FREE PARTICLE GAUSSIAN WAVEPACKET

Reading:
McIntyre Ch 6

GAUSSIAN WAVE PACKET - REVIEW

- *Time dependent Schrödinger equation*
- *Energy eigenvalue equation (time independent SE)*
- *Eigenstates*
- *Time dependence*
- *(Connection to separation of variables)*
- *Mathematical representations of the above*

Build a "wavepacket" from free particle eigenstates

- Ask 2 important questions:
- Given a particular superposition, what can we learn about the particle's location and momentum?

HEISENBERG UNCERTAINTY PRINCIPLE

- How does the wavepacket evolve in time?

GROUP VELOCITY

We have already discussed the principle of superposition & the time evolution of that superposition in the context of the discrete quantum mechanical states of the infinite potential energy well.

We now discuss how build a wave packet from harmonic waveforms (with a continuous frequency distribution).

We use the case of superposition of quantum mechanical states of the free particle, which are no longer discrete, and we choose to weight different frequency components more heavily than others.

Free particle eigenstates

$$\boxed{\psi_k(x,t) = e^{ikx} e^{-i\frac{E_k}{\hbar}t}}$$

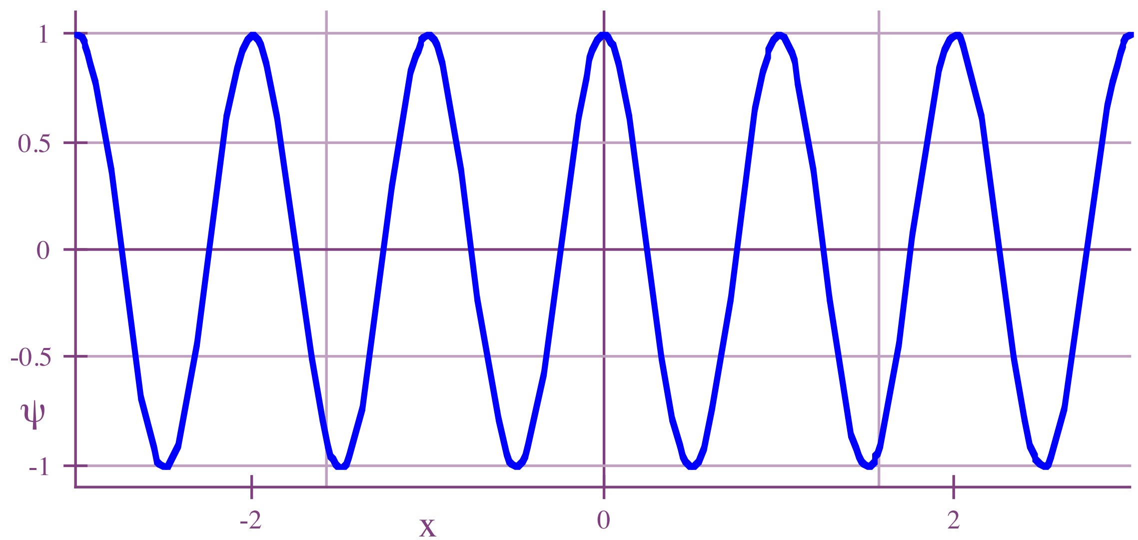
$$E_k = \frac{\hbar^2 k^2}{2m}$$

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

$$\boxed{\varphi_k(x) \equiv \psi_k(x,0)}$$

$$\boxed{\varphi_k(x) = e^{ikx}}$$

- Oscillating function
- Definite momentum $p = hk/2\pi$
- Subscript k on ω reminds us that ω depends on k
- What are E and ω in terms of given quantities?

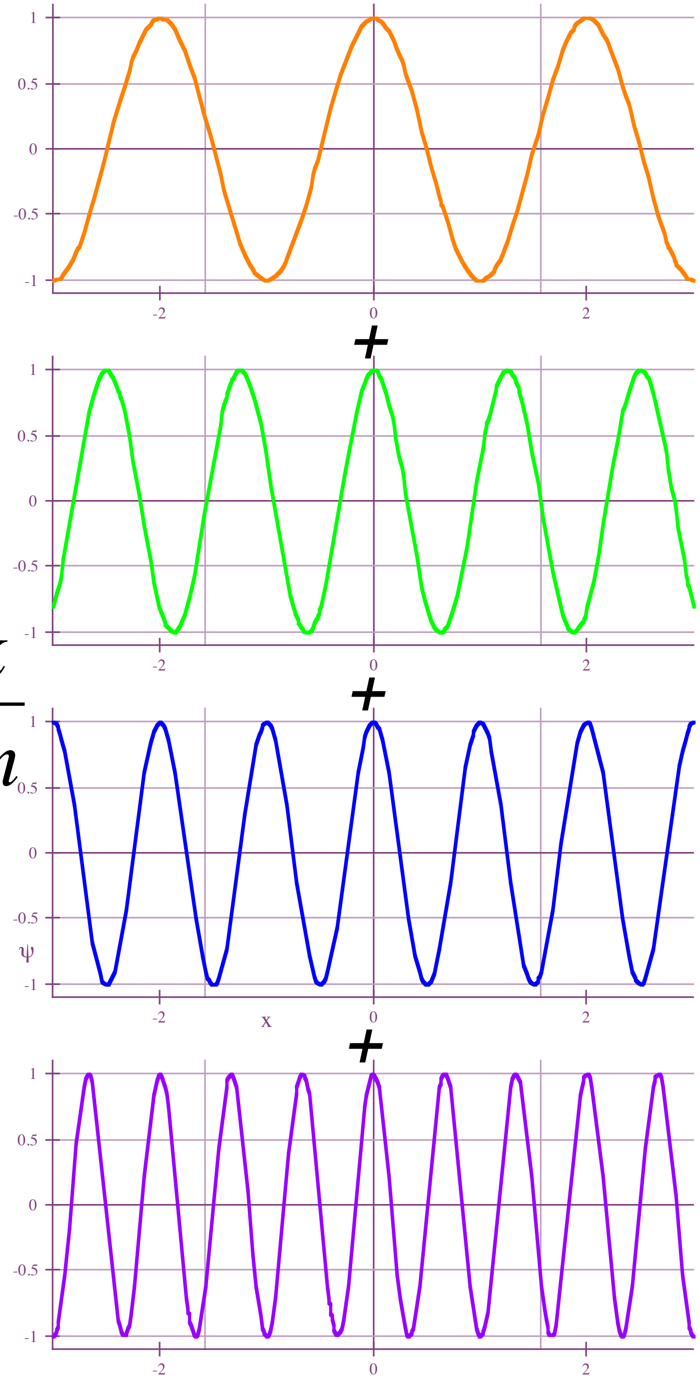


Superposition of eigenstates
(Fourier series)

$$\varphi(x) = \sum_k c_k \varphi_k(x)$$

$$\varphi_k(x) = e^{ikx}$$

$$E_k = \frac{\hbar^2 k^2}{2m} \qquad v_{phase,k} = \frac{\omega_k}{k} = \frac{E_k}{\hbar k} = \frac{\hbar k}{2m}$$



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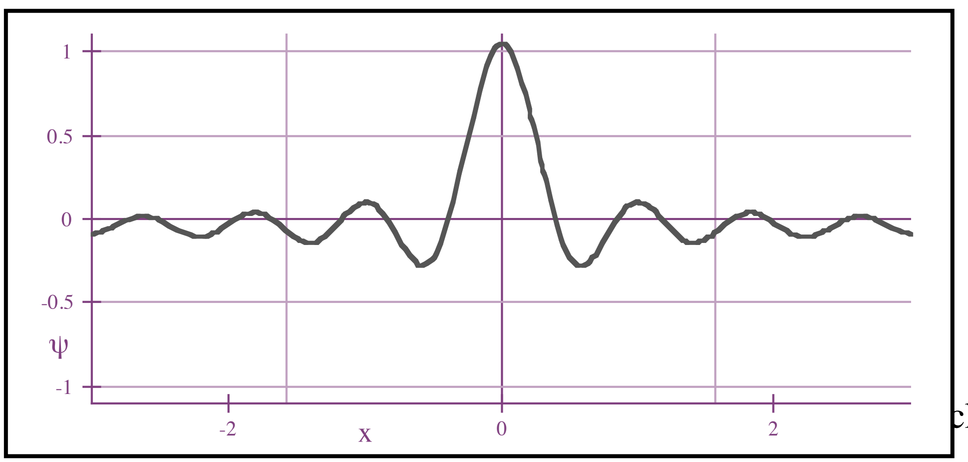

