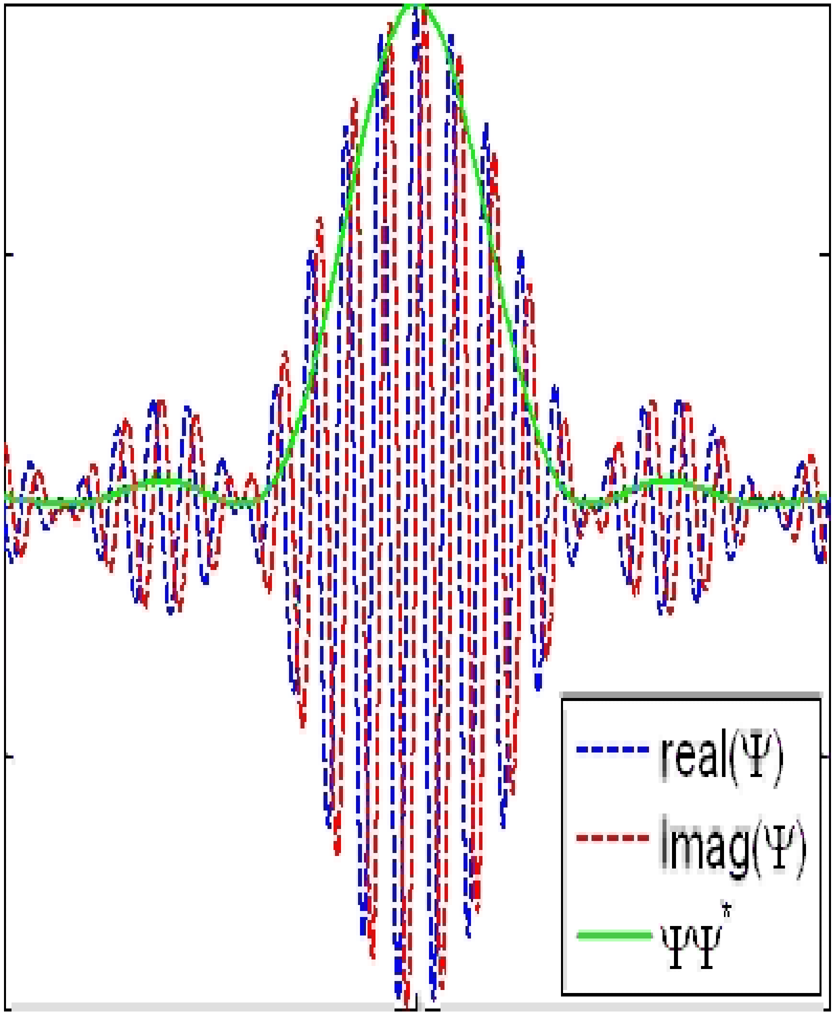
Lecture 12: 02/13/09

- Physical meaning of the Wave Function
  - Normalization
  - Expectation Values
  - Operators
- Stationary States
  - Properties
  - time-independent Schrödinger equation



Recap:

$II_{1,3}$ Plausibility Argument leading to Schrödinger's Equation:

Postulates: wave equation $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x,t)\Psi(x,t)$

wave function for free particle with const. E, p $\quad \Psi(x,t) = e^{i(kx-\omega t)}$ ← plane complex wave

Time-dependent Schrödinger equation: $i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi(x,t)$

$\hat{H}$: Hamiltonian operator: $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$

$II_{1,4}$ Physical Significance of the Wave Function $\Psi(x,t)$:

