Free Particle $V(x) = \emptyset$,

$$\hat{H}_{Free} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} \quad \text{because } V(x) = \emptyset$$

What are the energy eigenstates (stationary states)?

eigenvalue equation: $\frac{-\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} = E\,\varphi(x)$

$$\boxed{\varphi''(x) + \frac{2mE}{\hbar^2}\varphi(x) = \emptyset}$$

Solution:

$$\varphi(x) = A e^{ikx} + B e^{-ikx}, \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

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

Same solution as particle-in-a-box, but this time there's no boundary conditions.

Recall: Ae^{ikx} is an eigenstate of momentum.

Eigenstates of momentum are stationary states of the free particle Hamiltonian.

We will use the momentum eigenstates Ae^{ikx} to construct general solutions to free particle states

For Particle-in-a-box we have discrete stationary states:

$$\varphi_n(x) = \{\varphi_1(x),\ \varphi_2(x),\ \varphi_3(x),\ \ldots\}$$

Discrete Eigenvalues:

$$E_n = \{E_1,\ E_2,\ E_3,\ \ldots\}$$

General solution is a discrete sum:

$$\psi(x) = \sum_n a_n \varphi_n(x) = a_1 \varphi_1(x) + a_2 \varphi_2(x) + \ldots$$

Time dependent solution is

$$\Psi(x,t) = \sum_n a_n \varphi_n(x) e^{-i\omega_n t}, \quad \omega_n = E_n/\hbar.$$

For the free particle, we have a continuum of stationary states:

$$\varphi(x,k) = \{\ldots,\ e^{i(2.000)x},\ e^{i(2.001)x},\ e^{i(2.002)x},\ \ldots\}$$

k is continuous

A continuum of eigenvalues:

$$E(k) = \frac{(\hbar k)^2}{2m}, \quad k \text{ is continuum.}$$

What's the General Solution? A continuous sum over the continuous stationary states:

$$\psi(x) = \underbrace{\sum_n}_{\text{sum over discrete }(n)} a_n \varphi_n(x) \quad \xrightarrow{\text{becomes}} \quad \psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \underbrace{\phi(k)}_{\text{a continuous set of coefficients}} e^{ikx} \underbrace{dk}_{\text{sum over continuous }(k)}$$

What's the physical meaning of the coefficients $\phi(k)$?

For the particle-in-a-box, the $\{a_n\}$ are amplitudes to measure energy eigenvalues:

$$P(E_n) = |a_n|^2.$$

For the free particle, the $\phi(k)$ must be amplitudes to measure momentum eigenvalue $p=\hbar k$.

$$P(k)\, dk = |\phi(k)|^2 dk$$

need to multiply by a small interval dk because k is continuous.

We call $\phi(k)$ the "momentum space wavefunction" and $\psi(x)$ the "position-space" wavefunction.

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

Then $\phi(k)$ is the Fourier Transform of $\psi(x)$.

We can calculate the correct set of coefficients $\phi(k)$ like this: $\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx}\, dx$

Given $\Psi(x, t=0) = \psi(x)$.

How will $\psi(x)$ evolve in time?

Answer: Each stationary state gets its own phase factor $e^{-i\omega(k)t}$, where $\omega(k) = \frac{E(k)}{\hbar} = \frac{\hbar k^2}{2m}$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \left(e^{ikx}\right) e^{-i\omega(k)t}\, dk$$

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{ik\left(x - \frac{\hbar k}{2m} t\right)}\, dk}$$

General Strategy for free particle:

① Given the wavefunction at $t=0$ $\left(\psi(x)\right)$, we can calculate $\phi(k)$:

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

② As time goes forward, the state evolves as

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

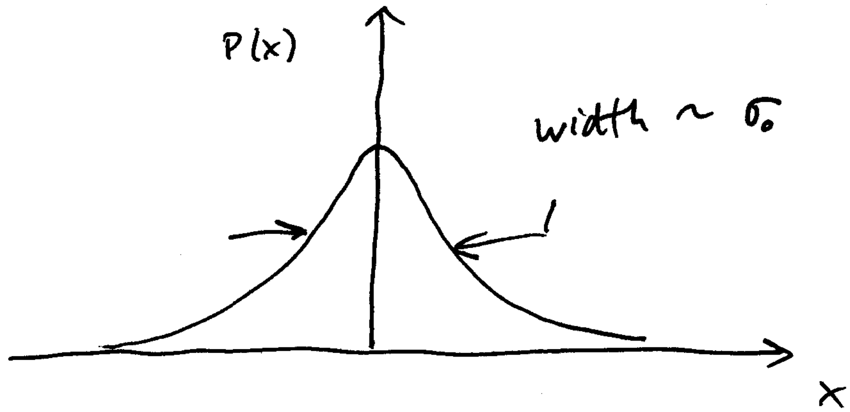
<u>Example</u> Gaussian wave packet

Suppose at $t = \emptyset$, $\psi(x) = \frac{1}{(2\pi)^{\frac{1}{4}}} \frac{1}{\sqrt{\sigma}} e^{ik_0 x} e^{-x^2/4\sigma_0^2}$

k_0 = a constant

σ_0 = width parameter. at $t = \emptyset$

Then $P(x) = \psi^* \psi = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_0} e^{-x^2/2\sigma_0^2}$ ← a Gaussian



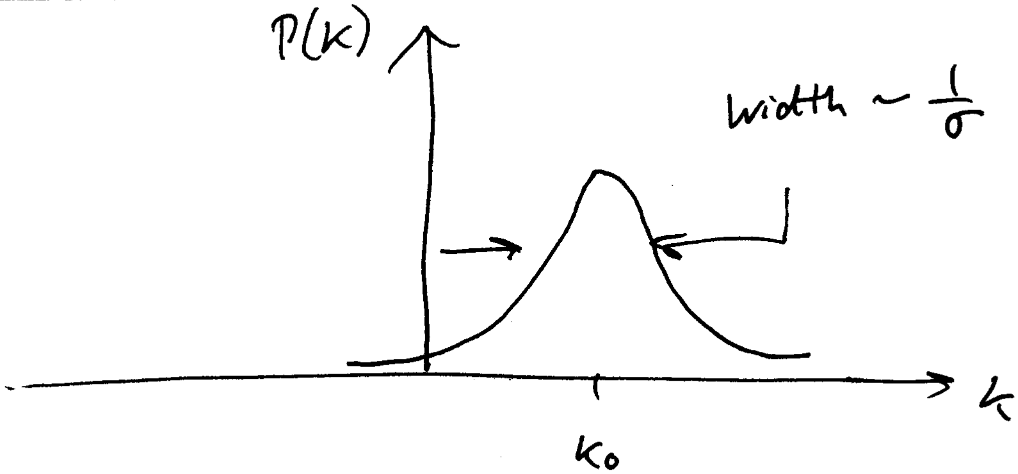
What's the momentum space wavefunction?

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \underbrace{\psi(x)}_{\uparrow \text{ substitute}}\, e^{-ikx} = \frac{1}{(2\pi)^{3/4}} \frac{1}{\sqrt{\sigma_0}} \int_{-\infty}^{\infty} dx\, e^{-x^2/4\sigma_0^2} e^{ix(k_0 - k)}$$

$$\phi(k) = \sqrt{\frac{2\sigma_0}{\sqrt{2\pi}}}\, e^{-\sigma_0^2 (k_0 - k)^2}$$

↑ A Gaussian in k, centered on k_0.

$$P(k) = |\phi(k)|^2 = \frac{2\sigma_0}{\sqrt{2\pi}} e^{-2\sigma_0^2 (k_0 - k)^2}$$



A ~~narrow~~ gaussian pulse which is narrow in x is wide in k, and vice versa. This is an illustration of the uncertainty principle

What happens as time goes forward? Plug $\phi(k)$ back in and integrate:

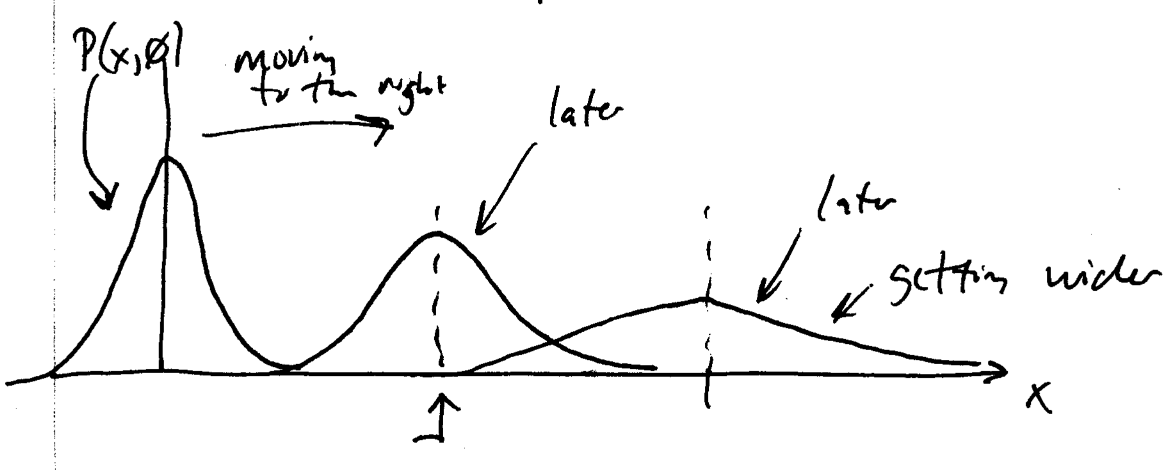
Answer:

$$P(x,t) = \Psi^*(x,t)\,\Psi(x,t)$$

$$= \cancel{\frac{1}{\sigma_0\sqrt{2\pi}}}$$

$$= \frac{1}{\sigma_0\sqrt{2\pi}} \underbrace{\frac{1}{\sqrt{1+t^2/\tau^2}}}_{\text{height gets smaller}} e^{-(x-(\hbar k_0/m)t)^2/2\sigma_0^2\underbrace{(1+t^2/\tau^2)}_{\text{Gaussian gets wider}}}$$

where $\tau \equiv$ spreading time constant $= \dfrac{2m\sigma^2}{\hbar}$



For a macroscopic object, say width $\sigma_0 = 1$ cm

and $m = 1$ gram,

Then $\tau \sim 10^{27}$ seconds $\sim 10^{20}$ years

Free particle

$\psi(x)$ can be written as a superposition of momentum eigenstates $\{e^{ikx}\}$:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \underbrace{\phi(k)}_{\text{a continuum of coefficients}} \underbrace{e^{ikx}\, dk}_{\text{a continuous sum over the continuous variable } k.}$$

This is useful because the $\{e^{ikx}\}$ are stationary states: each evolves in time by getting its own phase factor $e^{-i\omega t}$, where $\omega = \frac{E}{\hbar} = \frac{\frac{(\hbar k)^2}{2m}}{\hbar} = \frac{\hbar k^2}{2m}$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{ikx}\, e^{-i\omega t}\, dk$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{ik\left(x - \frac{\hbar k}{2m} t\right)}\, dk$$

How do we find the right function $\phi(k)$ for a particular $\psi(x)$?

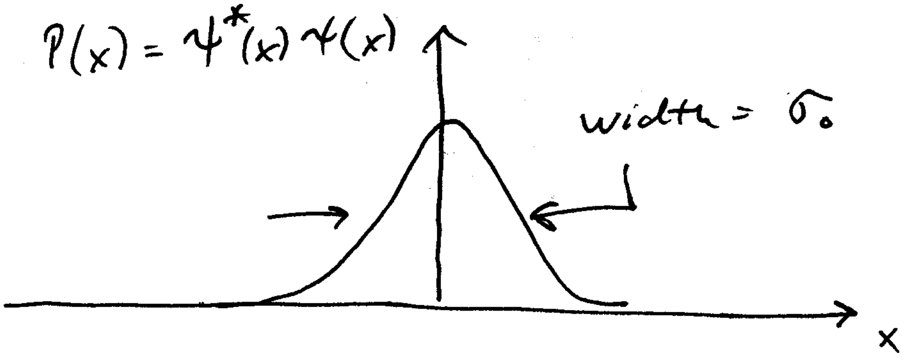
Answer: $\phi(k)$ is the Fourier Transform of $\psi(x)$:

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

<u>Example</u>: Gaussian wave packet

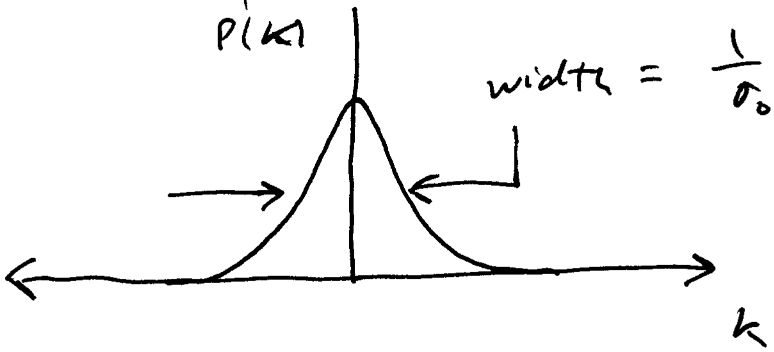
Suppose $\psi(x) = \frac{1}{(2\pi)^{1/4}} \frac{1}{\sqrt{\sigma_0}}\, e^{-x^2/4\sigma_0^2}$, σ_0 = width at $t=0$

$P(x) = \psi^*(x)\,\psi(x)$



Then $\phi(k) = \sqrt{\frac{2\sigma_0}{\sqrt{2\pi}}}\; e^{-\sigma_0^2 (k)^2}$

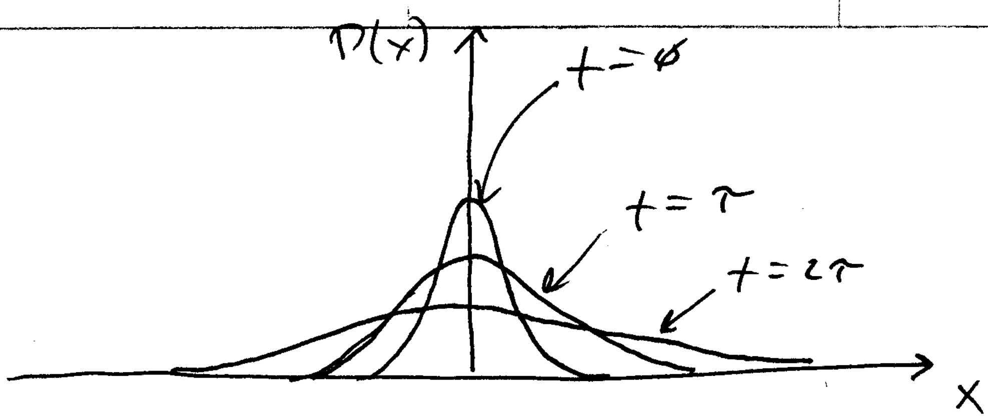
and $P(k) = |\phi(k)|^2$



And

$P(x) = \frac{1}{\sigma_0\sqrt{2\pi}} \frac{1}{\sqrt{1+t^2/\tau^2}}\; e^{-x^2/2\sigma_0^2 \underbrace{(1+t^2/\tau^2)}_{\text{Gaussian gets wider as time goes forward}}}$

where $\tau = \frac{2m\sigma_0^2}{\hbar}$ = spreading time constant



Why does it spread out at time goes forward? well, the gaussian is composed of many momentum eigenstates, all moving at their own speeds. So they cannot stay together.

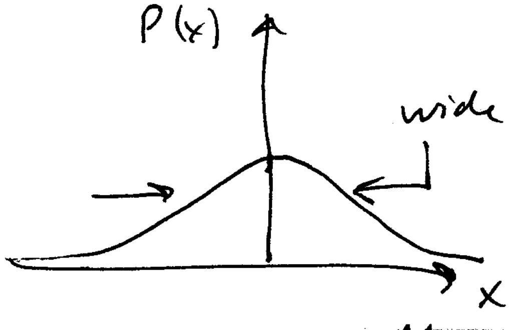
How long does it take? Suppose m = one gram and σ_0 = one cm, like a piece of chalk.

