Free Particle $V(x) = 0$,

$$H_{\text{free}} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \text{ because } V(x) = 0$$

**What are the energy eigenstates (stationary states)?**

Eigenvalue equation:

$$\frac{-\hbar^2}{2m} \frac{d^2 \phi(x)}{dx^2} = E \phi(x)$$

$$\phi''(x) + \frac{2mE}{\hbar^2} \phi(x) = 0$$

**Solution:**

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

Same solution as particle-in-a-box,

but this time there is no boundary conditions.

Recall: $A e^{ikx}$ is an eigenstate of momentum.

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

We will use the momentum eigenstates $A e^{ikx}$ to construct general solutions to free particle states.
For Particle-in-a-box we have discrete stationary states:

\( \alpha_n(x) = \{ \alpha_1(x), \alpha_2(x), \alpha_3(x), \ldots \} \)

Discrete Eigenvalues:

\( E_n = \{ E_1, E_2, E_3, \ldots \} \)

General solution is a discrete sum:

\[ \psi(x) = \sum_n a_n \alpha_n(x) = a_1 \alpha_1(x) + a_2 \alpha_2(x) + \ldots \]

Time dependent solution is:

\[ \psi(x,t) = \sum_n a_n \alpha_n(x) e^{-iE_n t} \]

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

\[ \alpha(x,k) = \{ \ldots, \alpha(2.000x), \alpha(2.001x), \alpha(2.002x), \ldots \} \]

\( k \) is continuous

A continuum of eigenvalues:

\[ E(k) = \frac{(nk)^2}{2m} \quad k \text{ is continuous} \]
What's the general solution? A continuous sum over the continuous stationary states:

\[ \psi(x) = \sum_n a_n \phi_n(x) \quad \Rightarrow \quad \psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)e^{ikx} \, dk \]

sum over
set of coefficients

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 \( E_n \):

\[ P(E_n) = |a_n|^2 \]

For the free particle, the \( \phi(k) \) must be amplitudes to measure momentum eigenvalue \( p = -i \hbar \frac{d}{dx} \).

\[ \int P(k) \, dk = |\phi(k)|^2 \, dk \]

\( \phi(k) \) the momentum space wavefunction,

\( \psi(x) \) the position-space wavefunction.

We call \( \phi(k) \) the "momentum space wavefunction" and \( \psi(x) \) the "position-space wavefunction."
Mathematically, since \( \psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} \text{d}k \)

Thus, \( \phi(k) \) is the Fourier Transform of \( \psi(x) \).

We can calculate the correct set of coefficients \( \phi(k) \) like this:

\[
\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} \text{d}x
\]

Given \( \Psi(x) = \psi(x) \), we can find how \( \psi(x) \) will evolve in time.

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

\[
\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)(e^{-i\omega(t)x}) e^{ikx} \text{d}k
\]

General strategy for free particle:

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

\[
\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} \text{d}x
\]
(2) As time goes forward, the state evolves

\[ \psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{-i\frac{k}{\hbar}(x - \frac{\hbar k}{\mu} t)} dk \]

**Example: Gaussian wave packet**

Suppose at \( t = 0 \),

\[ \psi(x) = \frac{1}{(2\pi)^{1/2} \sigma_0} e^{-\frac{x^2}{2\sigma_0^2}} \]

\( k_0 \) = a constant

\( \sigma_0 \) = width parameter at \( t = 0 \)

Then

\[ P(x) = \psi^* \psi = \frac{1}{2\pi} \frac{1}{\sigma_0} e^{-\frac{x^2}{2\sigma_0^2}} \leq \text{a Gaussian} \]

What's the momentum space wave function?

\[ \phi(k) = \frac{1}{(2\pi)^{1/2} \sigma_0} \int_{-\infty}^{\infty} dx \psi(x) e^{-ikx} = \frac{1}{(2\pi)^{1/2} \sigma_0} \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2\sigma_0^2} - ikx} \]

Substitute

\[ \phi(k) = \sqrt{\frac{2\sigma_0}{N\pi}} e^{-\frac{k_0^2}{2\sigma_0^2} - \sigma_0^2(k_0 - k)^2} \]

\[ P(k) = \left| \phi(k) \right|^2 = \frac{2\sigma_0}{N\pi} e^{-2\sigma_0^2(k_0 - k)^2} \leq \text{a Gaussian in } k, \text{ centered on } k_0. \]
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:**

$$P(x,t) = \sqrt{\frac{\tau}{2\pi \sigma_0^2}} e^{-\frac{(x - \frac{\hbar}{\sigma_0^2})^2}{2\sigma_0^2(1 + \frac{t^2}{\tau^2})}}$$

- $\sigma_0^2/(1 + t^2/\tau^2)$ height gets smaller
- $\tau$ = spreading time constant = $\frac{2\sigma_0^2}{\hbar}$

The pulse moves to the right, $P(x,t)$ getting wider.
For a macroscopic object, say width $d_o = 1 \text{ cm}$ and 

$m = 1 \text{ gram}$, 

Then $t \sim 10^{27} \text{ seconds} \sim 10^{20} \text{ years}$
Free particle

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

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

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

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

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

**Answer:** \( \phi(k) \) is the Fourier Transform of \( \Psi(x) \):

\[
\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) e^{-ikx} \, dx
\]
Example: Gaussian wave packet

