- Evolution in $x$ and $p$ basis.

- **Schrödinger Equation.**

\[ i\hbar \frac{\partial}{\partial t} \Psi = H \Psi \]

- **Inspired by classical mechanics.**

\[ H = \frac{\hat{p}^2}{2m} + V(\hat{x}). \]

- **Kinetic energy.**


- Potential is classical.

- **$x$-basis Schrödinger equation.**

\[ i\hbar \frac{\partial}{\partial t} \langle x | \Psi \rangle = \int dx' \langle x | H | x' \rangle \langle x' | \Psi \rangle \]

- **Evaluating $\langle x | H | x' \rangle$:**

i) \[ \langle x | \frac{\hat{p}^2}{2m} | x' \rangle = \frac{1}{2m} \delta(x-x') \left( -\frac{\partial}{\partial x} \right)^2 \]

\[ \int dx' \langle x | \frac{\hat{p}^2}{2m} | x' \rangle \langle x' | \Psi \rangle = -\hbar^2 \frac{\partial^2}{2m \partial x^2} \langle x | \Psi \rangle \]

ii) \[ \langle x | V(x') | x' \rangle = V(x) \delta(x-x') \]

\[ \int dx' \langle x | V(x') | x' \rangle \langle x' | \Psi \rangle = V(x) \langle x | \Psi \rangle. \]
Therefore, in $x$-basis, wave function satisfies the following Schrödinger Eq.

$$i\hbar \frac{\partial}{\partial t} \psi (x,t) = \left( - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi (x,t)$$

where we use $\psi (x,t)$. This notation to emphasize the wave function is time dependent.

In 3-dimension, this would be

$$i\hbar \frac{\partial}{\partial t} \psi (\vec{x},t) = \left( - \frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right) \psi (\vec{x},t).$$
- Continuity of probability flow.

Start with Schrödinger equation, and its complex conjugate, multiply by \( \psi^* \) and \( \psi \) on the left respectively.

1. \( \psi^* \frac{i \hbar}{\partial t} \psi = \psi^* \left( -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) \psi \)

2. \( \psi \left( -\frac{i \hbar}{\partial t} \psi^* \right) = \psi \left( -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) \psi^* \)

\[ \rightarrow \quad \implies \quad \begin{align*}
\frac{i \hbar}{\partial t} (\psi^* \psi) &= -\frac{\hbar^2}{2m} \left( \psi^* \nabla^2 \psi - \psi \nabla^2 \psi^* \right) \\
&= -\frac{\hbar^2}{2m} \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*)
\end{align*} \]

def
prob. density \( \rho = \psi^* \psi \).
prob. current \( \vec{J} = -\frac{i \hbar}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*) \).

\[ \rightarrow \frac{\partial}{\partial t} \rho + \nabla \cdot \vec{J} = 0 \]

Or, consider a volume \( V \) with closed surface \( S \).

\[ \frac{d}{dt} \int_V d^3x \rho = -\int_V d^3x \nabla \cdot \vec{J} = - \oint_S \vec{J} \cdot d\vec{s} \]

rate of prob. change in \( V \) = total prob in-flow curr
- If $H$ is independent of $t$, energy is conserved
  
  $H |\psi_i> = E_i |\psi_i>$, $|\psi_i>$ is energy eigenstate.

- In $x$-basis, Schrödinger Eq. of $\psi_i$ is
  
  \[ i\hbar \frac{\partial}{\partial t} \psi_i(x,t) = H \psi_i(x,t) = E_i \psi_i(x,t). \]

  \[ \Rightarrow \psi_i(x,t) = \psi_i(x) e^{-\frac{i}{\hbar}E_i t} \]

  $\psi_i(x) = \psi_i(x,t) \big|_{t=0}$, $\psi_i(x)$ independent of $t$

- For arbitrary state $|\psi, t>$
  
  - At $t=0$, we express it in terms of $|\psi_i>$
    \[ <x|\psi, t=0> = \sum_i \psi_i(x) \cdot a_i \]
    
    $a_i = \int dx \psi_i^*(x) \psi(x, t=0)$

- Then, at arbitrary later time $t$
  
  \[ <x|\psi, t> = \psi(x, t) = \sum_i a_i \psi_i(x) e^{-\frac{i}{\hbar}E_i t} \]
- Free particle, Plane wave

- Free particle
  \[ H = \frac{\hat{p}^2}{2m} \]

- \([\hat{p}, H] = 0\), \(|\psi\rangle\) is also energy eigenstate.
  \[ H |\psi\rangle = \frac{\hat{p}^2}{2m} |\psi\rangle, \quad E_\psi = \frac{p^2}{2m} \]