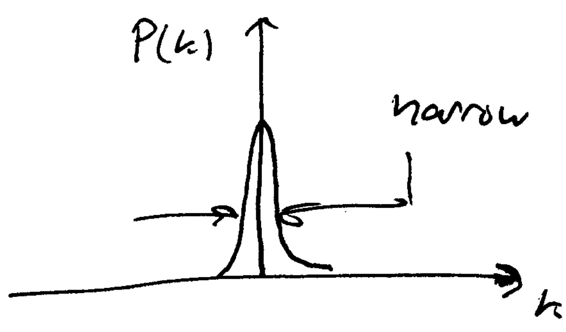
Then $\tau = \dfrac{2(10^{-3}\,kg)(10^{-2}\,m)^2}{(6\times 10^{-34}\,J\cdot s)} \sim \frac{1}{3}\times 10^{27}$ seconds

But if $m = 10^{-31}$ kg, like an electron, and $\sigma_0 = 10^{-10}$ m, like an atomic scale, then

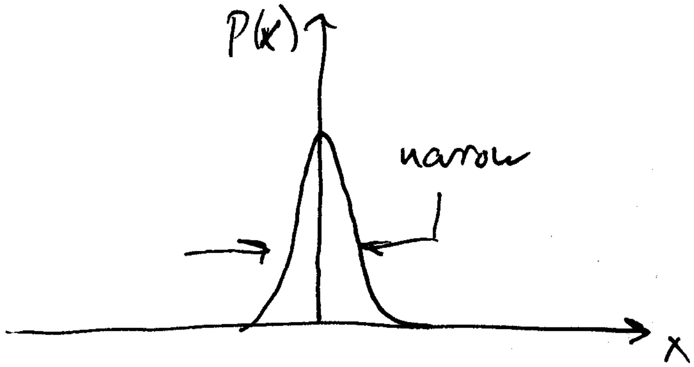
$$\tau \approx \frac{1}{3}\times 10^{-17} \text{ seconds}$$

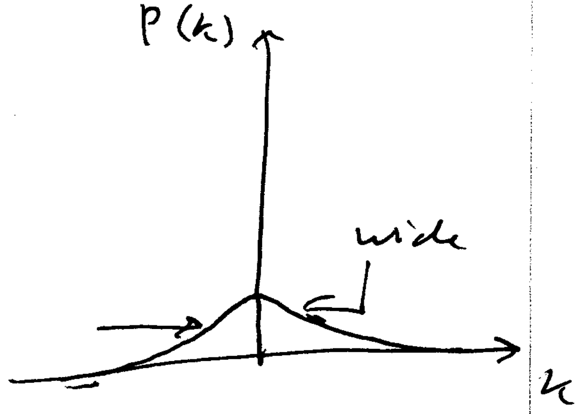
Note that the a $\psi(x)$ which is wide has a narrow $\phi(k)$:





And vice versa:





This is an illustration of the uncertainty principle. If we can be very certain of the position of the particle, then we are very uncertain of the momentum of the particle. And vice versa

~~Another example~~

Orthogonality of the $\{e^{ikx}\}$

For the particle-in-a-box, we had an orthogonality relation for the energy eigenstates:

$$\int_{-\infty}^{\infty} \psi_m^*(x)\,\psi_n(x)\,dx = \delta_{mn}$$

For the free particle, the energy eigenstates are the $\{e^{ikx}\}$. Do we have an orthogonality relation for these?

$$\cancel{\int_{-\infty}^{\infty}\left(e^{ikx}\right)^*\left(e^{ik'x}\right)dx = ?}$$

$$\int_{-\infty}^{\infty}\left(e^{ikx}\right)^*\left(e^{ik'x}\right)dx = ?$$

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

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk' \, e^{ik'x} \, \phi(k')$$

$$\therefore \; \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-ikx} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk' e^{ik'x} \, \phi(k') \right]$$

$$\phi(k) = \int_{-\infty}^{\infty} dk' \, \phi(k') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} dx \left(e^{ik'x} \right) \left(e^{ikx} \right)^{*} \right]$$