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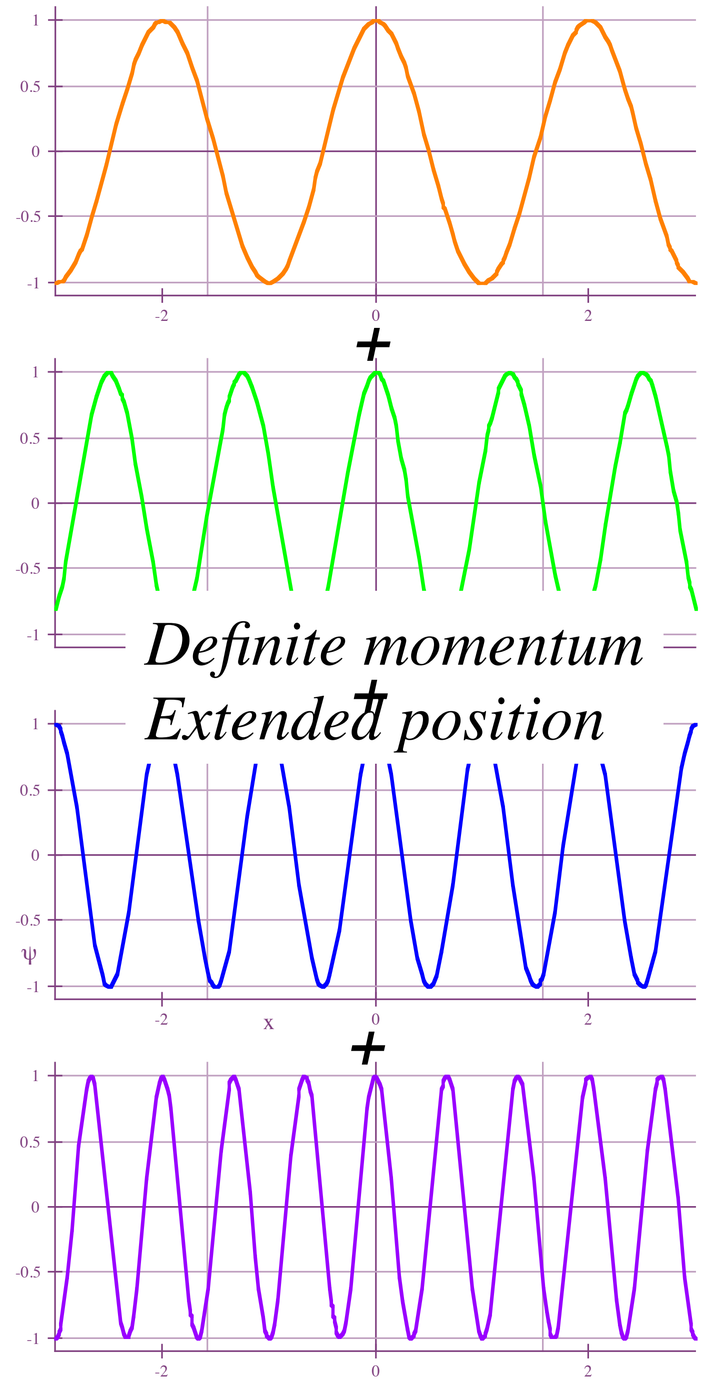
Superposition of eigenstates
(Fourier integral)

$$\varphi(x) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx}$$

$$n \rightarrow k$$

$$\sum_n \rightarrow \int dk$$

$$c_n \rightarrow A_k \rightarrow A(k)$$



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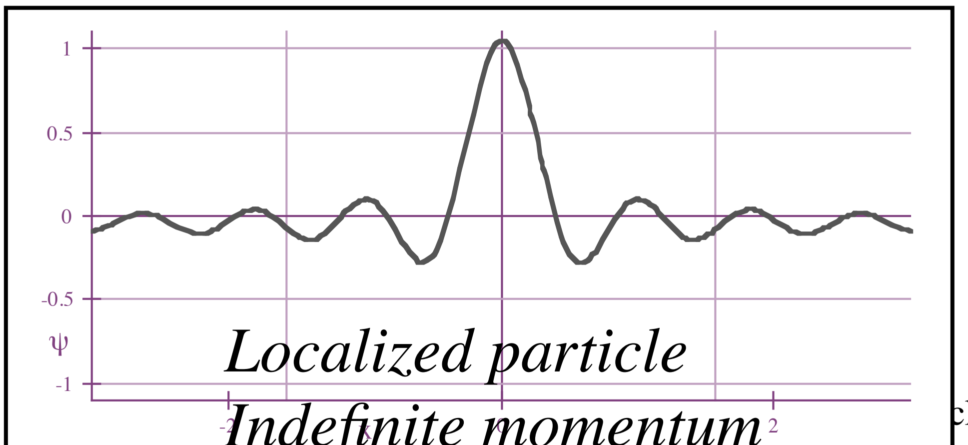

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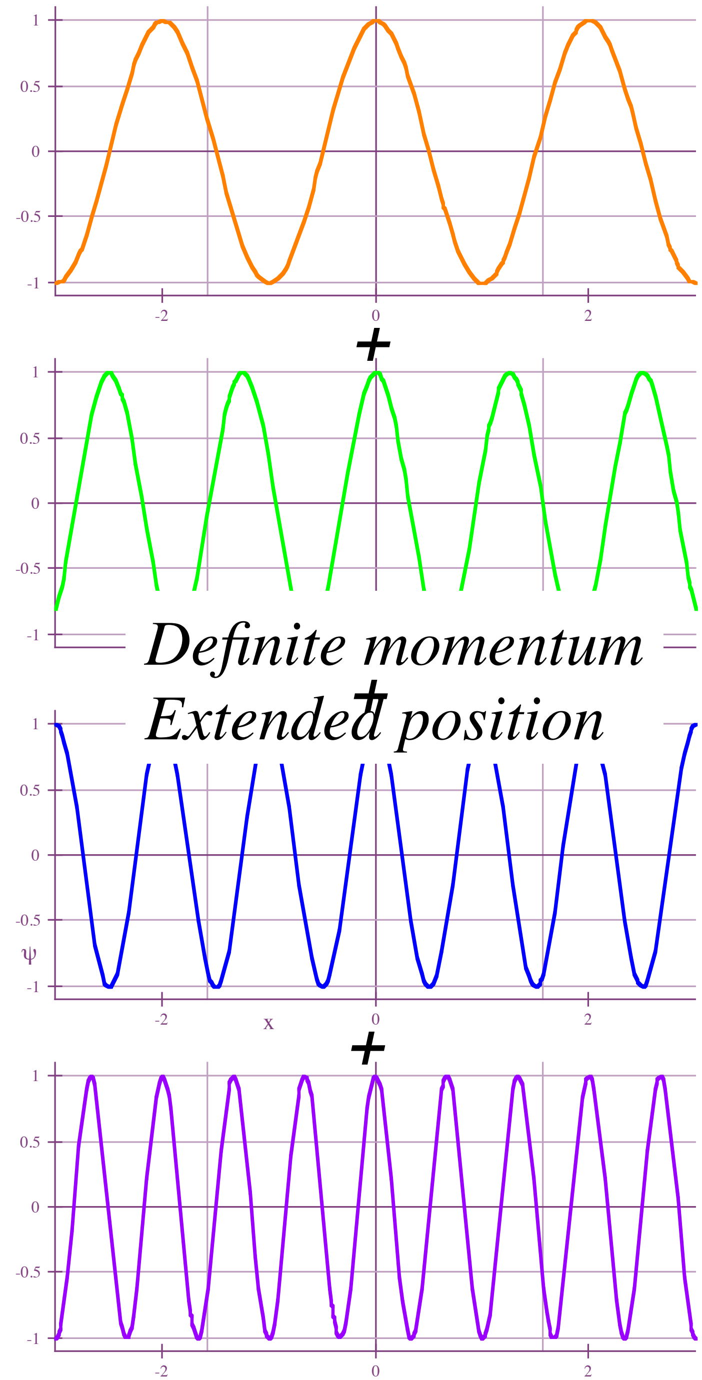
Superposition of eigenstates
How does it develop in time?

