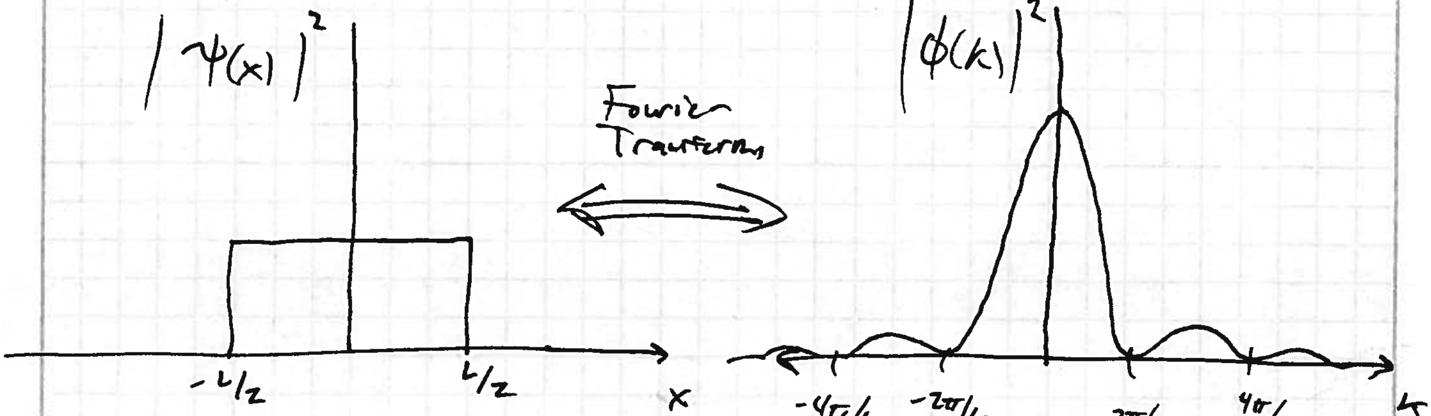
For the top-hat free particle, the momentum space wavefunction looks like



Comments #1

- If we confine $\psi(x)$ by making L smaller, then $\phi(k)$ gets wider ($2\pi/L$ becomes larger). So the widths of $\psi(x)$ and $\phi(k)$ are inversely related. Conversely, a less-confined $\psi(x)$ has a $\phi(k)$ which is narrower.

Qualitatively speaking,

$$\left(\text{width of } |\psi(x)|^2\right) \sim \frac{1}{\left(\text{width of } |\phi(k)|^2\right)}$$

or

$$\underbrace{(\Delta x)}_{\text{width of } |\psi(x)|^2} \underbrace{(\Delta p)}_{\text{width of } |\phi(k)|^2} \sim 1$$

Later we will show that the true, exact relation is

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

This is an example of the Uncertainty Principle. poorly know

For the top-hat wavefunction, $\Delta x \Delta p$ turns out to be larger than $\hbar/2$:

$$\Delta x \Delta p > \frac{\hbar}{2} \quad \text{(for the top-hat wavefunctio}$$

For a Gaussian wavefunction,

$$\Delta x \Delta p = \frac{\hbar}{2} \quad \text{(Gaussian Wavefunction)}$$

It turns out that no wavefunction at all can have a $\Delta x \Delta p$ less than the Gaussian wavefunction

