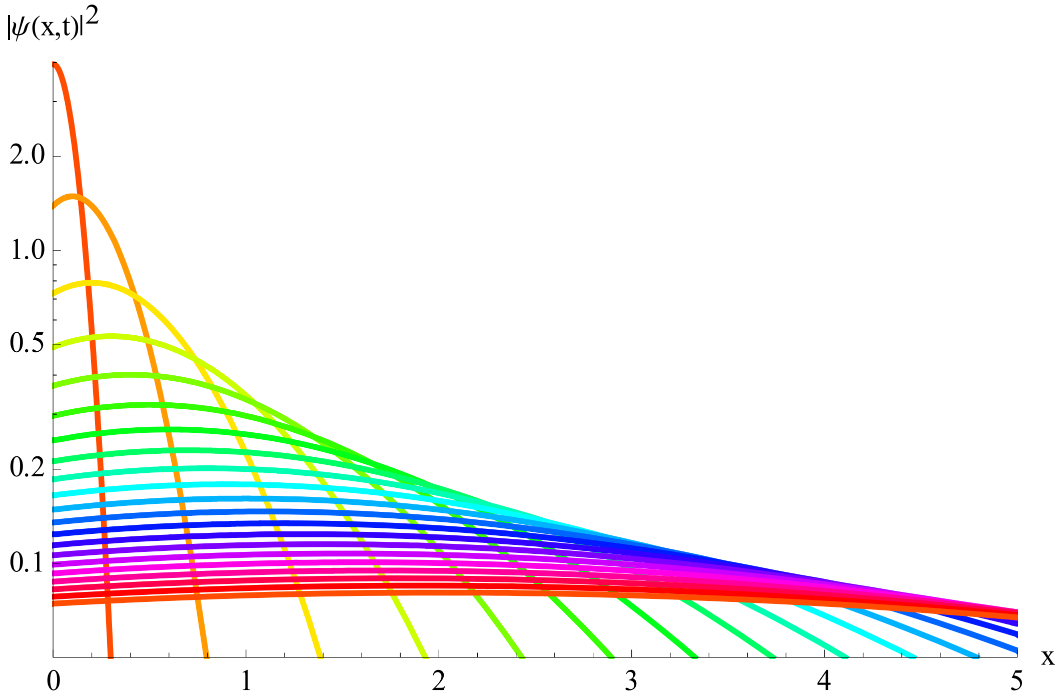

Fig. Propagation of Gaussian wave packet. Plot of $|\psi(x,t)|^2$ as a function of x. The time t is changed as a parameter; t = 0 - 1 with Δt = 0.05. m = 1. $\hbar = 1$. k_0 = 2. Δk = 7. x_0 = 0.

((**Mathematica**)) QM wavepacket

Evolution of Gaussian Wave packet Gaussian

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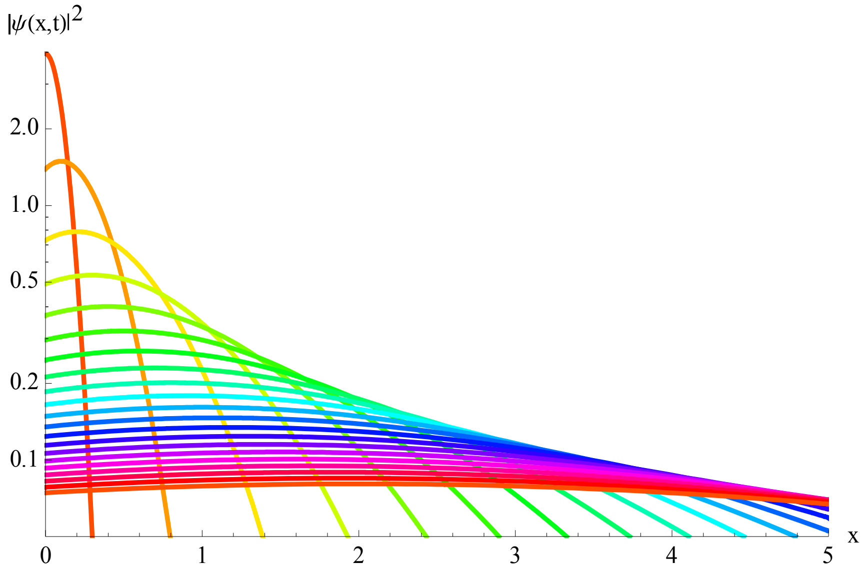
$$P\psi = \frac{e^{-\frac{\Delta k^2 \left(x - x0 - \frac{k0\, t\, \hbar}{m}\right)^2}{1 + \frac{t^2 \Delta k^4 \hbar^2}{m^2}}}}{\sqrt{\pi}\, \Delta k \sqrt{\frac{1}{\Delta k^4} + \frac{t^2 \hbar^2}{m^2}}};$$

```
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"}]
```



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

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

5. Fourier transform of Gaussian distribution function

The Gaussian distribution function is given by

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp(-\frac{x^2}{2\sigma^2}).$$

