Quantum Theory

Thornton and Rex, Ch. 6
Matter can behave like waves.

1) What is the wave equation?

2) How do we interpret the wave function \(\psi(x,t)\)?
Light Waves

Plane wave: \( y(x,t) = A \cos(kx-\omega t) \)

Wave (\( \omega, k \)) \( \square \) particle (\( E, p \)):

1) Planck: \( E = h\omega = \hbar\omega \)
2) De Broglie: \( p = h/\lambda = \hbar k \)

A particle relation:

3) Einstein: \( E = pc \)

A wave relation:

4) \( \omega = ck \) (follows from (1), (2), and (3))

The wave equation:

\[
\frac{1}{c^2} \frac{\partial^2 y}{\partial t^2} = \frac{\partial^2 y}{\partial x^2}
\]
Matter Waves

Equations (1) and (2) must hold.

\((\text{wave } (\psi, k) \rightarrow \text{ particle } (E, p))\)

Particle relation (non-relativistic, no forces):

3') \(E = \frac{1}{2} m v^2 = \frac{p^2}{2m}\)

The wave relation:

4') \(\hbar \psi = (\hbar k)^2/2m\)  
(follows from (1), (2), and (3'))

Require a wave equation that is consistent with (4') for plane waves.
The Schrödinger Equation

1925, Erwin Schrödinger wrote down the equation:

\[ i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \]
The Schrödinger Equation

\[ i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \]

(Assume \( V \) is constant here.)

A general solution is

\[ \psi(x,t) = A e^{i(kx-\omega t)} \]

\[ = A ( \cos(kx-\omega t) + i \sin(kx-\omega t) ) \]

\[ \hbar^2 = \frac{\hbar^2k^2}{2m} + V \]

\[ E = \frac{p^2}{2m} + V \]
What is $\psi(x,t)$?

Double-slit experiment for light:

$$I(x) \approx |E(x)|^2 + |B(x)|^2$$

Probability of photon at $x$ is $I(x)$.

Max Born suggested:

$|\psi(x,t)|^2$ is the probability of finding a matter particle (electron) at a place $x$ and time $t$. 
Probability and Normalization

The probability of a particle being between \( x \) and \( x + dx \) is:

\[
P(x) \, dx = |\psi(x,t)|^2 \, dx = \bar{\psi}(x,t)\psi(x,t) \, dx
\]

The probability of being between \( x_1 \) and \( x_2 \) is:

\[
P = \int_{x_1}^{x_2} \bar{\psi}(x,t)\psi(x,t) \, dx
\]

The wavefunction must be normalized:

\[
P = \int_{-\infty}^{\infty} \bar{\psi}(x,t)\psi(x,t) \, dx = 1
\]
Properties of valid wave functions

1. \( \psi \) must be finite everywhere.

2. \( \psi \) must be single valued.

3. \( \psi \) and \( \frac{d\psi}{dx} \) must be continuous for finite potentials (so that \( \frac{d^2\psi}{dx^2} \) remains single valued).

4. \( \psi \to 0 \) as \( x \to \pm \infty \).

These properties (boundary conditions) are required for physically reasonable solutions.
Heisenberg’s Uncertainty Principle

Independently, Werner Heisenberg, developed a different approach to quantum theory. It involved abstract quantum states, and it was based on general properties of matrices.

Heisenberg showed that certain pairs of physical quantities ("conjugate variables") could not be simultaneously determined to any desired accuracy.
We have already seen:

\[ D_x D_p \geq \hbar/2 \]

It is impossible to specify simultaneously both the position and momentum of a particle.

Other conjugate variables are \((E, t)\) \((L, q)\):

\[ D_t D_E \geq \hbar/2 \]

\[ D_L D_L \geq \hbar/2 \]
Expectation Values

Consider the measurement of a quantity (example, position $x$). The average value of many measurements is:

$$\overline{x} = \frac{\sum_{i} N_i x_i}{\sum_{i} N_i}$$

For continuous variables:

$$\overline{x} = \frac{\int_{-\infty}^{\infty} P(x) x \, dx}{\int_{-\infty}^{\infty} P(x) \, dx}$$

where $P(x)$ is the probability density for observing the particle at $x$. 
Expectation Values (cont’d)

In QM we can calculate the “expected” average:

\[ \langle x \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \psi x \, dx}{\int_{-\infty}^{\infty} \psi^* \psi \, dx} = \int_{-\infty}^{\infty} \psi^* \psi x \, dx \]

The expectation value.

Expectation value of any function \( g(x) \) is:

\[ \langle g(x) \rangle = \int_{-\infty}^{\infty} \psi^* g(x) \psi \, dx \]
What are the expectation values of $p$ or $E$?