Comment #2

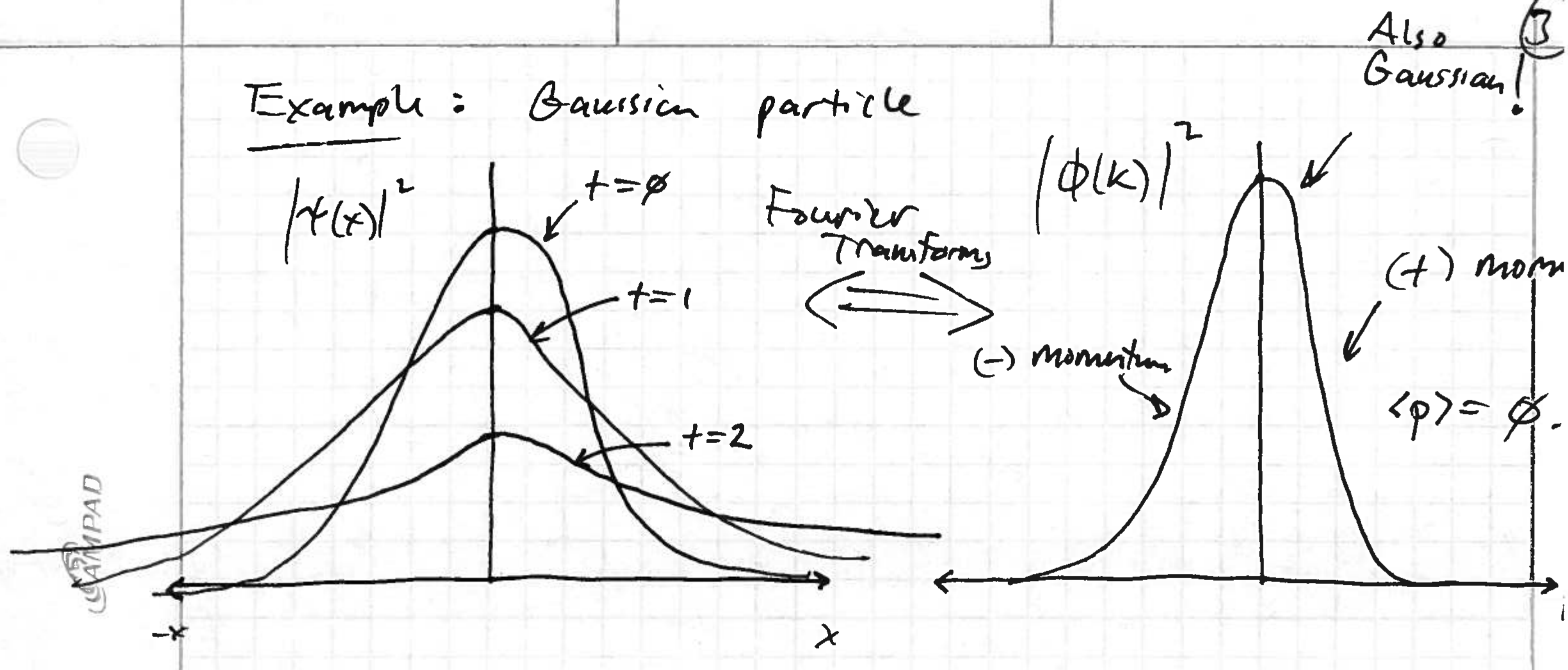
For ~~the~~ our top-hat wavefunction, $\phi(k)$ is symmetric around $k = \emptyset$, so $\langle p \rangle = 0$ ⇐ "Quantum mechanical particle at rest".

~~But suppose we wait~~

Question: Does this mean that $\psi(x)$ will not change as time goes forward?

Answer: No! $\psi(x)$ contains equal numbers of $(+k)$ and $(-k)$ components. These represent plane waves moving in the $(+x)$ and $(-x)$ directions. As time goes forward, $\psi(x)$ becomes wider, but remains centered on $x=0$ because it spreads equally in both directions.

Example: Gaussian particle



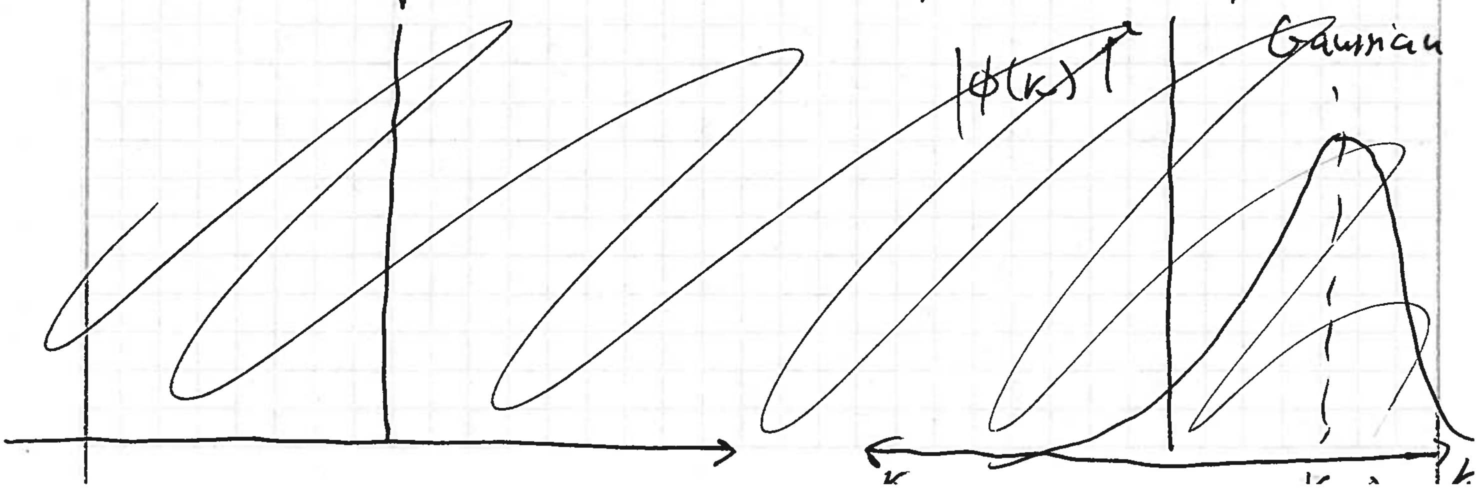
The spatial wavefunction spreads out in time.