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

$$\varphi(x,t) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx} e^{-iE_k t/\hbar}$$

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



Definite momentum
Extended position

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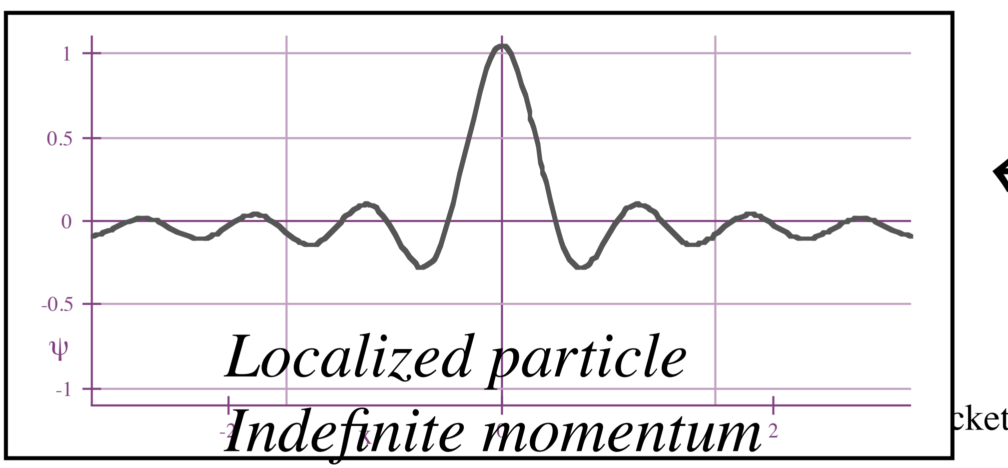
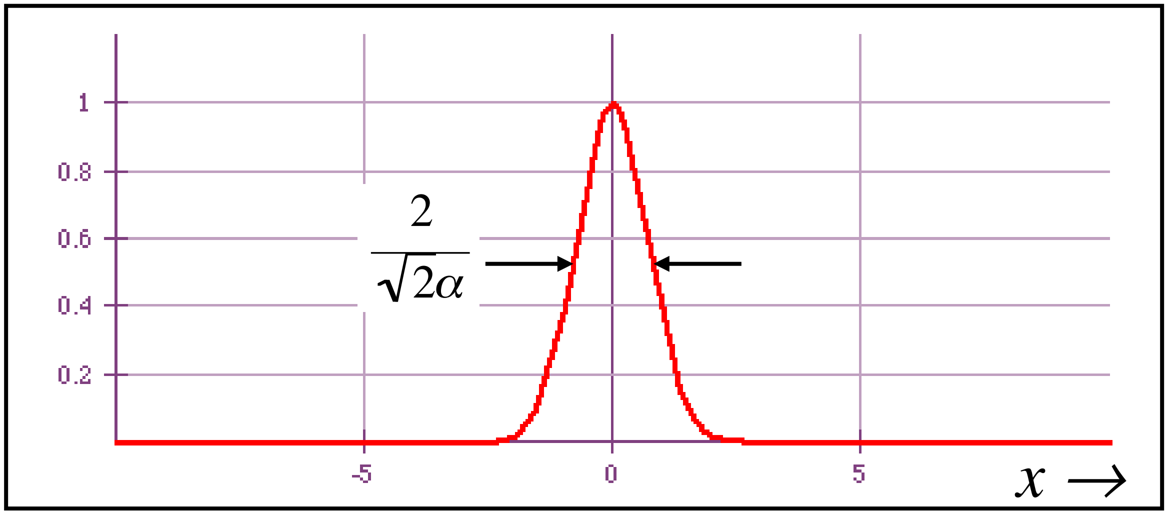


Localized particle
Indefinite momentum

Build
Gaussian wave packet

$$\varphi(x,0) = \left(\frac{2\alpha^2}{\pi}\right)^{\frac{1}{4}} e^{-\alpha^2 x^2}$$

What is $A(k)$?



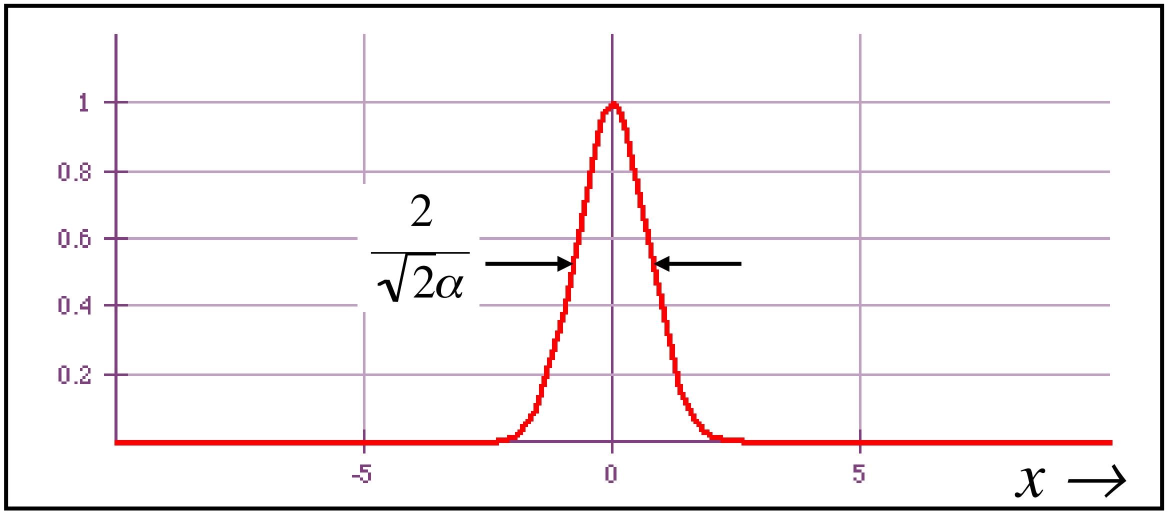
We'll ignore overall constants that are not of primary importance (there are conventions about factors of 2π that are important to take care of to get numerical results, but we're after the physics!)

$$\boxed{A(k) = \langle \varphi_k | \varphi \rangle_{t=0}}$$

Projection of general function on eigenstate

Gaussian wave packet

$$\boxed{\varphi(x,0) = \left(\frac{2\alpha^2}{\pi}\right)^{\frac{1}{4}} e^{-\alpha^2 x^2}}$$



$$A(k) = \langle \varphi_k | \varphi_{t=0} \rangle = \int_{-\infty}^{\infty} dx\, \varphi_k^*(x)\varphi(x,0)$$

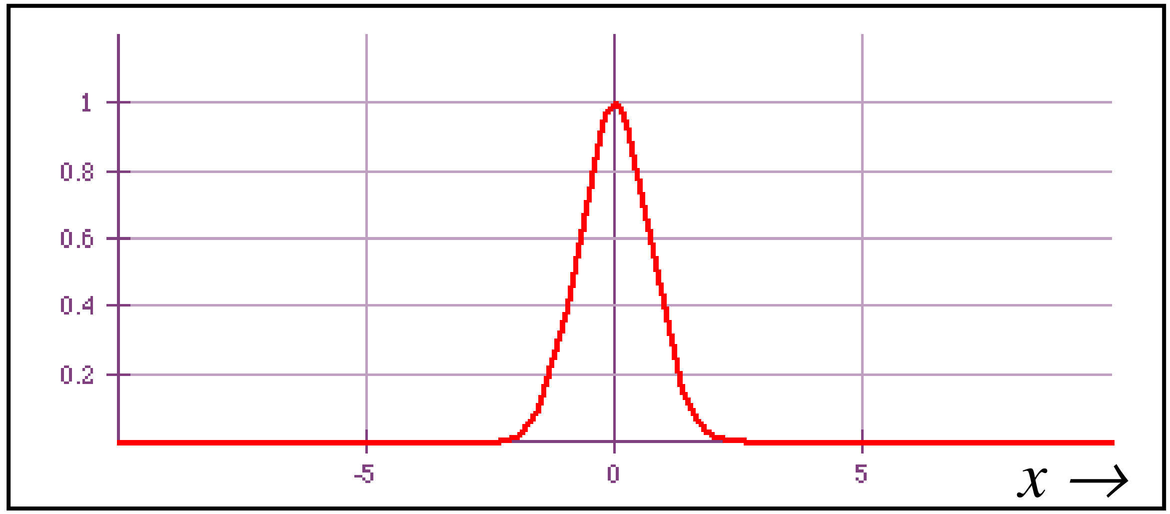
$$A(k) = \langle \varphi_k | \varphi_{t=0} \rangle \cong \int_{-\infty}^{\infty} dx\, e^{-ikx} e^{-\alpha^2 x^2}$$