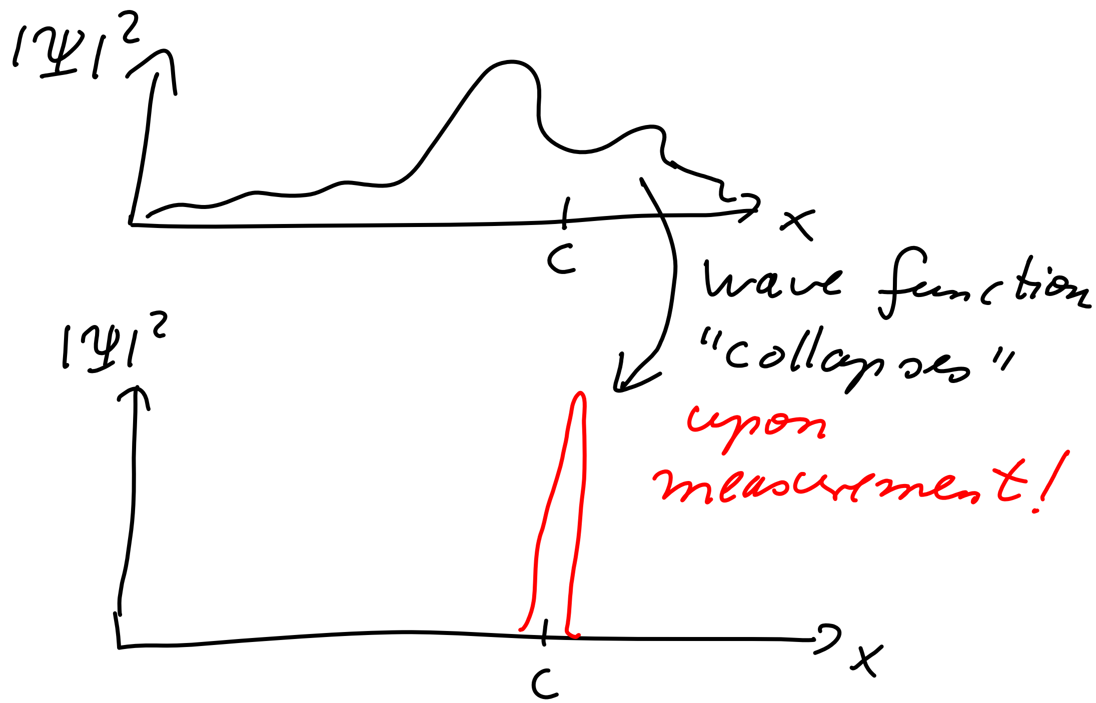
$$\int_a^b |\Psi|^2 dx = \int_a^b \underbrace{\Psi^* \Psi\, dx}_{= P(x,t)dx} = \left\{ \begin{array}{l} \text{probability of finding the} \\ \text{particle between a and b} \\ \text{at time } t \end{array} \right\}$$

$= P(x,t)dx$: probability density

Measurement:

- $|\Psi|^2$ just before measurement

- $|\Psi|^2$ immediately after measurement has found particle at point "c"



For a proper wave function, $\int_{-\infty}^{\infty} \left|\Psi(x,t)\right|^2 dx = ?$

A. 0

B. 1

C. infinite

D. Something else

Probability of finding the particle somewhere must be $= 1$!

– Normalization:

require $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1$ Normalization condition

(Probability of finding particle somewhere $\stackrel{!}{=} 1$)