All localized ~~[illegible]~~ free particles in QM always spread out in time. We can't keep them confined without a binding potential. However, since $\langle p \rangle = 0$, the center of the wavefunction remains at $x=0$.

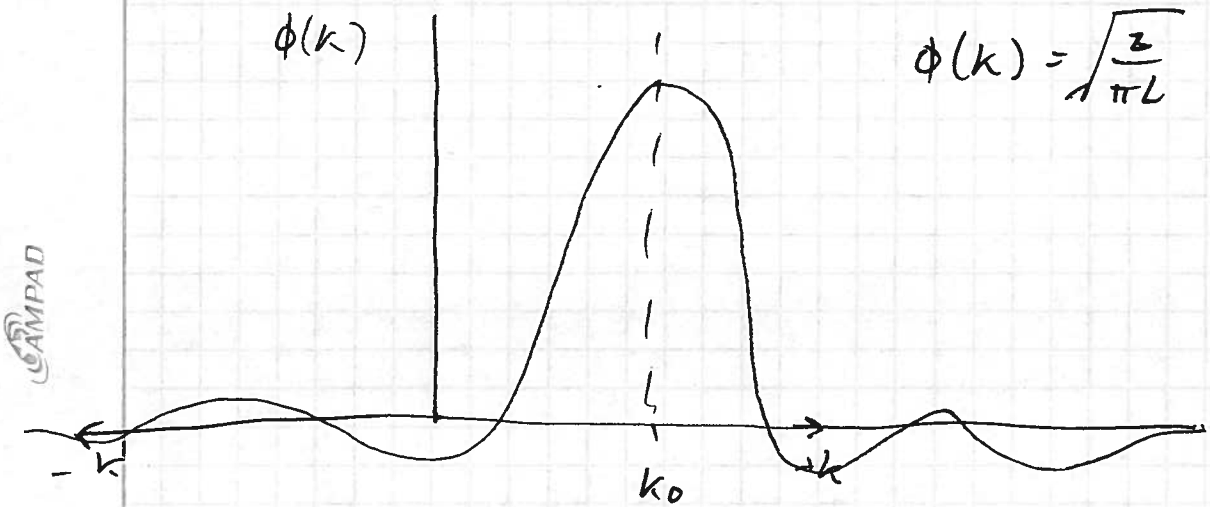
This is the closest thing to a particle at rest in QM.

Comment # 3 How can we represent a moving free particle?

Answer: Displace the $\phi(k)$ away from $k=0$:



For example, suppose we displace $\phi(k)_{\text{top-hat}}$ away from $k=0$:



$$\phi(k) = \sqrt{\frac{2}{\pi L}}\ \frac{\sin((k-k_0)L/2)}{(k-k_0)}.$$

What will $\psi(x)$ look like? A top-hat?

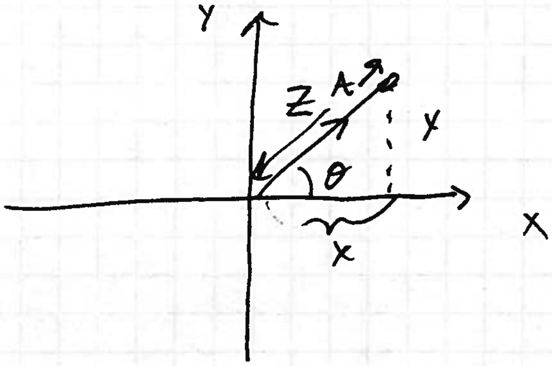
Yes, but with a phase factor

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\, \phi(k) e^{+ikx} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk \sqrt{\frac{2}{\pi L}}\ \frac{\sin((k-k_0)L/2)}{(k-k_0)} \times e^{ikx}$$

$$= \begin{cases} \frac{1}{\sqrt{L}}\, e^{ik_0 x}, & -\frac{L}{2} < x < \frac{L}{2} \\ 0, & \text{otherwise} \end{cases}$$

plane wave phase factor represents moving free-particle.

Complex numbers



$$z = x + iy = Ae^{i\theta}$$

$$|z|^2 = z^* z$$

$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$\theta = \tan^{-1}(y/x)$$

$$A = \sqrt{x^2 + y^2}$$

$$x = A\cos\theta$$

$$y = A\sin\theta$$

Differential Eqs.

$$\frac{dy(t)}{dt} = A \Rightarrow y(t) = At + C$$

$$\frac{dy(t)}{dt} = Ay(t) \Rightarrow y(t) = Ce^{At}$$

$$\frac{d^2y(t)}{dt^2} + Ay(t) = 0 \Rightarrow y(t) = C_1 e^{i\sqrt{A}t} + C_2 e^{-i\sqrt{A}t}$$

Constants C_1, C_2 determined by initial conditions

Wave Dictionary

λ = wavelength

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

T = period

ν = freq. $= \frac{1}{T}$

$\omega = 2\pi\nu = \frac{2\pi}{T}$

phase change due to $\Delta x = k\Delta x$

" $\Delta t = \omega\Delta t$

Planck Formula for energy of a photon: $E = h\nu = \hbar\omega$

DeBroglie Wavelength - $\lambda = \frac{h}{p}$ ← particle momentum.