First, represent them in terms of $x$ and $t$:

$$\frac{\partial \hat{\mathbf{r}}}{\partial x} = \frac{\partial}{\partial x} (Ae^{i(kx-\omega t)}) = ik \hat{\mathbf{r}} = \frac{ip}{\hbar} \hat{\mathbf{r}}$$

$$\hat{\mathbf{p}} \hat{\mathbf{r}} = -i\hbar \frac{\partial \hat{\mathbf{r}}}{\partial x}$$

Define the **momentum operator**:

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

Then:

$$\langle p \rangle = \int_{-\infty}^{\infty} \hat{\mathbf{r}}^* \hat{p} \hat{\mathbf{r}} \, dx = -i\hbar \int_{-\infty}^{\infty} \hat{\mathbf{r}}^* \frac{\partial \hat{\mathbf{r}}}{\partial x} \, dx$$
Similarly, 

\[ \frac{\partial \square}{\partial t} = -i \square \hat{\square} = \frac{-iE}{\hbar} \hat{\square} \]

\[ \hat{\square} \square E \hat{\square} = i\hbar \frac{\delta \square}{\delta t} \]

so the **Energy operator** is:

\[ \hat{E} = i\hbar \frac{\delta \square}{\delta t} \]

and

\[ \langle E \rangle = \int_{-\infty}^{\infty} \hat{\square} \hat{E} \hat{\square} \, dx = i\hbar \int_{-\infty}^{\infty} \frac{\delta \hat{\square}}{\delta t} \hat{\square} \, dx \]
A self-consistency check:

The classical system obeys:

\[ E = K + V = \frac{p^2}{2m} + V \]

Replace \( E \) and \( p \) by their respective operators and multiplying by \( \hat{\square} \):

\[ \hat{E} \hat{\square} = \left( \frac{\hat{p}^2}{2m} + V \right) \hat{\square} \]

The Schrodinger Equation!
Time-independent Schrödinger Equation

In many (most) cases the potential $V$ will not depend on time. Then we can write:

$$\Psi(x,t) = \Psi(x) e^{-i\omega t}$$

$$i\hbar \frac{\partial \Psi}{\partial t} = i\hbar (-i\omega) \Psi = \hbar \omega \Psi = E \Psi$$

This gives the time-independent S. Eqn:

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

The probability density and distributions are constant in time:

$$\Psi^*(x,t) \Psi(x,t) = \Psi^*(x) e^{i\omega t} \Psi(x) e^{-i\omega t} = \Psi^*(x) \Psi(x)$$
The infinite square well potential

The particle is constrained to $0 < x < L$. Outside the "well" $V = \infty$,

\[ \square \square = 0 \]

for $x<0$ or $x>L$. 
Inside the well, the t-independent Schrödinger Equation:

\[ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E \psi \]

\[ \frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2} \psi = -k^2 \psi \]

(with \( k = \sqrt{\frac{2mE}{\hbar^2}} \))

A general solution is:

\[ \psi(x) = A \sin kx + B \cos kx \]

Continuity at \( x=0 \) and \( x=L \) give

\[ \psi(x=0) = 0 \]
\[ \psi(x=L) = 0 \]
\[ B = 0 \]

and

\[ \psi(x=L) = 0 \]

Therefore:

\[ \psi(x) = A \sin kx \]

With \( kL = n \pi \) \( n=1,2,3,\ldots \)
Normalization condition gives

\[ A = \sqrt{\frac{2}{L}} \]

so the normalized wave functions are:

\[ y_n(x) = \sqrt{\frac{2}{L}} \sin(\frac{n\pi x}{L}) \quad n=1,2,3,\ldots \]

with \( k_n = \frac{n\pi}{L} = \sqrt{\frac{2mE_n}{\hbar^2}} \)

\[ E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \]

The possible energies (Energy levels) are quantized with \( n \) the quantum number.
Consider a particle of energy $E < V_0$. Classically, it will be bound inside the well. Quantum Mechanically, there is a finite probability of it being outside of the well (in regions I or III).
Regions I and III:

\[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = (E - V_0) \psi\]

\[\psi \quad \frac{d^2 \psi}{dx^2} = \psi^2 \quad \text{with } \psi^2 = 2m(V_0 - E)/\hbar^2 > 0\]

The solutions are exponential decays:

\[\psi_I(x) = A e^{\psi x} \quad \text{Region I } (x<0)\]

\[\psi_{III}(x) = B e^{-\psi x} \quad \text{Region III } (x>L)\]

In region II (in the well) the solution is

\[\psi_{II}(x) = C \cos(kx) + D \sin(kx)\]

with \(k^2 = 2mE/\hbar^2\) as before.

Coefficients determined by matching wavefunctions and derivatives at boundaries.
The 3-dimensional infinite square well

S. time-independent eqn in 3-dim:

\[ \frac{-\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V = E \]

The solution:

\[ \psi = A \sin(k_1x) \sin(k_2y) \sin(k_3z) \]

with \( k_1 = n_1 \frac{\pi}{L_1} \), \( k_2 = n_2 \frac{\pi}{L_2} \), \( k_3 = n_3 \frac{\pi}{L_3} \).