We did this integral (by hand).

using:
$$\int_{-\infty}^{\infty} dy\, e^{vy} e^{-uy^2} = \sqrt{\frac{\pi}{u}}\, e^{\frac{v^2}{4u}}$$

Gaussian wave packet

$$\boxed{\varphi(x,0) = \left(\frac{2\alpha^2}{\pi}\right)^{\frac{1}{4}} e^{-\alpha^2 x^2}}$$

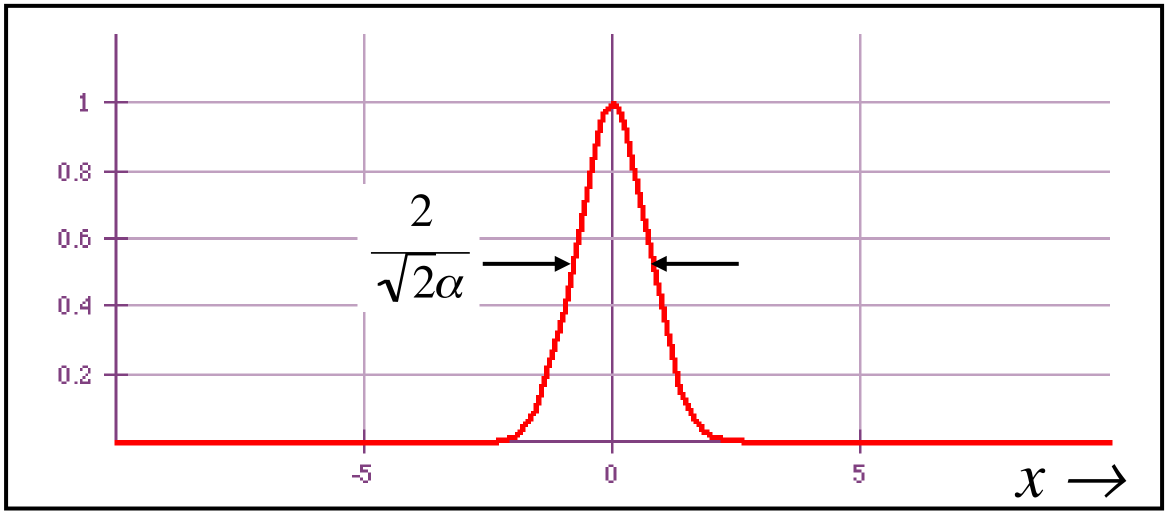


$$A(k) = \langle \varphi_k | \varphi_{t=0} \rangle \cong \int_{-\infty}^{\infty} dx\, e^{-ikx} e^{-\alpha^2 x^2}$$

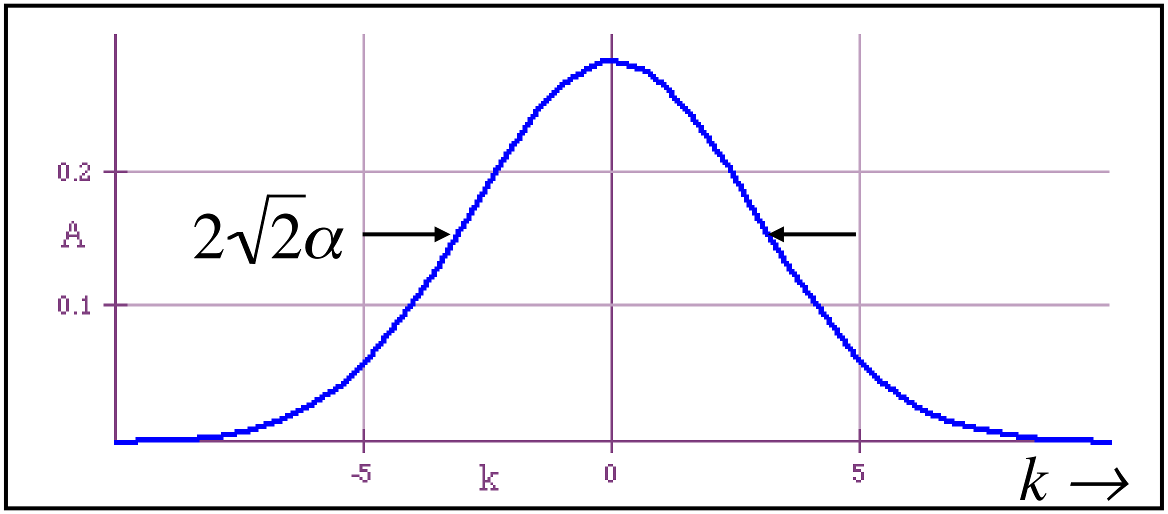
$$A(k) \cong e^{-k^2/4\alpha^2}$$

Gaussian wave packet

$$\boxed{\varphi(x) \cong e^{-\alpha^2 x^2}}$$

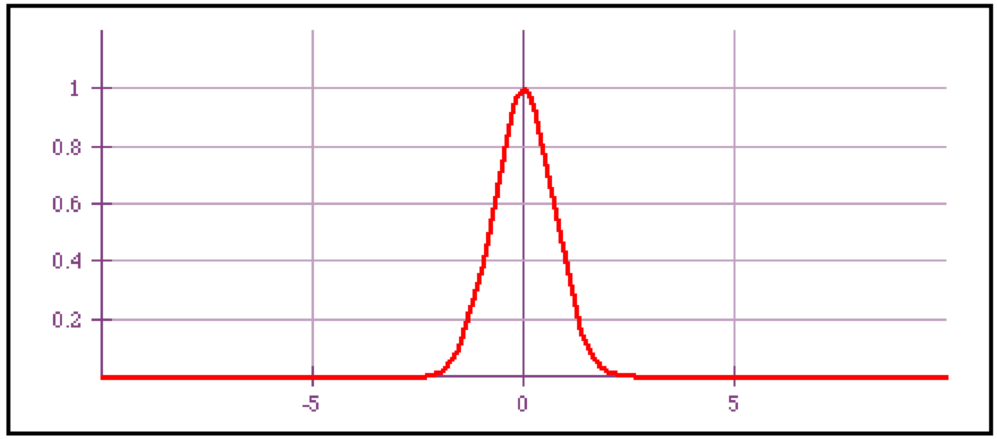


$$\boxed{A(k) \cong e^{-k^2/4\alpha^2}}$$

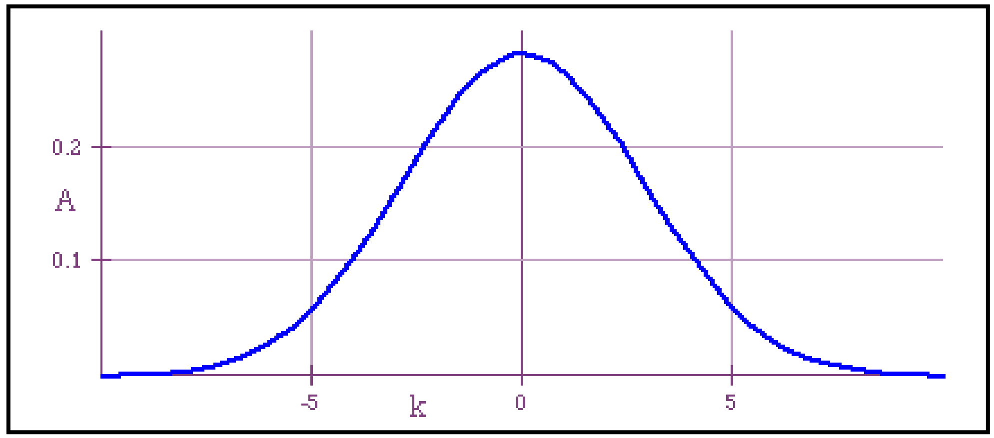


If φ(x) is wide, A(k) is narrow and vice versa.

