Wave packet

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: August, 12, 2011)

1. Schrödinger equation

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

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

Time dependent Schrödinger equation.

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

We assume that

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

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

or

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

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

or

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

$$H(\mathbf{r})\varphi_n(\mathbf{r}) = E\varphi_n(\mathbf{r})$$

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:

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

$$H\varphi_k = E_k\varphi_k$$

or

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi_k(x) = E_k\varphi_k(x) \qquad \text{or} \qquad \frac{\partial^2}{\partial x^2}\varphi_k(x) = -k^2\varphi_k(x)$$

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

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

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

phase velocity: $v_p = \frac{E_k}{\hbar k} = \frac{\hbar k}{2m} = \frac{p}{2}$

group velocity: $v_g = \frac{1}{\hbar}\frac{\partial E_k}{\partial k} = \frac{\hbar k}{m} = p$

$|\psi_k(x,t)|^2 = |A|^2$, 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

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

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

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

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

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:

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

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:

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

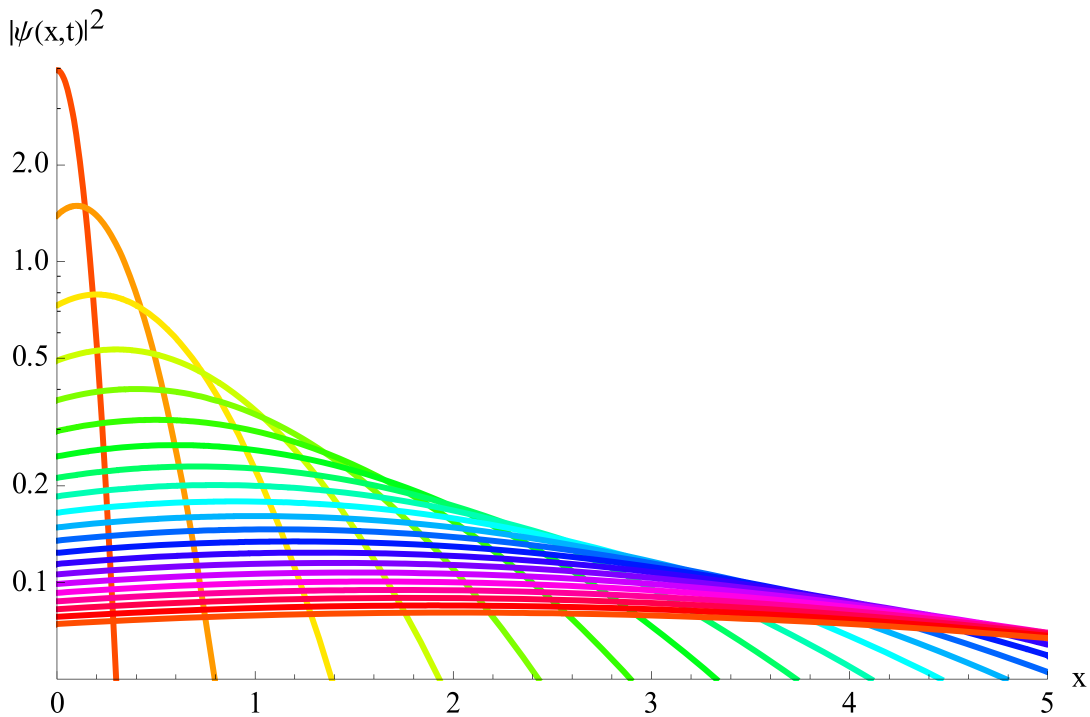


Fig. Propagation of Gaussian wave packet. Plot of $|\psi(x,t)|^2$ as a function of x. The time t is changed as a parameter; t = 0 - 1 with Δt = 0.05. m = 1. $\hbar = 1$. k_0 = 2. Δk = 7. x_0 = 0.

((**Mathematica**)) QM wavepacket

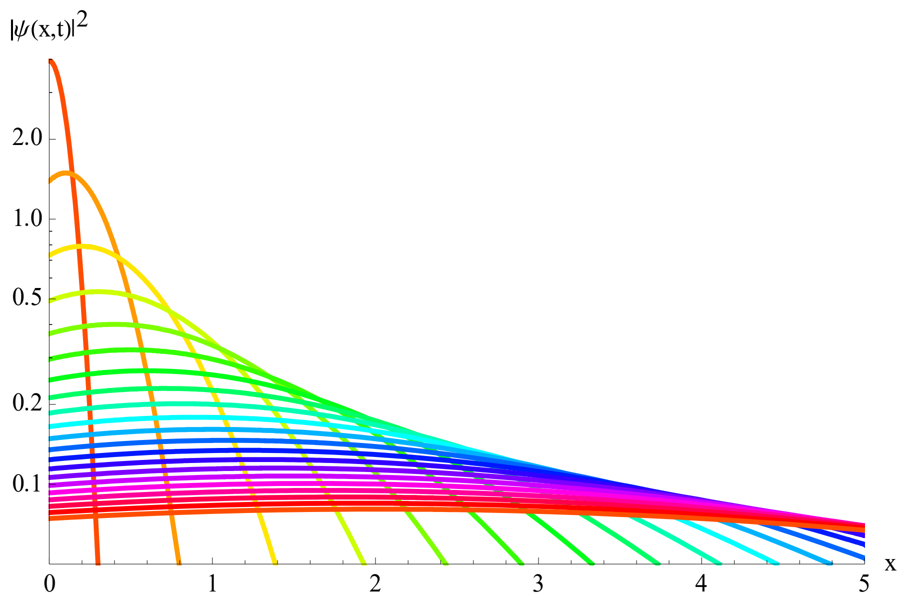
Evolution of Gaussian Wave packet Gaussian

```
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[m^2 Δk^2 / (m^2 + t^2 Δk^4 ℏ^2)] > 0}]
```

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