Suppose \( \psi(x) = \frac{1}{(2\pi)^{1/4}} \frac{1}{\sigma_0} e^{-x^2/4\sigma_0^2} \)

\( \sigma_0 = \text{width at } t=0 \)

\[ P(x) = \psi^*(x) \psi(x) \]

width = \( \sigma_0 \)

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

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

width = \( \frac{1}{\sigma_0} \)

And

\[ P(x) = \frac{1}{\sigma_0 \sqrt{2\pi}} \frac{1}{\sqrt{1 + \frac{t^2}{\tau^2}}} e^{-x^2/2\sigma_0^2(1+t^2\tau^2)} \]

when \( \tau = \frac{2m\sigma_0^2}{\hbar} = \text{speeding} \)

\( \text{time } \to \text{ wider } \)

constant \( \to \text{ goes forward} \)
Why does it spread out as 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 \( \sigma_0 = \) one cm, like a piece of chalk.

Then \( \tau = \frac{2(10^{-3} \text{ kg})(10^{-2} \text{ m})^2}{(6 \times 10^{-3} \text{ s} 	imes 5.5)} \approx \frac{1}{3} \times 10^{-27} \text{ seconds} \)

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

Then \( \tau \approx \frac{1}{3} \times 10^{-17} \text{ seconds} \)

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

\[
\int_{-\infty}^{\infty} (e^{ikx})^{*} (e^{-ik'x}) \, dx = ?
\]

\[
\int_{-\infty}^{\infty} (e^{ikx})^{*} (e^{ik'x}) \, dx = ?
\]
\[ \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-ikx} \, \varphi(x) \]

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

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

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

This looks like the definition of the Dirac Delta function:

\[ \delta(x) = \int_{-\infty}^{\infty} dx' \, \varphi(x') \delta(x-x') \]

So we must have

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

So we must have

\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \, (e^{ikx})^* (e^{ikx})^* = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k'-k)x} \, dx = \delta(k'-k) \]
So, for particle in the box
\[ \int_{-\infty}^{\infty} dx \, \phi_n^*(x) \phi_m(x) = \delta_{nm} \]

\[ \oint \frac{1}{2\pi i} \int_{-\infty}^{\infty} dx \left( e^{ik\cdot x} \right) \left( e^{-ik\cdot x} \right) = \delta(k, -k) \]

Physical Interpretation
Suppose we have a particle in a perfect momentum eigenstate:
\[ \chi(x) = \frac{1}{\sqrt{2\pi}} e^{ik'x} \]

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

\[ \phi(k) = \delta(k' - k) \]
The momentum space wavefunction is a perfect spike at $k = k'$:

$|\phi(k)|^2$

perfect plane wave \[ \xrightarrow{x} \]

What is the width of $|\phi(x)|^2$? Answer: $\Delta k \rightarrow \infty$.

What is the width of $|\phi(k)|^2$? Answer: $\Delta k \rightarrow 0$.

Again, we have an inverse relation:

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

This is an extreme example of the uncertainty principle.
Postulates II

Observable $A$ has an operator $\hat{A}$
eigenfunction: $\psi$
eigenvalues: $a$

Then are defined by $\hat{A}\psi = a\psi$

$\uparrow$ a constant

The eigenvalues are the possible results of measurements of $A$.

Immediately after a measurement of $A$, the wavefunction will collapse to an eigenfunction of $A$.

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

Postulate II

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

$\frac{\psi^*(x)\psi(x)dx}{|\psi(x)|^2}dx = p(x)dx$

$\frac{\psi^*(x)\psi(x)}{|\psi(x)|^2}|x_k\rightarrow x_{k+dx}|$

Prob $\chi(x, x + dx)$
\[ \langle A \rangle = \int_{-\infty}^{\infty} \rho^A(x) \, dx \]

Consequence: If we expand \( \psi(x) \) as a sum of energy eigenfunctions, the expansion coefficients \( \{a_n^2\} \) are amplitudes to measure the energy eigenvalues \( \{E_n\} \):

**Discrete - eigenfunctions**

\[
\psi(x) = a_1 \phi_1 + a_2 \phi_2 + a_3 \phi_3 + \ldots
\]

\[
= \sum_n a_n \phi_n
\]

The \( P(E_i) = |a_i|^2 \)

\( P(E_1) = |a_1|^2 \)

**Discrete amplitudes**

\( P(E_2) = |a_2|^2 \)

\( P(E_3) = |a_3|^2 \)

**Continuum - eigenfunction**

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

just like in the \( \{a_n^2\} \)

but \( \phi(k) \)

is continuous

\[ E = \frac{(\hbar k)^2}{2m} \]
\( \phi(k) \) is the amplitude to measure momentum \( k \):

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

\( P(k) \) : 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:

\[
\frac{i}{\hbar} \frac{\partial \psi(x,t)}{\partial t} = \hat{H} \psi(x,t)
\]

**Consequence**

1. Discrete energy eigenfunction:

\[
\psi(x,t) = \sum_n a_n e^{-i\omega_n t}
\]

The \( \psi(x,t) = \sum_n a_n e^{-i\omega_n t} \), \( \omega_n = E_n / \hbar \).
(2) Continuous energy eigenfunctions (free particle)

\[ \Phi(x) \equiv \chi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \phi(k) e^{ikx} \]

Then \( \Phi(x) \) is

\[ \Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \phi(k) e^{ikx} - i\omega(k) + \frac{\hbar^2 k^2}{2m} \]

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