$$\boxed{\varphi(x) \cong e^{-\alpha^2 x^2}}$$



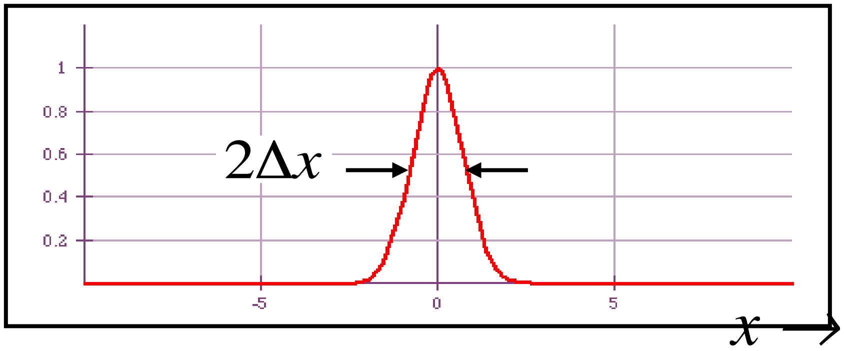
$$\boxed{A(k) \cong e^{-k^2/4\alpha^2}}$$



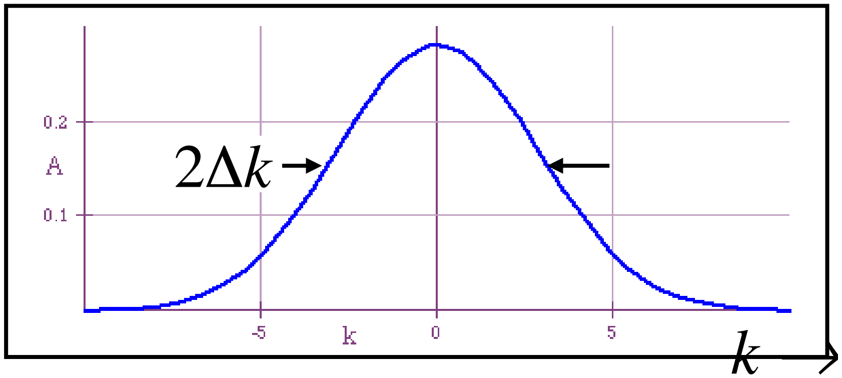
$A(k)$ is the projection of $\varphi(x)$ on the momentum eigenstates e^{ikx}, and thus represents the amplitude of each momentum eigenstate in the superposition.

We need the contribution of a wide spread of momentum states to localize a particle. If we have the contribution of just a few, the location of the particle is uncertain

$$\left|\varphi(x)\right|^2 \cong e^{-2\alpha^2 x^2}$$

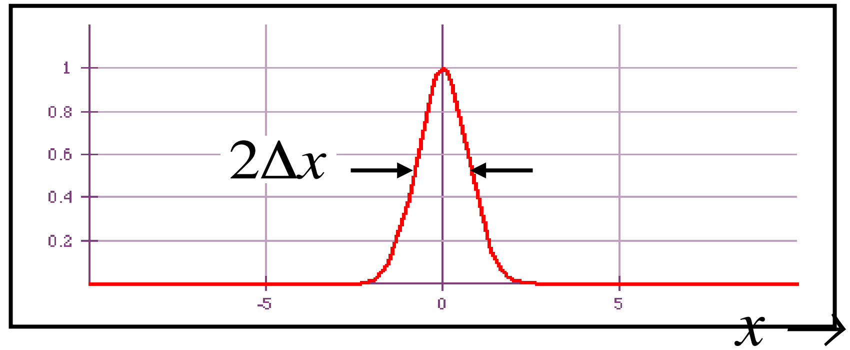


$$\left|A(k)\right|^2 \cong e^{-2k^2/4\alpha^2}$$



To define "uncertainty" in position or momentum, we must consider probability, not wave function.

$$|\varphi(x)|^2 \cong e^{\boxed{-2\alpha^2 x^2}}$$



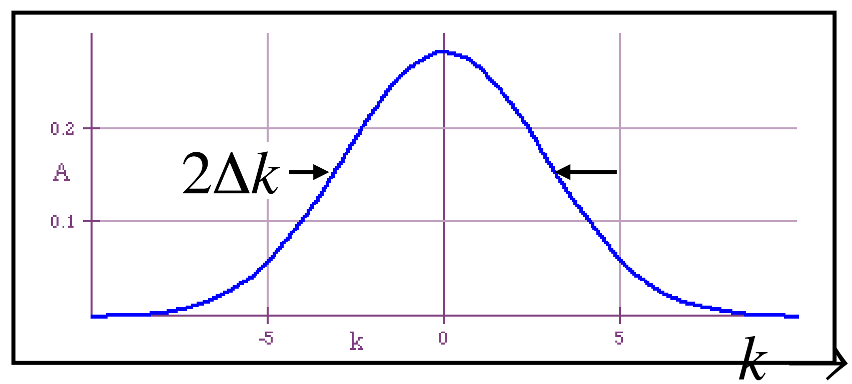
$$\Delta x = \frac{1}{2\alpha}$$

$$|f(z)|^2 \cong e^{\boxed{-\frac{z^2}{2\Delta z_z^2}}}$$

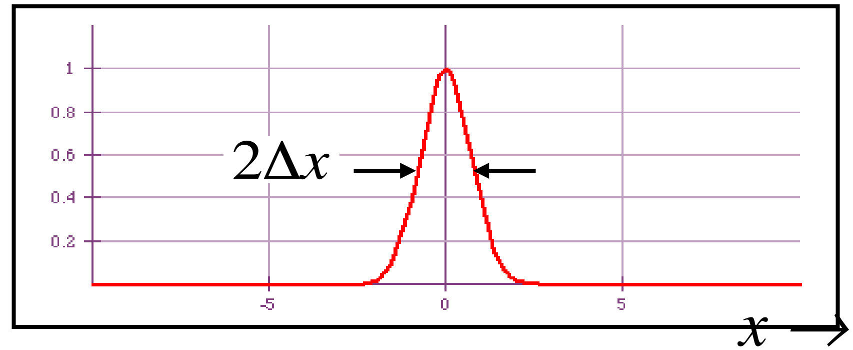
$$\Delta k = \alpha$$

$$|A(k)|^2 \cong e^{\boxed{-2k^2/4\alpha^2}}$$

Wavepacket



$$\boxed{\left|\varphi(x)\right|^2 \cong e^{-2\alpha^2 x^2}}$$



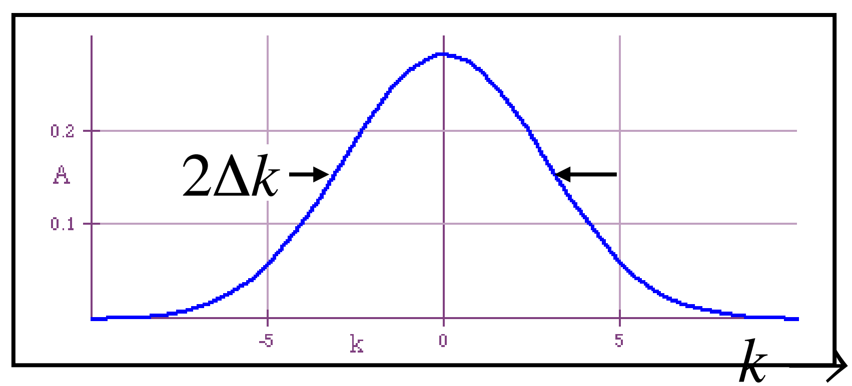
HEISENBERG UNCERTAINTY PRINCIPLE

$$\Delta p \Delta x = \hbar \Delta k \Delta x = \hbar \alpha \frac{1}{2\alpha}$$

$$\boxed{\Delta p \Delta x = \frac{\hbar}{2}}$$

$$\boxed{\left|A(k)\right|^2 \cong e^{-2k^2/4\alpha^2}}$$

Wavepacket



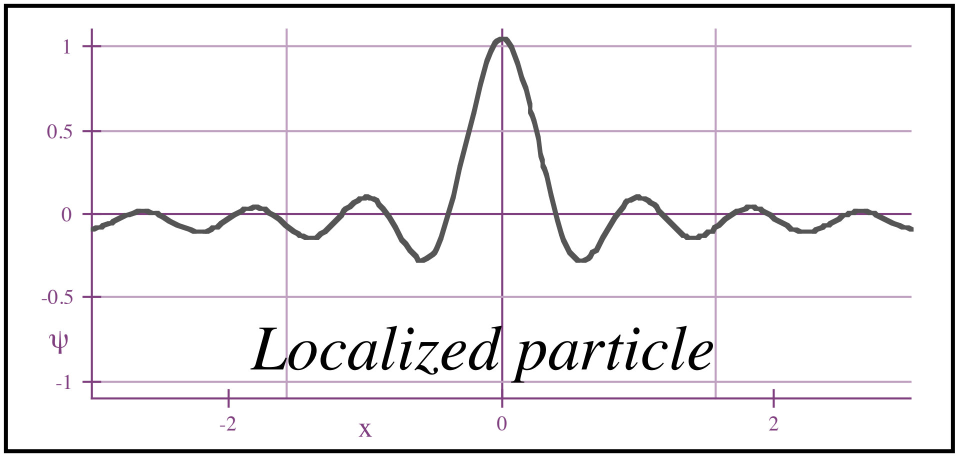
Next, we'll ask how a general wave packet propagates, And deal with the particular example of the Gaussian wavepacket.