- Suppose
  \[ \psi(x, t=0) = |\psi\rangle = \frac{1}{\sqrt{2\pi \hbar}} e^{\frac{i}{\hbar} px} \quad \text{"Plane wave"} \]

- Since it is already energy eigenstate, the time evolution is simply
  \[ \psi(x, t \rightarrow \infty) = \langle x |\psi\rangle e^{-\frac{i}{\hbar} E_\psi t} = \frac{1}{\sqrt{2\pi \hbar}} e^{\frac{i}{\hbar} (px - \frac{p^2}{2m} t)} \]
• Gaussian wave packet in $p$-basis

$$
\psi_p = \int dx \langle \varphi(x) | x \rangle
$$

$$
= A \int dx \exp \left( \frac{i}{\hbar} (p_0 - p) x - \frac{x^2}{2\sigma^2} \right), \quad A = \frac{1}{\sigma \sqrt{2\pi \hbar}}
$$

$$
= A \int dx \exp \left( -\frac{1}{2\sigma^2} \left( x + \frac{i}{\hbar} \sigma^2 (p_0 - p) \right)^2 - \frac{\sigma^2 (p - p_0)^2}{\hbar^2} \right)
$$

$$
\psi(p) = \frac{\sigma^{1/2}}{(\pi \sigma^2 \hbar)^{1/4}} e^{-\frac{\sigma^2}{2\hbar^2} (p - p_0)^2}.
$$

From this, we obtain

$$
\langle p \rangle = \langle p_0 \rangle, \quad \langle p^2 \rangle = \frac{\hbar^2}{2\sigma^2} + \langle p \rangle^2.
$$

$$
\langle \Delta p^2 \rangle = \frac{\hbar^2}{2\sigma^2}.
$$

• $\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle = \frac{\hbar^2}{4}$

Saturates uncertainty relation.

"Minimal wave packet"
- Gaussian Wave packet.

- Definition
  \[ \psi(x) = \frac{1}{(\sigma^2 \pi)^{1/4}} e^{\frac{i}{\hbar} px - \frac{x^2}{2\sigma^2}} \]

- Gaussian integral formula.
  \[ \int_{-\infty}^{\infty} dx \ e^{-a^2 x^2} = \frac{1}{a} \sqrt{\pi} \]

- \( \langle x \rangle \)
  \[ = \int dx \ x \ \psi^*(x) \psi(x) = \int dx \ x \ \frac{1}{(\sigma^2 \pi)^{1/4}} e^{-\frac{x^2}{\sigma^2}} \]
  \[ = 0 \text{ since the integrand odd under } x \rightarrow -x \]

- \( \langle x^2 \rangle \)
  \[ = \int dx \ x^2 \ \frac{1}{(\sigma^2 \pi)^{1/2}} e^{-\frac{x^2}{\sigma^2}} = \frac{\sigma^2}{2} \]

- \( \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 = \frac{\sigma^2}{2} \).
Gaussian wave packet demonstrates the general phenomenon that if one "squeeze" the wave packet of a particle in $x(p)$, its size in $p(x)$ will grow correspondingly.

In this case: $|\langle \Delta x \rangle| = \frac{\hbar}{\sqrt{2} \sigma}$, $|\langle \Delta p \rangle| = \frac{\hbar}{\sqrt{2} \sigma}$.

This gives us some intuition about the "size" of a particle.

i) It cannot be localized exactly at a point. If so, $\Delta x \rightarrow 0$, $\Delta p \rightarrow \infty$. However, infinite momentum means infinite energy is necessary to localize it. From $E = mc^2$, we know that injecting infinite amount of energy leads creation of many new particles. This invalidates the picture of one localized particle.

ii) This line of reasoning gives us an estimate of the size of a particle with mass $M$.

To avoid particle creation, the injected energy $E < Mc^2$. 

$\therefore$
b) Correspondingly, the momentum transfer, or the "jitter" the particle experiences during the measurement

$$\Delta p < \sqrt{\frac{E}{c}} = Mc$$

c) Therefore, the spread of the particle wave packet, the "size" of the particle, is

$$\Delta x \geq \frac{\hbar}{\Delta p_{\text{max}}} = \frac{\hbar}{Mc}$$
• Time evolution of Gaussian wave packet.

We assume the particle is free. \( H = \frac{\hat{p}^2}{2m} \).