Then $p = \frac{h}{\lambda} = \hbar k$

Expectation Value : $\langle c \rangle = \bar{c} = \sum_{i=1}^{N} P_i c_i$

probability to observe c_i

or $\langle c \rangle = \int_{\text{all possible } c\text{'s.}} c \, P(c) \, dc$

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

Variance : $\sigma^2 = (\Delta c)^2 = \frac{1}{N} \sum_{i=1}^{N} \left(c_i - \langle c \rangle \right)^2$

$= \langle c^2 \rangle - \langle c \rangle^2$

Standard Dev: $\sigma = \Delta c = \sqrt{\langle c^2 \rangle - \langle c \rangle^2}$

Postulates of QM

I : For any observable A, we have $\hat{A} \phi = a \phi$
$\hat{A}$: an operator , a : an eigenvalue , ϕ : an eigenfunct
Measurement of A always returns an eigenvalue (a).

II : The system is described by $\Psi(x,t)$.
Expectation values are calculated : $\langle c \rangle = \int \Psi^* \hat{C} \Psi \, dx$
$|\Psi|^2 dx$ is the probability to find the particle between x & $x + dx$.

III : Collapse of the Wavefunction. If A is measured, and e.v. (a) results, the wavefunction will be left in e.f. ϕ_a.

IV : $\Psi(x,t)$ evolves in time as (when the system is not measured)
$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$, $\hat{H}$ = Hamiltonian = Energy Operator

Common Operators	e.v. equation	Sol'n
$\hat{p} = -i\hbar \frac{d}{dx}$	$-i\hbar \frac{d}{dx}\varphi(x) = p\,\varphi(x)$	$\varphi(x) = Ae^{ik}$
$\hat{x} = x$	$\hat{x}\,\delta(x) = x\,\delta(x)$	$\delta(x)$ = Dirac Delta Function
$\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$ $= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$	$\hat{H}\varphi = E\varphi$	Sol'n depends on $V(x)$.

General Solution to the TDSE.

$$\Psi(x,t) = \sum_n a_n \varphi_n(x)\, e^{-iE_nt/\hbar} \quad \text{for discrete } \varphi_n.$$

Coeff. Determined by $\Psi(x,t=0) = \psi(x)$; e.f. of $\hat{H}$.

Define $\omega_n \equiv E_n/\hbar$.

We call ~~φ_n~~ the e.f. of $\hat{H}$ "stationary states" because all probabilities & expectation values are constant in time if $\Psi(x,t)$ is an e.f. of $\hat{H}$.

~~Particle in a Box : $V(x) = \begin{cases} 0, & 0<x<L \\ +\infty, & \text{otherwise} \end{cases}$~~

~~Sol'ns $\varphi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}$, $E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}$~~

For a particular intial state, $\{a_n\}$ can be calculated by

$$a_m = \int \varphi_m^*(x)\,\psi(x)\,dx$$

$|a_m|^2$ can be interpreted as the probability to measure E_m, a particular energy e.V.

$$|a_m|^2 = P(E_m)$$

Particle-in-a-Box $\quad V(x) = \begin{cases} \emptyset & 0<x<L \\ +\infty, & \text{otherwise} \end{cases}$

$$\varphi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

$\{\varphi_n\}$ are ortho-normal:

$$\int \varphi_m^* \varphi_n \, dx = \delta_{mn} = \begin{cases} 1, & m=n \\ \emptyset, & \text{otherwise} \end{cases}$$

$\{\varphi_n\}$ are standing waves. Their form is determined by the boundary conditions.

Free-Particle

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

$\hat{H}$ & $\hat{p}$ have common e.f.
All e.f. of $\hat{p}$ are also e.f. of $\hat{H}$.

$$\{\varphi(x)\} = \{A e^{ikx}\}$$

a continuum of e.f. & e.V.

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

$\varphi_k(x)$ are not normalizable, but we can use them to construct normalizable states

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} \, dk \quad \text{for some } \phi(k).$$

Then $\quad \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx}\, dx$

$\phi(k)$ is the momentum space wavefunction.

$|\phi(k)|^2 dk =$ probability to observe momentum between k & $k+dk$.

General Soln: for free particle

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{+i(kx - \hbar k^2 t/2m)}\, dk$$

where $\quad \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx}\, dx.$