In short, we simply attach the exp(-iE(k)t/hbar) factor to each eigenstate and let time run.

Difference to non-dispersive equation: not all waves propagate with same velocity. "Packet" does not stay intact! Need to invoke "group velocity" to follow the progress of the "bump".

Superposition of eigenstates
How does it develop in time?

$$\varphi(x,t) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx} e^{-i\omega_k t}$$



If ω depends on *k*, the different eigenstates (waves) making up this "packet" travel at different speeds, so the feature at x=0 that exists at t=0 may not stay intact at all time.
It may stay identifiably intact for some reasonable time, and if it does, how fast does it travel?
The answer is "it travels at the group velocity dω/d*k*"

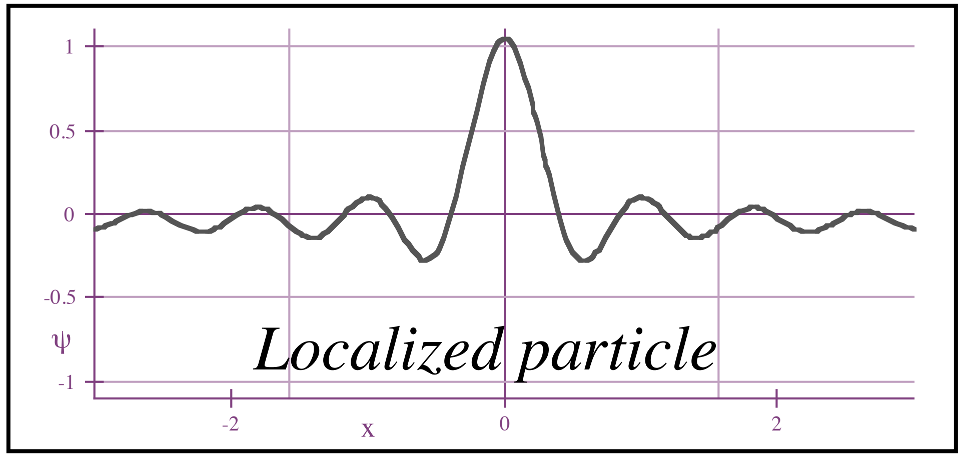
$$\omega_k \equiv \frac{E_k}{\hbar} = \frac{\hbar k^2}{2m}$$

$$\boxed{v_{group} = \frac{d\omega}{dk} = \frac{\hbar k}{m}}$$

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

Superposition of eigenstates
How does it develop in time?

$$\varphi(x,t) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx} e^{-i\omega_k t}$$



The quantity dω/dk may (does!) vary depending on the k value at which you choose to evaluate it. So it must be evaluated at a particular value k_0 that represents the center of the packet. The next few pages spend time deriving the basic result. The derivation is not so important. The **result** is important:

$$\boxed{v_{group} = \left.\frac{d\omega}{dk}\right|_{k_0} = \frac{\hbar k_0}{m}}$$

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

Particular example of the Gaussian wavepacket.

$$\varphi(x,t) \cong \int_{-\infty}^{\infty} dk\, e^{-k^2/4\alpha^2} e^{ikx} e^{-i\omega t}$$

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

$$\varphi(x,t) \cong \int_{-\infty}^{\infty} dk\, e^{-\left[\frac{1}{4\alpha^2} + i\frac{\hbar}{2m}t\right]k^2} e^{ikx}$$

Use same integral as before

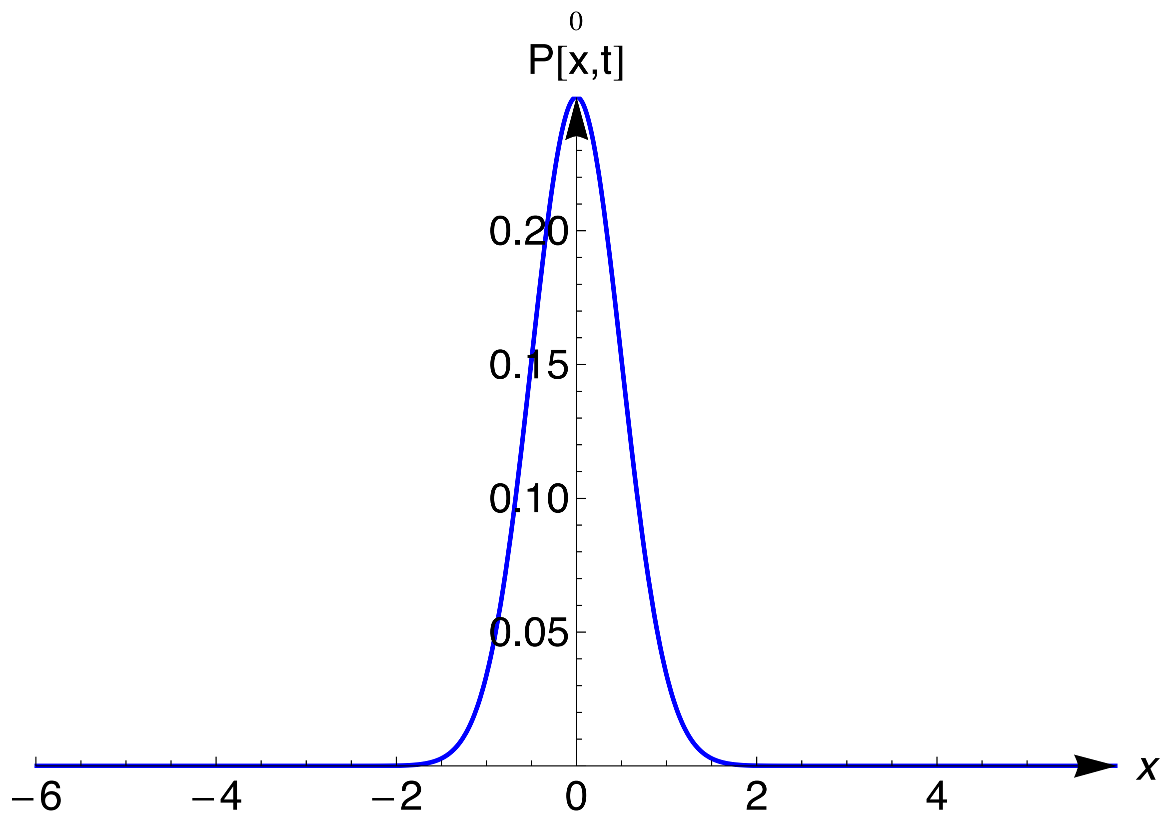
$$\boxed{\varphi(x,t) \cong \frac{1}{\sqrt{1+it/\tau}}\, e^{-\alpha^2 x^2/[1+it/\tau]}}$$