This looks like the definition of the Dirac Delta Function:

$$\cancel{f(x) = \int_{-\infty}^{\infty} dx' \, f(x') \, \delta(x-x')}$$

~~So we must have~~

$$\phi(k) = \int_{-\infty}^{\infty} dk' \, \phi(k') \, \delta(k-k')$$

So we must have

$$\boxed{\frac{1}{2\pi} \int_{-\infty}^{\infty} dx \left(e^{ik'x} \right) \left(e^{ikx} \right)^{*} = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k'-k)x} = \delta(k'-k)}$$

So, for particle in the box and for the free particle

$$\int_{-\infty}^{\infty} dx\; u_n^*(x)\, u_m(x) = \delta_{nm}$$

↑ Discrete, Kronecker Delta

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dx \left(e^{ik'x}\right)\left(e^{ikx}\right)^* = \delta(k'-k)$$

↑ Continuous, Dirac Delta

Physical Interpretation

Suppose we have a particle in a perfect momentum eigenstate:

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\, e^{ik'x}, \quad k' = \text{constant} = \text{some particular wave number}$$

Then $\psi(x)$ extends to infinity in both directions. We are equally likely to find the particle anywhere on the x-axis.

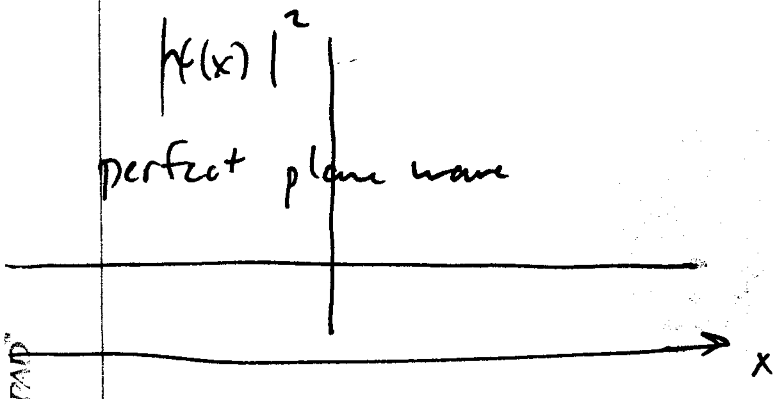
Question What is the momentum-space wavefunction?

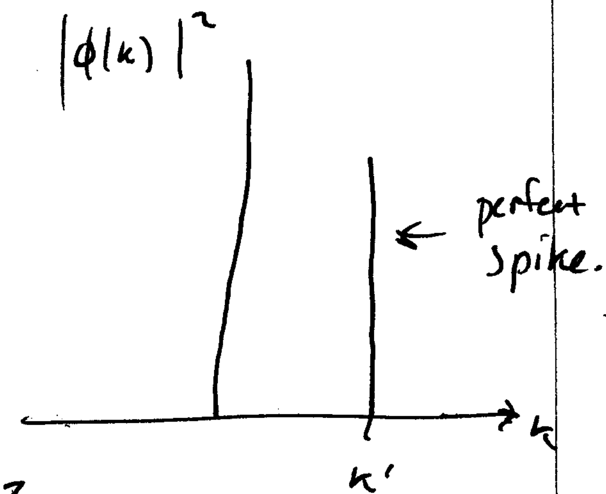
Answer:

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\; \psi(x)\, e^{-ikx} = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx \left(e^{ik'x}\right)\left(e^{-ikx}\right)$$

$$\boxed{\phi(k) = \delta(k'-k)}$$

The momentum space wavefunction is a perfect spike at $k = k'$:





What is the width of $|\psi(x)|^2$? Answer: $\Delta x \to \infty$

What is the width of $|\phi(k)|$? Answer $\Delta k \to \emptyset$.

Again, we have an inverse relation:

$$\Delta x \sim \frac{1}{(\Delta k)}$$

This is an extreme example of the uncertainty principle.

Postulates I & III Observable A has
an operator : $\hat{A}$
eigenfunction : α
eigenvalues : a

These are defined by $\hat{A}\alpha = a\alpha$
$\uparrow$ a constant

The eigenvalues are the possible results of measurements of A.