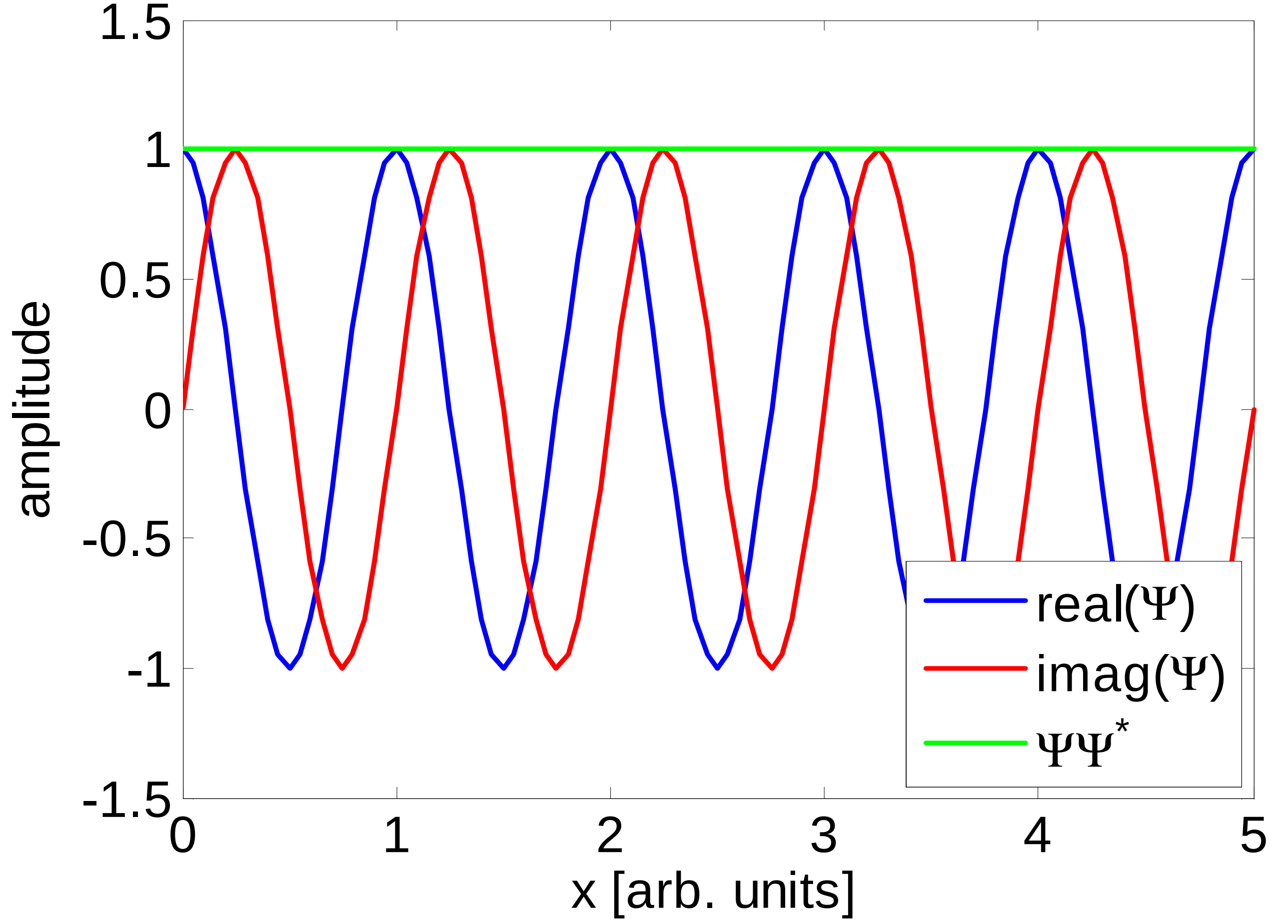
Note: If $\Psi(x,t)$ is solution of S.E. $\Rightarrow c\,\Psi(x,t)$ is too!

$\Rightarrow$ if $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = a$ normalized wave function $= \frac{1}{\sqrt{a}}\Psi(x,t)$

$\Rightarrow$ Note: If a wave function is normalized at time $t=0$ it will stay normalized as time goes on!

Examples: ① Plane complex wave: free particle with constant E, p

$\Psi = A e^{i(kx - \omega t)}$ $\Rightarrow$ $P(x,t) = |A|^2 = \text{const}$!



$\Rightarrow$ Problem: can not be normalized $\Rightarrow$ not physical!