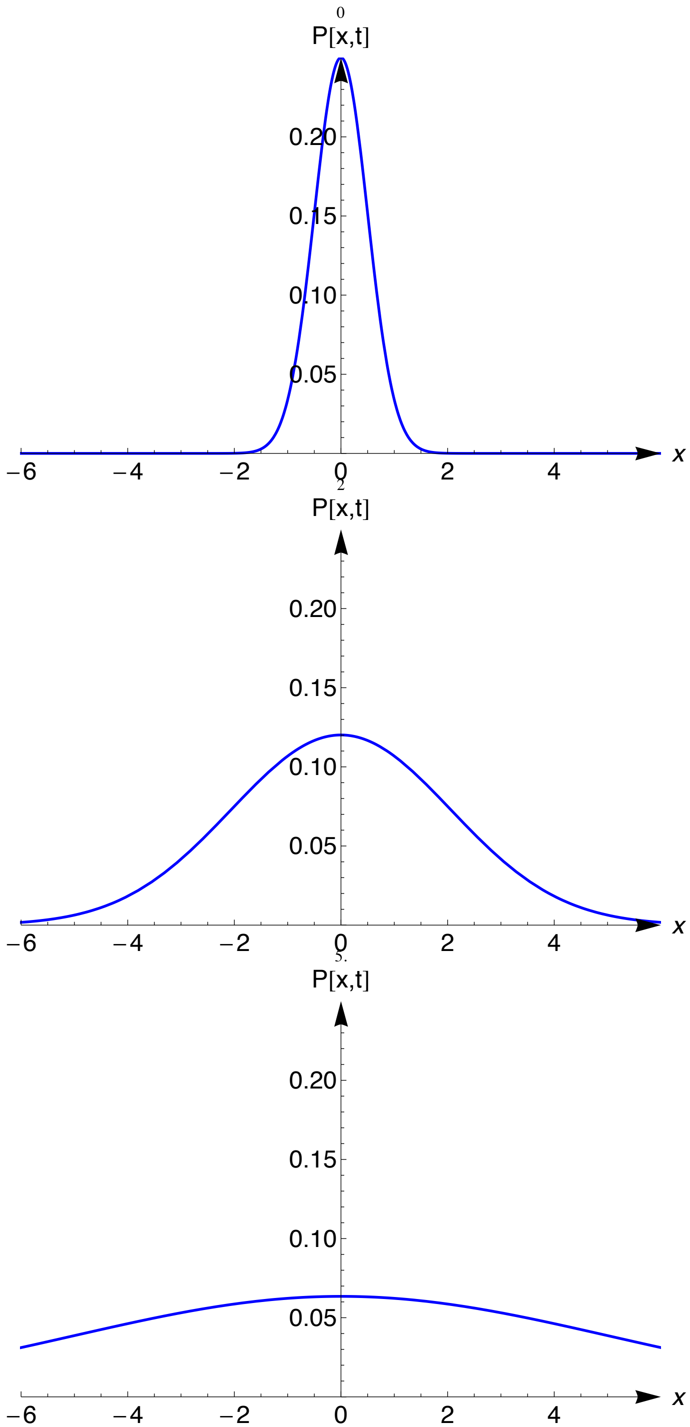
$$\tau = \frac{m}{2\hbar\alpha^2}$$

$$\boxed{P(x,t) \cong \frac{1}{\sqrt{1+t^2/\tau^2}}\, e^{-2\alpha^2 x^2/\left[1+t^2/\tau^2\right]}}$$

$$\boxed{P(x,t) \cong \frac{1}{\sqrt{1 + t^2/\tau^2}} e^{-2\alpha^2 x^2 / \left[1 + t^2/\tau^2\right]}}$$

$$\tau = \frac{m}{2\hbar\alpha^2}$$

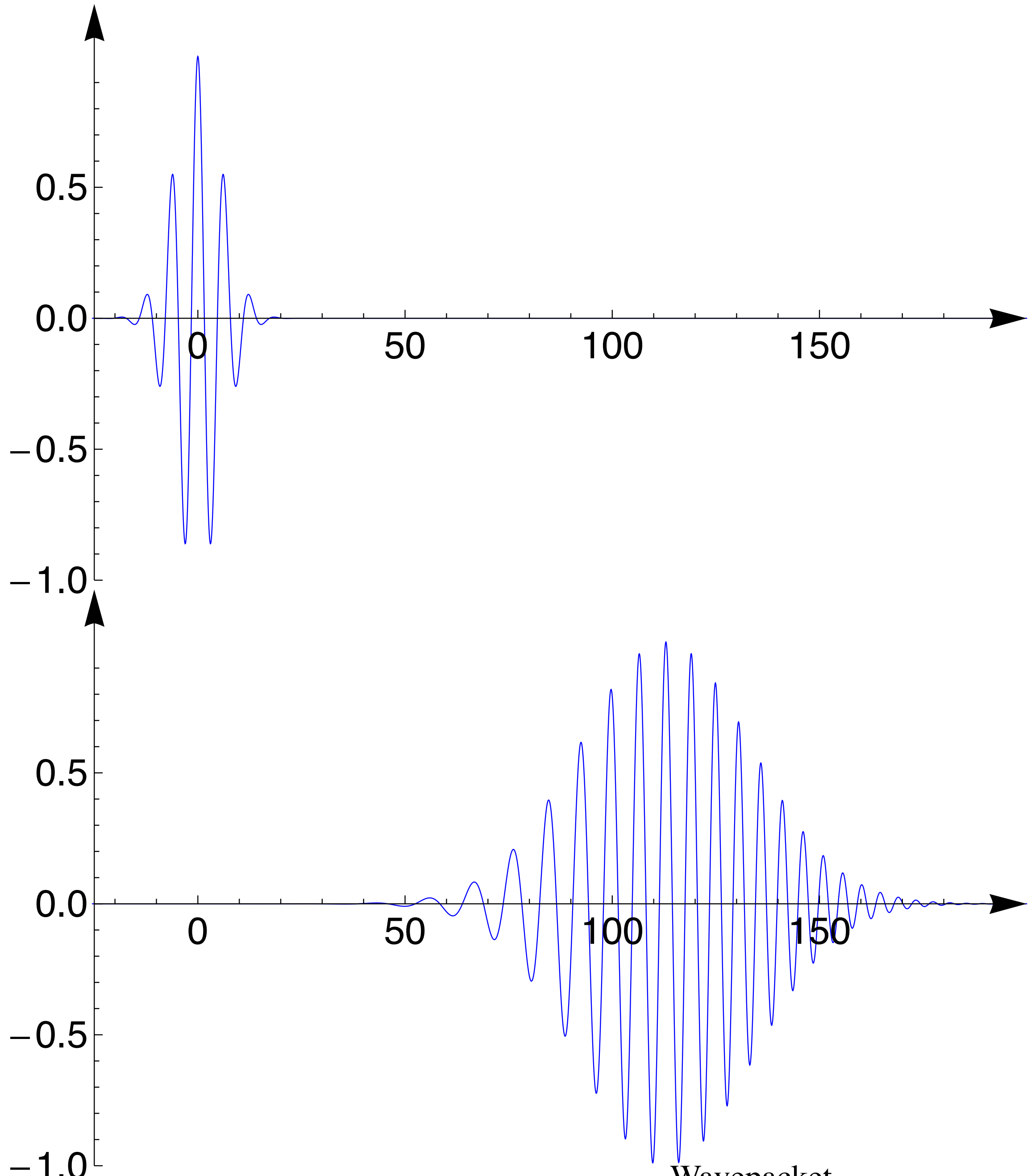




$$\boxed{P(x,t) \cong \frac{1}{\sqrt{1+t^2/\tau^2}}\, e^{-2\alpha^2 x^2/\left[1+t^2/\tau^2\right]}}$$

$$\boxed{\varphi(x,t) \cong \frac{1}{\sqrt{1+it/\tau}}\, e^{-\alpha^2 x^2/\left[1+it/\tau\right]}}$$

Zero-momentum wavepacket:
Spreads but doesn't travel!
It has many positive k components as it has negative k components.



Finite-momentum wavepacket:
Spreads and travels!

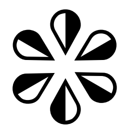
$$P(x,t) \cong \frac{1}{\sqrt{1 + t^2/\tau^2}} e^{-2\alpha^2 x^2/\left[1+t^2/\tau^2\right]}$$

τ is characteristic time for wavepacket to spread

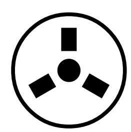
$$\tau = \frac{m}{2\hbar\alpha^2}$$

τ for macroscopic things:
$m \approx 10^{-3}$kg; $1/\alpha \approx 10^{-2}$ m
$\tau \approx 10^{27}$ s $\approx 10^{20}$ yr   !! long

τ for atomic scale:
$m \approx 10^{-?}$kg; $1/\alpha \approx 10^{-?}$ m
$\tau \approx 10^{-?}$ s



τ for nuclear scale:
$m \approx 10^{-?}$kg; $1/\alpha \approx 10^{-?}$ m
$\tau \approx 10^{-?}$ s