We start at \( t=0 \) with

\[
\psi(\mathbf{r},0) = \frac{1}{(2\pi \sigma^2)^{1/4}} e^{\frac{i}{\hbar} \hat{p}_0 \mathbf{r} - \frac{\mathbf{r}^2}{2\sigma^2}}
\]

\[
= \frac{1}{\sqrt{2\pi \hbar}} \int d\mathbf{p} \, e^{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}} \psi(\mathbf{p}).
\]

Then

\[
\psi(\mathbf{r},t) = \frac{1}{\sqrt{2\pi \hbar}} \frac{\sqrt{\frac{1}{2}}}{\pi^{1/4} \hbar^{1/2}} \int d\mathbf{p} \, e^{\frac{i}{\hbar} \mathbf{p} \cdot (\mathbf{r} - \mathbf{r}_0)} e^{\frac{-\sigma^2}{2\hbar^2} (\mathbf{p} - \mathbf{p}_0)^2} e^{\frac{i}{\hbar} (\mathbf{p} \cdot \mathbf{r} - E_p t)}
\]

where \( E_p = \frac{\mathbf{p}^2}{2m} \).

Carrying out the Gaussian integral, we find,

\[
\psi(\mathbf{r},t) = \left( \frac{4\sigma^2}{\pi} \right)^{1/4} \frac{1}{\left(4\sigma^2 + \frac{\hbar^2 t^2}{m^2}\right)^{1/4}} \exp \left( -\frac{(\mathbf{r} - \frac{\mathbf{p}_0}{m} t)^2}{2 \left( \frac{\sigma^2}{4} + \frac{i\hbar t}{m} \right)} \right)
\]

\[
\times e^{i\mathbf{p}_0 \cdot \mathbf{r}} e^{\frac{i}{\hbar} \mathbf{p}_0 \cdot (\mathbf{r} - \frac{\mathbf{p}_0}{2m} t)}.
\]
\[ |\psi(x, t)|^2 = \sqrt{\frac{1}{\pi \sigma^2}} \cdot \frac{1}{\sqrt{1 + \frac{\hbar^2 t^2}{m^2 \sigma^2}}} \times \exp \left( - \frac{(x - \frac{p_0}{m} t)^2}{\sigma^2 + \frac{\hbar^2 t^2}{m^2 \sigma^2}} \right) \]

- We observe that
  i) At time \( t \), it is still a Gaussian wave packet centering at \( x_0 = \frac{p_0}{m} t \).
  The center of the wave packet moves at speed
  \[ \dot{x}_{\text{center}} = \frac{p_0}{m} \]
  ii) The wave packet spreads (in \( x \)).
  \[ \langle \Delta x^2 \rangle = \frac{\sigma^2}{2} + \frac{\hbar^2 t^2}{2m^2 \sigma^2} \]
iii) In contrast with classical particles.

For a collection of classical particles with different velocities, spanning over

$$\Delta v = \frac{\Delta p}{m}.$$ 

For comparison, take $$\Delta p = \frac{\hbar}{\sqrt{2m}}.$$ 

The induced spread in position at time $$t$$

$$\Delta x_{\text{classical}} = \Delta v \cdot t = \frac{\hbar}{m} \frac{1}{2\sigma^2} \cdot t.$$ 

Quantum mechanical result approaches classical result at very large $$t$$.
1-D problem

- In general, we solve Schrödinger Eq.

\[ i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi(x,t). \]

\[ \psi(x,t) = \sum_{n} \psi_n(x) e^{-\frac{i}{\hbar} E_n t}. \]

\[ E_n; \text{nth eigenvalue of } H, \]

with

\[ \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi_n(x) = E_n \psi_n(x). \]

- General properties of solutions.

1) \( \psi_n(x) \) forms a complete set.

2) If \( V(-x) = V(x) \); 
   a) if \( \psi(x) \) is a solution, \( \psi(-x) \) is also a solution.
   b) We can express solutions with definite parity
      \( \psi(\mp x) = \pm \psi(x) \).

3) Matching conditions.
   a) In most cases, \( \psi(x), \psi'(x) \) continuous.
   b) Exception is if \( V(x) \to \infty \) for some \( x \), such as \( V(x) = \delta(x) \).

4) bound state.

\[ \psi(x) \to 0 \quad \text{as} \quad x \to \pm \infty. \]
1-D problem references.

- 1-D problem has been covered in detail in many places. Here is a list of references.
  - Infinite square well: Griffiths 2.2, Shankar 5.2, Resnick 6.8
  - Finite square well: Griffiths 2.6, Resnick 6.7
  - Scattering/step potential: Resnick 6.3, 6.4.
  - Scattering/barrier: Resnick 6.5, 6.6
  - Simple harmonic Oscillator: Griffiths 2.3, Resnick 6.9, Shankar 8.7.