Examples: ① Plane complex wave: free particle with constant E, p

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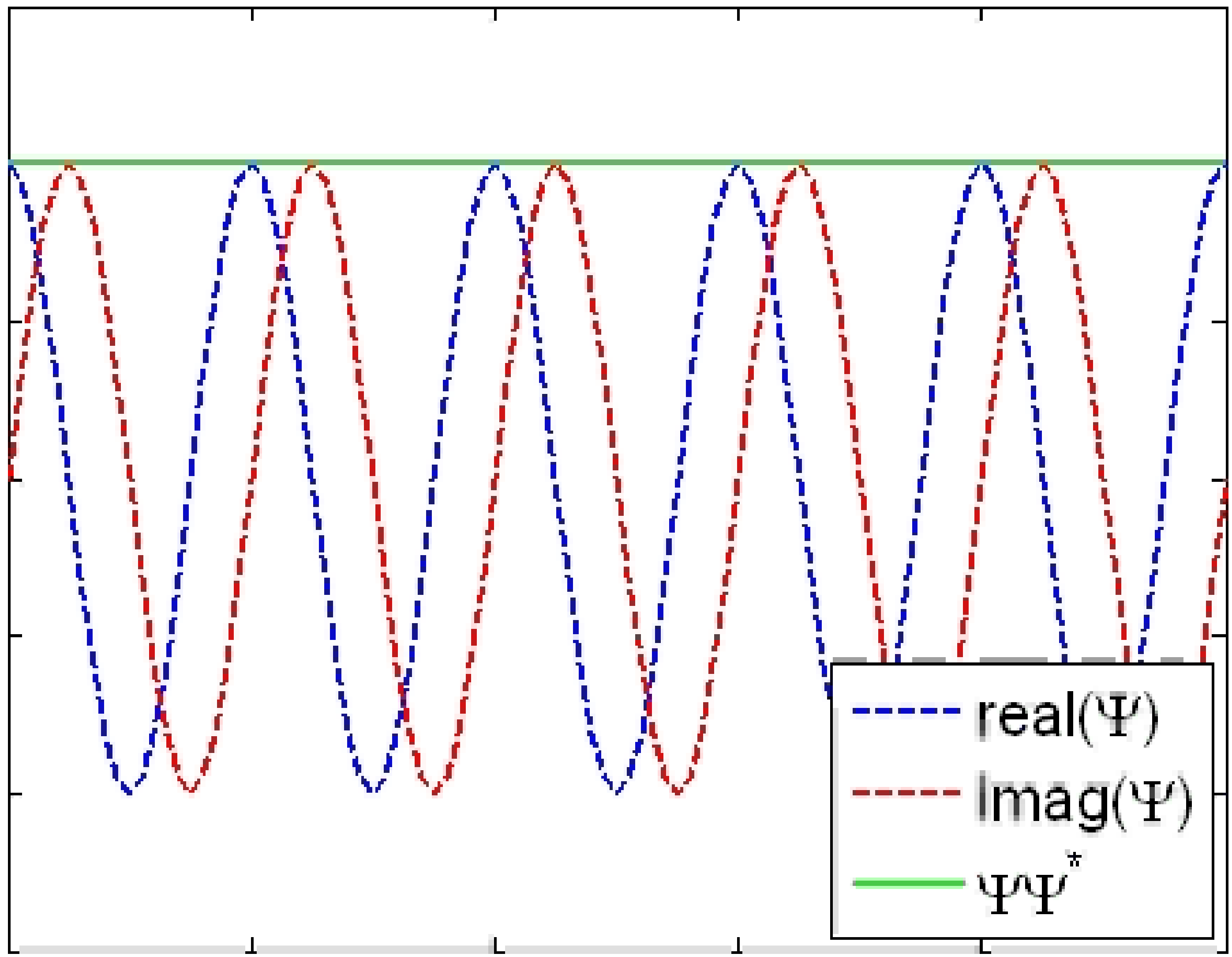
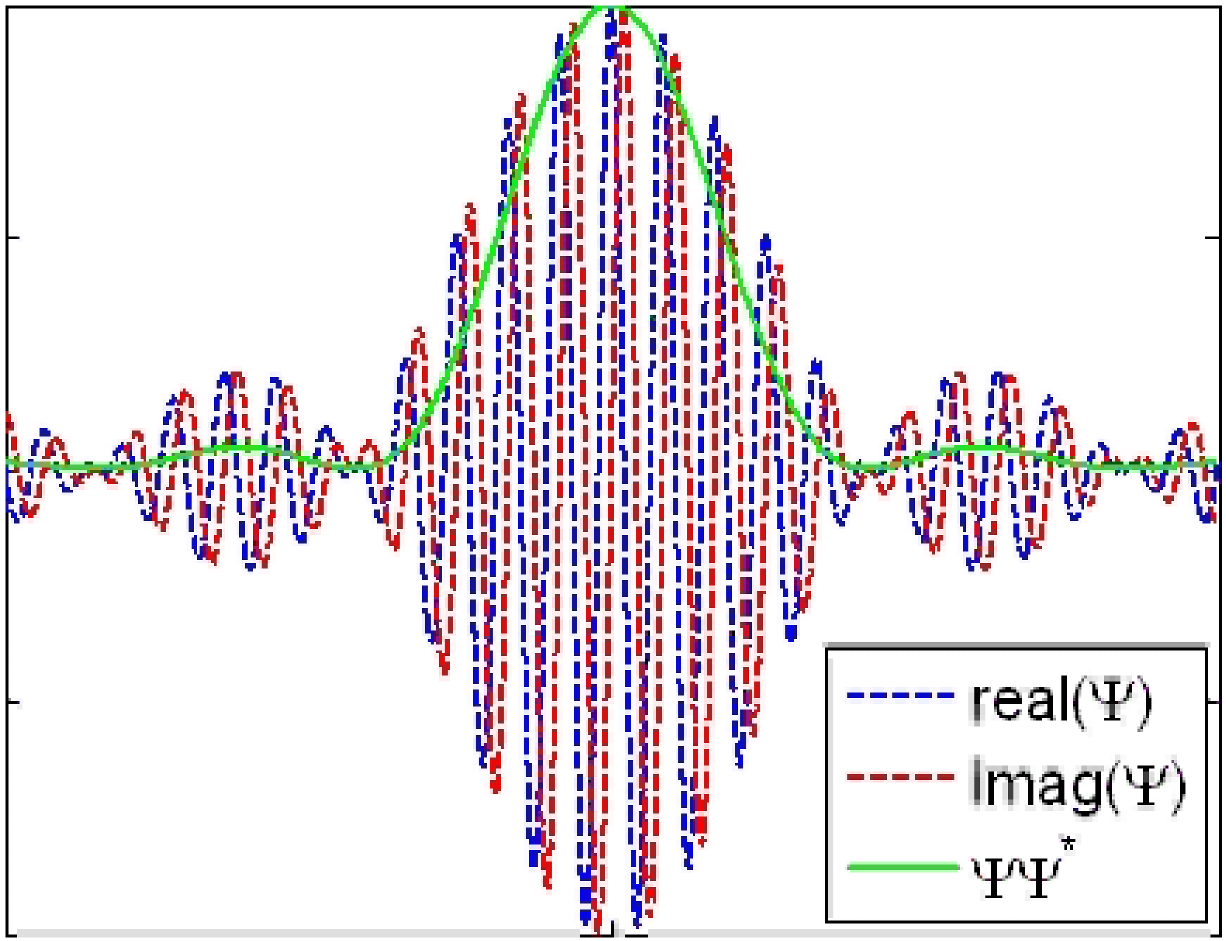
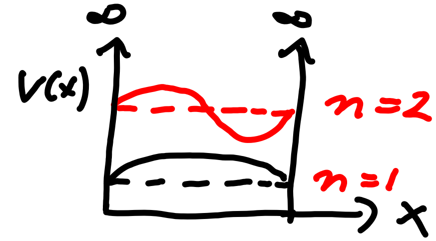