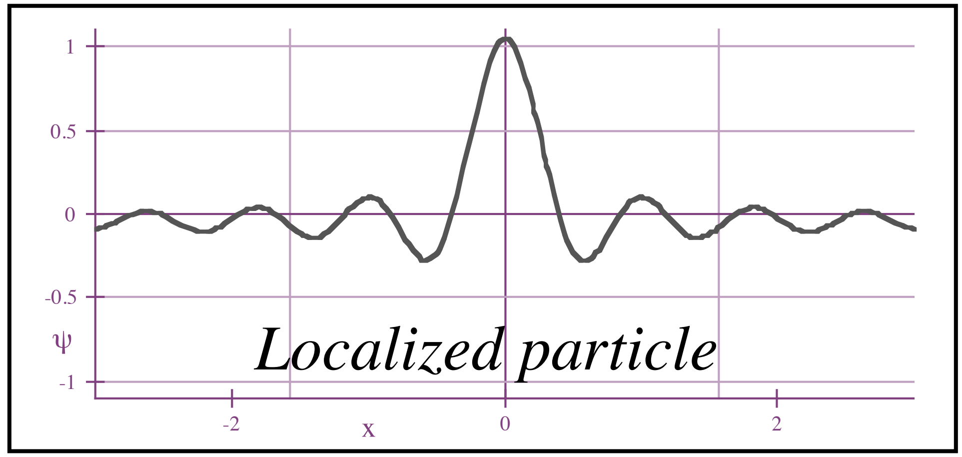


FREE PARTICLE QUANTUM WAVEPACKET - REVIEW

- *Gaussian superposition of free-particle eigenstates (of energy and momentum!)*
- *Localized in space means dispersed in momentum and vice versa.*
- *Look at time-dependent probability distribution: packet broadens and moves*

For those of you who want more about the group velocity:

$$\varphi(x,t) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx} e^{-i\omega_k t}$$



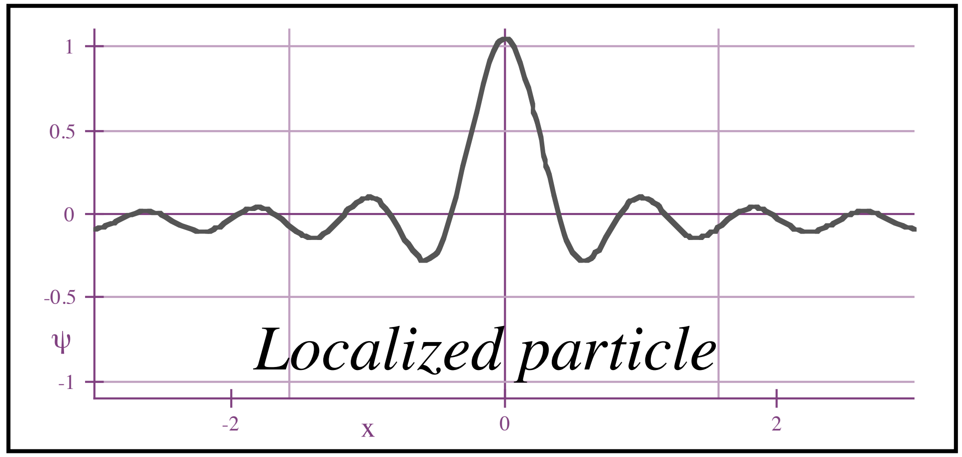
$$\omega(k) = \omega_0 + \left.\frac{d\omega}{dk}\right|_{k=k_0} \left(k - k_0\right)$$

ω is a smooth function of k and $\omega_0 = \omega(k_0)$

$$\varphi(x,t) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx} e^{-i\left(\omega_0 + \left.\frac{d\omega}{dk}\right|_{k=k_0} \left(k - k_0\right)\right)t}$$

$$k - k_0 = s$$

For those of you who want more about the group velocity:



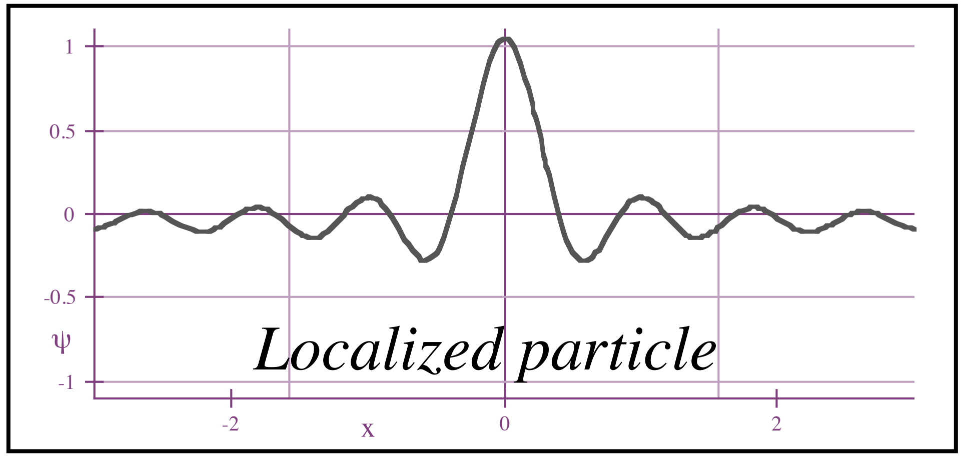
$$\varphi(x,t)=\int_{-\infty}^{\infty} dk\,A(k)e^{ikx}e^{-i\left(\omega_0+\left.\frac{d\omega}{dk}\right|_{k_0}(k-k_0)\right)t}$$

$$k-k_0=s$$

$$\varphi(x,t)=\int_{-\infty}^{\infty} d\left(k_0+s\right)A(k_0+s)e^{i(k_0+s)x}e^{-i\left(\omega_0+\left.\frac{d\omega}{dk}\right|_{k_0}(k_0+s-k_0)\right)t}$$

$$\varphi(x,t)=e^{-i\left(\omega_0-k_0\left.\frac{d\omega}{dk}\right|_{k_0}\right)t}\int_{-\infty}^{\infty} d\left(k_0+s\right)A(k_0+s)e^{i(k_0+s)\left(x-\left.\frac{d\omega}{dk}\right|_{k_0}t\right)}$$

For those of you who want more about the group velocity:



$$k = k_0 + s$$

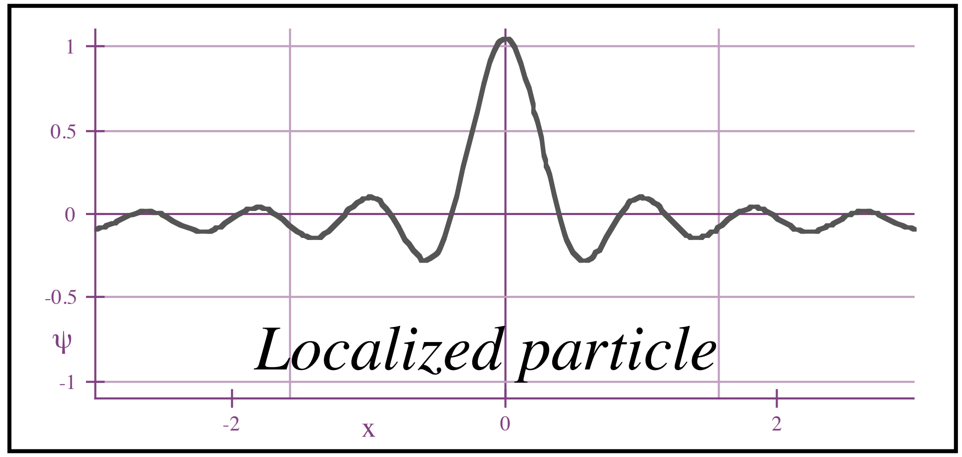
$$\varphi(x,t) = e^{-i\left(\omega_0 - k_0 \left.\frac{d\omega}{dk}\right|_{k_0}\right)t} \int_{-\infty}^{\infty} d\left(k_0 + s\right) A(k_0 + s) e^{i(k_0+s)\left(x - \left.\frac{d\omega}{dk}\right|_{k_0} t\right)}$$

$$\varphi(x,t) = e^{-i\left(\omega_0 - k_0 \left.\frac{d\omega}{dk}\right|_{k_0}\right)t} \int_{-\infty}^{\infty} dk\, A(k) e^{ik\left(x - \left.\frac{d\omega}{dk}\right|_{k_0} t\right)}$$

Phase factor - goes to 1 in probability

For those of you who want more about the group velocity:

$$\boxed{\varphi(x,0) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx}}$$



$$\varphi(x,t) = phase \int_{-\infty}^{\infty} dk\, A(k) e^{ik\left(x - \left.\frac{d\omega}{dk}\right|_{k_0} t\right)}$$

$$\varphi(x,t) = phase \int_{-\infty}^{\infty} dk\, A(k) e^{ik\left(x - v_g t\right)} = \varphi(x - v_g t, 0)$$

Wavepacket

$$\boxed{v_g = \left.\frac{d\omega}{dk}\right|_{k=k_0}}$$