Allowed energies:

\[ E = \frac{-\hbar^2}{2m} \left( \frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right) \]
If \( L_1 = L_2 = L_3 = L \) (a cubical box) the energies are:

\[
E = \frac{\hbar^2}{2mL^2} \left( n_1^2 + n_2^2 + n_3^2 \right)
\]

The ground state \((n_1 = n_2 = n_3 = 1)\) energy is:

\[
E_0 = \frac{3\hbar^2}{2mL^2}
\]

The first excited state can have \((n_1, n_2, n_3) = (2,1,1)\) or \((1,2,1)\) or \((1,1,2)\)

There are 3 different wave functions with the same energy:

\[
E_1 = \frac{6\hbar^2}{2mL^2}
\]

The 3 states are degenerate.
Simple Harmonic Oscillator

Spring force: \( F = -k x \)

\[ V(x) = \frac{1}{2} k x^2 \]

A particle of energy \( E \) in this potential:

\[ -\frac{\hbar^2}{2m} \frac{d^2\square}{dx^2} + \frac{1}{2} \square x^2 \square = E \square \]
\[
\frac{d^2 \psi}{dx^2} = \left( \frac{2m E}{\hbar} x^2 - \frac{m \hbar}{\hbar^2} \right) \psi
\]

with

\[
\hbar = \frac{2m E}{\hbar} \quad \text{and} \quad \hbar^2 = \frac{m \hbar}{\hbar^2}
\]

The solutions are:

\[
\psi_n(x) = H_n(x) \ e^{-\frac{x^2}{2}}
\]

Hermite Polynomial

Gaussian

(oscillates at small \(x\))

(exponential decay at large \(x\))
The energy levels are

\[ E_n = ( n + 1/2 ) \hbar \omega \]

where \( \omega^2 = \frac{k}{m} \) is the classical angular frequency.

The minimum energy \((n=0)\) is

\[ E_0 = \frac{\hbar \omega}{2} \]

This is known as the **zero-point energy**.
The lowest energy state saturates the Heisenberg uncertainty bound:

\[ \Delta x \Delta p = \hbar / 2 \]

We can use this to calculate \( E_0 \).

In the SHM, \( \langle PE \rangle = \langle K \rangle = E/2 \).

\[ \Delta \langle x^2 \rangle / 2 = \langle p^2 \rangle / (2m) = E/2 \]

\[ \Delta \Delta x^2 = \Delta p^2 / m = E \]

\[ \Delta x = \Delta p / \sqrt{m} \]

From uncertainty principle: \( \Delta x = \hbar / (2\Delta p) \)

So \( E = \Delta \Delta x \Delta x = \Delta (\Delta p / \sqrt{m}) (\hbar / (2\Delta p)) \)

\[ = (\hbar / 2) \sqrt{\Delta p / m} = \hbar \Delta p / 2 \]
Barriers and Tunneling

A particle of total energy $E$ approaches a change in potential $V_0$. Assume $E>V_0$:

Classically, the particle slows down over the barrier, but it always makes it past into region III.

Quantum Mechanically, there are finite probabilities of the particle being reflected as well as transmitted.
Solutions:

Region I

$$ \Phi_I = A e^{ikx} + B e^{-ikx} $$

Region II

$$ \Phi_{II} = C e^{ik'x} + D e^{-ik'x} $$

Region III

$$ \Phi_{III} = F e^{ikx} $$

with

$$ k = \sqrt{\frac{2mE}{\hbar^2}} \quad k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} $$
Coefficients determined by continuity of \( y \) and derivative at boundaries.

The probability of reflection is

\[
R = \frac{|B|^2}{|A|^2}
\]

The probability of transmission is

\[
T = \frac{|F|^2}{|A|^2}
\]

In general there will be some reflection and some transmission.

The result for transmission probability is

\[
T = \frac{1}{1 + \frac{V_0^2 \sin^2(k'L)}{4E(E - V_0)}}
\]

(Note \( T=1 \) for \( k'L=n\pi \), \( n=1,2,3,\ldots \))
If \( E < V_0 \) → no transmission classically.

But in QM, probability of transmission is nonzero.

For \( E < V_0 \) intermediate wavefunctions are:

\[
\psi_{II} = C e^{a x} + D e^{-a x}
\]

where \( a^2 = 2m(V_0 - E)/\hbar^2 \)

The intermediate solution decays exponentially, but there is a finite probability for the particle to emerge on the other side.

This process is called tunneling.
The probability for transmission is

\[ T \approx 16 \left( \frac{E}{V_0} \right) \left( 1 - \frac{E}{V_0} \right) e^{-2aL} \]

for \( aL \gg 1 \)
Applications of tunneling:

1) **Scanning Tunneling Microscope**
Consider two metals separated by vacuum:

![Diagram of two metals with distance L and work function](attachment://diagram.png)

Apply a voltage difference between the metals:

- The current $\sim$ Tunneling Probability $\sim e^{-\frac{\Phi}{L}}$
- Very sensitive to distance $L$
- With thin metal probe can map the surface contours of the other metal at the atomic level.
2) **Nuclear 𝛼-Decay**

The potential seen by the 𝛼-particle looks like:

Because the decay is limited by the probability of tunneling, small changes in the potential or energy of the 𝛼-particle lead to large changes in the nuclear lifetime.

\[ ^{232}\text{Th} \quad \alpha \approx 2 \times 10^8 \text{ yr} \]
\[ ^{212}\text{Po} \quad \alpha \approx 4 \times 10^{-7} \text{ s} \]

\[ \] 24 orders of magnitude!