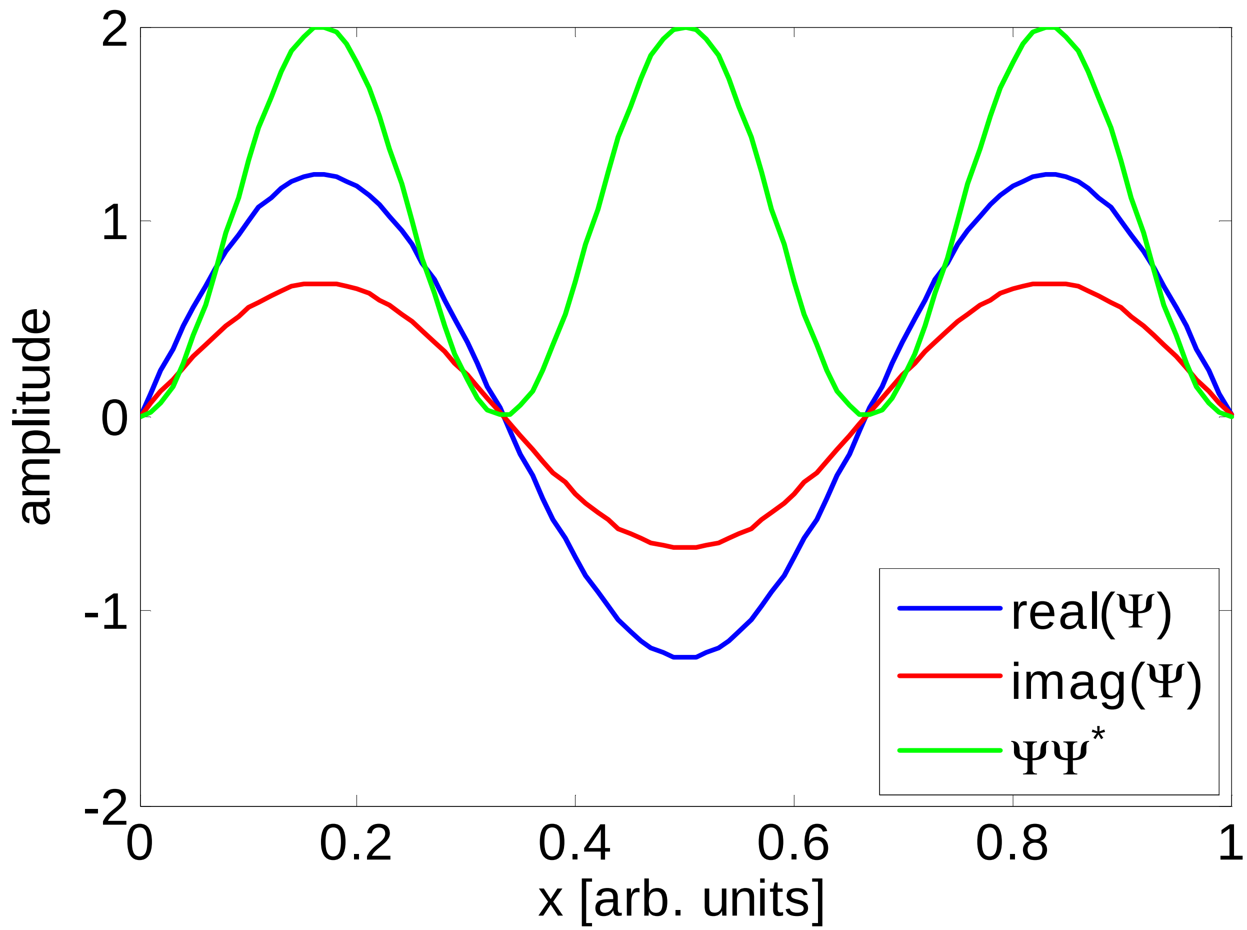
② Wave packet:



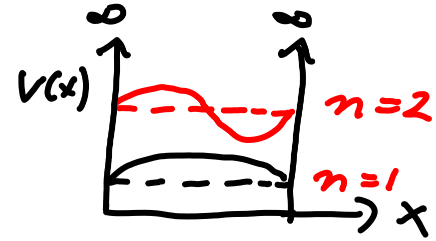
③ Particle in a 1D-box:



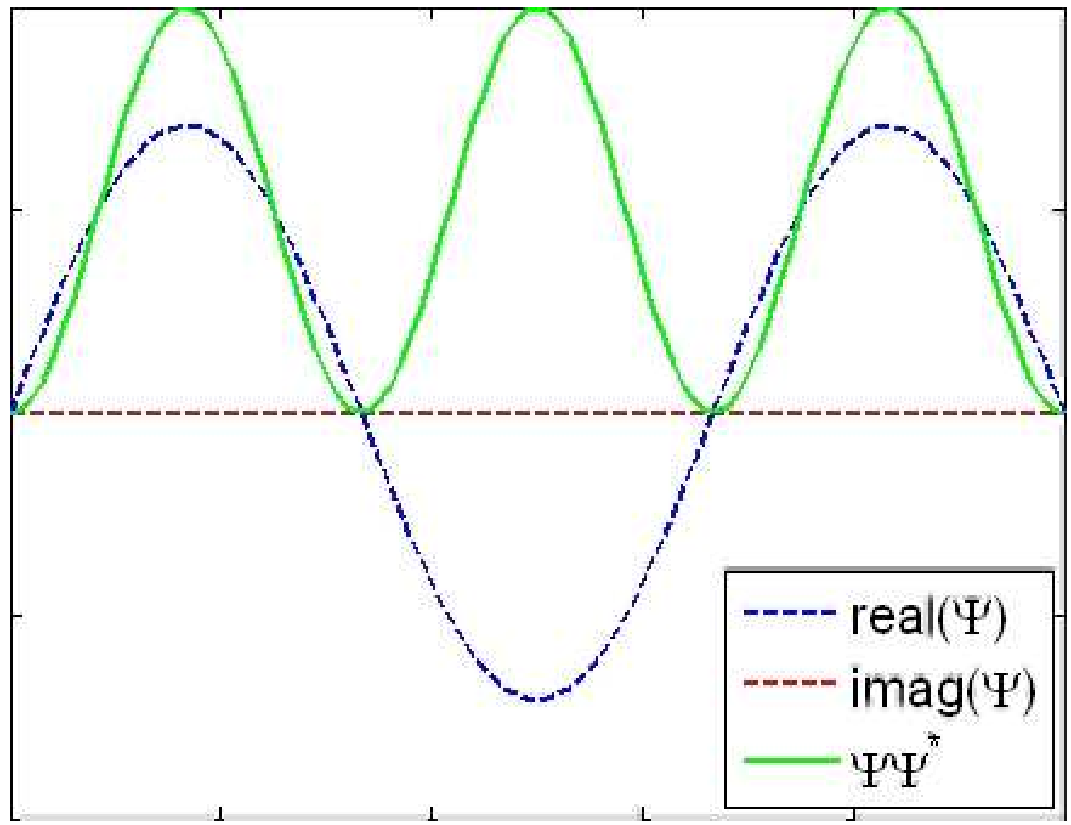
n = 3 state



③ Particle in a 1D-box:



n=3 state



$|\Psi|^2 = \Psi^* \Psi \rightarrow$ time independent! $\Rightarrow$ stationary state

Note: $\Psi(x,t)$ itself is still time dependent!

$II_{1,5}$ Expectation Values

- start with position:

wave function spreads over certain space → can not give definite position value for particle

but: specify average measured position of a particle = expectation value of the x-coordinate

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \, P(x,t) \, dx$$

value of x — probability of observing that value

⇒ Born's postulate $P(x,t) = \Psi^* \Psi$

$$\Rightarrow \quad \langle x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) \, x \, \Psi(x,t) \, dx$$

Note: The expectation value is the average of repeated measurements on an ensemble of identically prepared systems!

It is not what you would get if you measure the position of one particle over and over again!

A particle is associated with the following wave function:

$$\Psi(x,t)=\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right)e^{-i\omega t}$$ **for –L/2<x<L/2**

$$\Psi(x,t)=0$$ **elsewhere**

If the position *x* of the particle would be measured, the result would be:

A. x=0

B. Something between –L/2 and +L/2

C. Something between –∞ and +∞

D. Something else

A particle is associated with the following wave function: $\Psi(x,t) = \sqrt{\frac{2}{L}}\cos(\frac{\pi x}{L})e^{-i\omega t}$ **for –L/2<x<L/2**

$\Psi(x,t) = 0$ **elsewhere**

What is the expectation value of the position <*x*>?