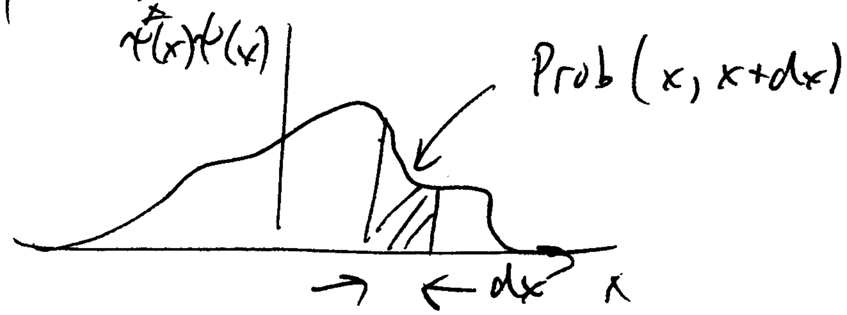
After a measurement of A, the wavefunction will collapse to an eigenfunction of A.

What does $\hat{A}\alpha = a\alpha$ tell us? It tells us what the possible eigenvalues a eigenfunctions are for A. It does not tell us the result of a particular measurement.

Postulate II

$\psi(x)$ = a continuum of quantum mechanical amplitudes

$$\psi^*(x)\psi(x)dx = |\psi(x)|^2 dx = P(x)\,dx$$



Also

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi \, dx$$

Consequence: If we expand $\psi(x)$ as a sum of energy eigenfunctions, the expansion coefficients $\{a_n\}$ are amplitudes to measure the energy eigenvalues $\{E_n\}$:

Discrete eigenfunctions:

$$\psi(x) = a_1 \varphi_1 + a_2 \varphi_2 + a_3 \varphi_3 + \dots$$

normalized energy eigenfunctions

$$= \sum_n a_n \varphi_n$$

Then

$$P(E_1) = |a_1|^2$$
$$P(E_2) = |a_2|^2$$
$$P(E_3) = |a_3|^2$$
$$\vdots$$

Discrete amplitudes

Continuous eigenfunctions

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

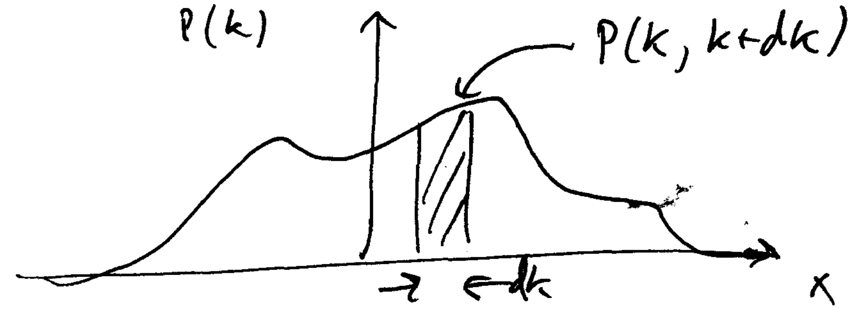
just like the $\{a_n\}$, but $\phi(k)$ is continuous

just like the φ_n, but (k is) continuous.

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

$\phi(k)$ is the amplitude to measure ~~the~~ momentum k:

$$P(k)\,dk = |\phi(k)|^2 dk$$



$\psi(x)$: a continuum of amplitudes to measure (x)

$\phi(k)$: a continuum of amplitudes to measure (k)

$\{a_n\}$: a discrete set of amplitudes to measure energy eigenvalues $\{E_n\}$ ⇐ only relevant when the $\{a_n\}$ are discrete

Postulate IV : Time evolution.

When no measurements are made, $\psi(x)$ goes forward in time:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\, \Psi(x,t)$$

Consequence

(1) Discrete energy eigenfunctions:

$$\Psi(x, t=0) = \psi(x) = \sum_n a_n \varphi_n$$

Then $\Psi(x,t) = \sum_n a_n \varphi_n e^{-i\omega_n t}$, $\omega_n = E_n/\hbar$.

2 Continuous energy eigenfunctions (free particle)

$$\Psi(x, t=0) = \psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \phi(k)\, e^{ikx}$$

Then

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

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \phi(k)\, e^{ikx}\, e^{-i\omega(k) t}$$

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