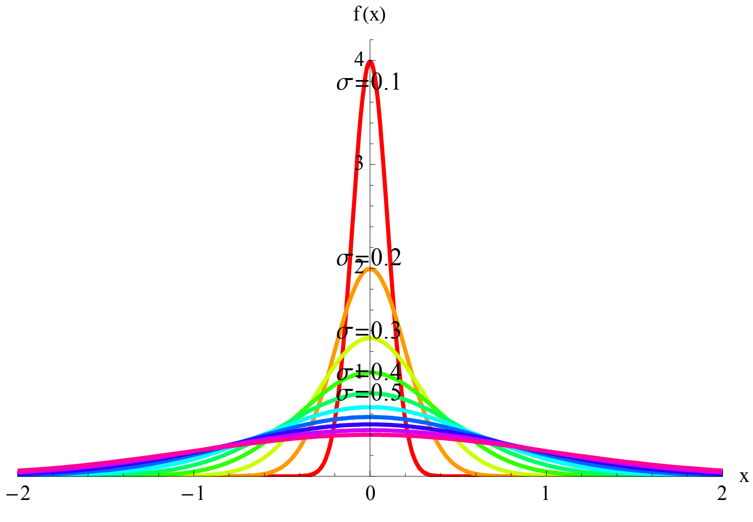
The full-width at half-maximum, Δx, is given by

$$\Delta x = (2\sqrt{2}\ln 2)\sigma,$$

since

$$\exp(-\frac{x^2}{2\sigma^2}) = \frac{1}{2}.$$

The line width Δx increases with increasing σ.



The Fourier transform of $f(x)$ is given by

$$F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx} f(x)dx = \frac{1}{\sqrt{2\pi}}\exp(-\frac{1}{2}k^2\sigma^2)$$

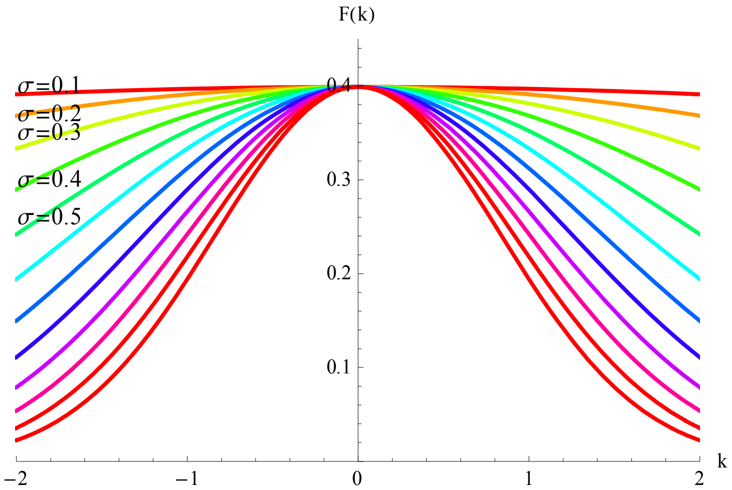
which also shows the Gaussian distribution. The full-width at half-maximum, Δk, is given by

$$\Delta k = \frac{(2\sqrt{2}\ln 2)}{\sigma},$$

since

$$\exp(-\frac{\sigma^2 k^2}{2}) = \frac{1}{2}.$$

The width of the line, *Δk*, shape decreases with increasing *σ*.



Thus we have the relation

$$\Delta x \Delta k = (2\sqrt{2}\ln 2)\sigma(2\sqrt{2}\ln 2)\frac{1}{\sigma} = (2\sqrt{2}\ln 2)^2 = 3.84>1$$

which satisfies the Heisenberg's principle of uncertainty.

6. Group velocity and phase velocity

6.1 Result from special relativity

The total energy *E* and the momentum p are expressed by

$$E = \frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}} = E_0 + K \,, \qquad\qquad p = \frac{mv}{\sqrt{1-\frac{v^2}{c^2}}}$$

where v is the particle velocity (group velocity). The energy dispersion relation is given by

$$E = \sqrt{m^2c^4 + c^2 p^2} = c\sqrt{m^2c^2 + p^2} = E_0 + K$$

Since

$$c^2(m^2c^2 + p^2) = (E_0 + K)^2$$

or

$$c^2 p^2 = (E_0 + K)^2 - E_0^{\,2}$$

we get the expression for p,

$$p = \frac{\sqrt{(E_0 + K)^2 - E_0^{\,2}}}{c} = \frac{\sqrt{K^2 + 2KE_0}}{c}$$

where K is the kinetic energy and E_0 is the energy at rest mass.

$$E_0 = mc^2$$

When $E_0 >> K$, p can be approximated by

$$p \approx \frac{\sqrt{2KE_0}}{c} = \sqrt{2mK}$$

6.2 Group velocity v_g

The group velocity is defined as

$$v_g = \frac{\partial E}{\partial p} = \frac{cp}{\sqrt{m^2c^2 + p^2}}$$

$$= \frac{cp}{\frac{E}{c}} = \frac{c^2 p}{E} = v$$

$$= \frac{c\sqrt{K^2 + 2KE_0}}{K + E_0}$$

In other words, the group velocity is identical with the particle velocity. In the limit of $K \ll E_0$, we get

$$v_g \approx \frac{c\sqrt{2KE_0}}{E_0} = c\sqrt{\frac{2K}{E_0}} = \sqrt{\frac{2K}{m}}$$

6.3 Phase velocity v_p

The phase velocity v_p is defined as

$$v_p = \frac{E}{p} = \frac{mc^2}{mv} = \frac{c^2}{v}$$

Since $v = v_g$, we have the relation between v_g and v_p as

$$v_g v_p = c^2$$

6.4 Classical limit

Classically, we have the energy dispersion relation

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

The group velocity is

$$v_g = \frac{\partial E_c}{\partial p} = \frac{p}{m} = v$$

(d) phase velocity

$$v_{ph} = \frac{E}{p} = \frac{c^2}{v} = \frac{c}{\beta}$$

or

$$v_g v_p = c^2$$

Since $v_g<c$, v_p is larger than c.

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