- **A. <x> = 0**
- **B. <x> = L/2**
- **C. <x> = -L/2**
- **D. <x> ≈ L/4**
- **E. Something else**

Symmetry of probability density about x=0! -> <x> =0

• Expectation value of the particle momentum:

want: $\langle p \rangle = m \langle v \rangle = m \dfrac{d\langle x \rangle}{dt}$

start with: $\dfrac{d\langle x\rangle}{dt} = \displaystyle\int_{-\infty}^{+\infty} x \frac{\partial}{\partial t} |\Psi|^2 dx$

$$\frac{\partial}{\partial t}|\Psi(x,t)|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t}\Psi$$

↑ product rule

use Schrödinger's equation:

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi$$

complex conjugate:

$$\frac{\partial \Psi^*}{\partial t} = \frac{-i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V \Psi^*$$

$$\Rightarrow \frac{\partial}{\partial t}|\Psi|^2 = \frac{i\hbar}{2m}\left(\Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi^*}{\partial x^2}\Psi\right) = \frac{\partial}{\partial x}\left\{\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\right\}$$

$$\Rightarrow \frac{d\langle x\rangle}{dt} = \int_{-\infty}^{+\infty} x \frac{\partial}{\partial t}|\Psi|^2 dx = \frac{i\hbar}{2m}\int_{-\infty}^{+\infty} \underbrace{x}_{f} \frac{\partial}{\partial x} \underbrace{\left\{ \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi \right\}}_{g} dx$$

use integration by parts:

$$\frac{d}{dx}(fg) = f\frac{dg}{dx} + \frac{df}{dx}\cdot g \Rightarrow \int_a^b f\frac{dg}{dx}dx = -\int_a^b \frac{df}{dx} g\, dx + fg\Big|_a^b$$

$$\Rightarrow \frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}\int_{-\infty}^{+\infty} 1\cdot\left\{\Psi^*\frac{\partial\Psi}{\partial x} - \underbrace{\frac{\partial \Psi^*}{\partial x}}_{\partial g/\partial x}\underbrace{\Psi}_{f}\right\}dx + \underbrace{fg\Big|_{-\infty}^{+\infty}}_{=0}$$

$=0$, $|\Psi| \xrightarrow[x\to\pm\infty]{} 0$ so that Ψ can be normalized

2^{nd} integration by parts on 2^{nd} term:

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}\int_{-\infty}^{+\infty} 2\Psi^*\frac{\partial\Psi}{\partial x}dx = -\frac{i\hbar}{m}\int_{-\infty}^{+\infty}\Psi^*\frac{\partial\Psi}{\partial x}dx = \langle v\rangle$$

expectation value for velocity

$$\Rightarrow \text{finally: } \langle p\rangle = m\langle v\rangle = -i\hbar\int_{-\infty}^{+\infty}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)dx$$

$$\Rightarrow \langle p \rangle = \int_{-\infty}^{+\infty} \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi \, dx \quad \Big\} \text{ expectation value of particle momentum}$$

- operator $\frac{\hbar}{i} \frac{\partial}{\partial x}$ $\longleftrightarrow$ "represents" momentum in quantum mechanics

  x $\longleftrightarrow$ "represents" position

$\Rightarrow$ For other quantities:

- Recipe: 1) express quantity as function of position and momentum
  2) replace "p" by $\frac{\hbar}{i} \partial/\partial x$, "replace" x by x

$$\Rightarrow \langle Q(x,p) \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\, \hat{Q}\left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}\right) \Psi(x,t)\, dx$$

Example: $\langle x^2 \rangle = \int_{-\infty}^{+\infty} \Psi^* x^2 \Psi \, dx$ $\Rightarrow$ variance: $\sigma_x^2 \equiv \langle x^2 \rangle - \langle x \rangle^2$

- potential energy : $\langle V \rangle = \int_{-\infty}^{+\infty} \Psi^* V(x,t)\, \Psi \, dx$

- kinetic energy : $KE = \frac{p^2}{2m} \Rightarrow \langle KE \rangle = \int_{-\infty}^{+\infty} \Psi^* \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \Psi \, dx$

- total energy $\langle E \rangle = \langle KE \rangle + \langle V \rangle = \int_{-\infty}^{+\infty} \Psi^* \Big(\underbrace{-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t)}_{= \hat{H}} \Big) \Psi \, dx$

$= \hat{H}$: Hamiltonian operator!