Modern Physics 6a – Intro to Quantum Mechanics
Physical Systems, Thursday 15 Feb. 2007, EJZ

Plan for our last four weeks:
• week 6 (today), Ch.6.1-3: Schrödinger Eqn in 1D, square wells
• week 7, Ch.6.4-6: Expectation values, operators, quantum harmonic oscillator, applications
• week 8, Ch.7.1-3: Schrödinger Eqn in 3D, Hydrogen atom
• week 9, Ch.7.4-8: Spin and angular momentum, applications

Outline – Intro to QM
• How to predict a system’s behavior?
• Schrödinger equation, energy & momentum operators
• Wavefunctions, probability, measurements
• Uncertainty principle, particle-wave duality
• Applications

How can we describe a system and predict its evolution?

Classical mechanics:
Force completely describes a system:
Use $F = ma = m \frac{dp}{dt}$ to find $x(t)$ and $v(t)$.

Quantum mechanics:
Wavefunction $\psi$ completely describes a QM system

Energy and momentum operators

$$E = \frac{hc}{\lambda} = pc \quad p = \frac{h}{\lambda}$$

$p = \frac{h}{\lambda} = \frac{\hbar}{2\pi} \approx \hbar k \approx i\hbar \frac{\partial}{\partial x}$

Similarly, from uncertainty principle, construct energy operator:

$$E t \approx \hbar \quad E \approx i\hbar \frac{\partial}{\partial t}$$
Energy conservation ⇒ Schroedinger eqn.

\[ E = T + V \]

\[ E \psi = T \psi + V \psi \]

where \( \psi \) is the wavefunction and operators depend on \( x, t \), and momentum:

\[ \hat{p} = i \hbar \frac{\partial}{\partial x} \quad \hat{E} = i \hbar \frac{\partial}{\partial t} \]

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

Solve the Schroedinger eqn. to find the wavefunction, and you know *everything* possible about your QM system.

Schrödinger Eqn

We saw that quantum mechanical systems can be described by wave functions \( \Psi \).

A general wave equation takes the form:

\[ \Psi(x,t) = A[\cos(kx-\omega t) + i \sin(kx-\omega t)] = e^{i(kx-\omega t)} \]

Substitute this into the Schrodinger equation to see if it satisfies energy conservation.

Derivation of Schrödinger Equation

Wave function and probability

EXAMPLE Q7.1

Problem: Consider the wavefunction \( \psi(x) \) shown in Figure Q7.1a. If we do an experiment to locate the quantum, what result is most likely? Least likely?

Figure Q7.1: (a) An example wavefunction. (b) The square of the same wavefunction.

Probability that a measurement of the system will yield a result between \( x_1 \) and \( x_2 \) is:

\[ \int_{x_1}^{x_2} |\psi(x,t)|^2 dx \]
Measurement collapses the wave function

• This does not mean that the system was at X before the measurement - it is not meaningful to say it was localized at all before the measurement.
• Immediately after the measurement, the system is still at X.
• Time-dependent Schrödinger eqn describes evolution of $\psi$ after a measurement.

Exercises in probability: qualitative

Q7T.1 Imagine that at a certain time a quanton has the wave function shown in Figure Q7.9. If we were to perform an experiment to locate the quanton, what would be the most likely result or results?

Exercises in probability: quantitative

1. Probability that an individual selected at random has age=15?
4. Average = expectation value of repeated measurements of many identically prepared system:
5. Average of squares of ages =
6. Standard deviation $\sigma$ will give us uncertainty principle...

Exercises in probability: uncertainty

Standard deviation $\sigma$ can be found from the deviation from the average: $\Delta j = j - \langle j \rangle$
But the average deviation vanishes: $\langle \Delta j \rangle = 0$
So calculate the average of the square of the deviation: $\sigma^2 = \langle (\Delta j)^2 \rangle$

Exercise: show that it is valid to calculate $\sigma$ more easily by:
$\sigma^2 = \langle j^2 \rangle - \langle j \rangle^2$
HW: Find these quantities for the exercise above.
Expectation values

Most likely outcome of a measurement of position, for a system (or particle) in state $\psi$:

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x,t)|^2 dx$$

Most likely outcome of a measurement of position, for a system (or particle) in state $\psi$:

$$\langle p \rangle = m \frac{d \langle x \rangle}{dt} = -i\hbar \int_{-\infty}^{\infty} \left( \psi^* \frac{\partial \psi}{\partial x} \right) dx$$

Uncertainty principle

Position is well-defined for a pulse with ill-defined wavelength. Spread in position measurements = $\sigma_x$

Momentum is well-defined for a wave with precise $\lambda$. By its nature, a wave is not localized in space. Spread in momentum measurements = $\sigma_p$

We saw last week that $\sigma_x \sigma_p \geq \hbar$

Particles and Waves

Light interferes and diffracts - but so do electrons! e.g. in Ni crystal

Electrons scatter like little billiard balls - but so does light! in the photoelectric effect

Applications of Quantum mechanics

Blackbody radiation: resolve ultraviolet catastrophe, measure star temperatures

Photoelectric effect: particle detectors and signal amplifiers

Bohr atom: predict and understand H-like spectra and energies

Structure and behavior of solids, including semiconductors

Scanning tunneling microscope

Zeeman effect: measure magnetic fields of stars from light

Electron spin: Pauli exclusion principle

Lasers, NMR, nuclear and particle physics, and much more...

Sign up for your Minilectures in Ch.7
Part 2: Stationary states and wells

- Stationary states
- Infinite square well
- Finite square well

- Next week: quantum harmonic oscillator
- Blackbody

Stationary states

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

If evolving wavefunction $\Psi(x,t) = \psi(x)f(t)$ can be separated, then the time-dependent term satisfies

$$i\hbar \frac{1}{f} \frac{df}{dt} = E$$

Everyone solve for $f(t) = \text{______}$

Separable solutions are stationary states...

Separable solutions:

1. are stationary states, because $|\Psi(x,t)|^2 = |\psi(x)|^2$
   - probability density is independent of time [2.7]
   - therefore, expectation values do not change

2. have definite total energy, since the Hamiltonian is sharply localized: [2.13] $\sigma_{\hbar^2} = 0$

3. $\psi_i$ = eigenfunctions corresponding to each allowed energy eigenvalue $E_i$.

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n e^{-iE_n t/\hbar}$$

General solution to SE is [2.14]

Show that stationary states are separable:

Guess that SE has separable solutions $\Psi(x,t) = \psi(x)f(t)$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

sub into SE=Schrodinger Eqn

$$i\hbar \frac{\partial \psi}{\partial t} = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} + V\psi$$

Divide by $\psi(x)f(t)$:

$LHS(t) = RHS(x) = \text{constant}=E$. Now solve each side:

You already found solution to LHS: $f(t) = \text{______}$

$$\frac{-\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V\psi = E\psi$$

RHS solution depends on the form of the potential $V(x)$. 
Now solve for $\psi(x)$ for various $V(x)$

Strategy:
* draw a diagram
* write down boundary conditions (BC)
* think about what form of $\psi(x)$ will fit the potential
* find the wavenumbers $k_n=\frac{2\pi}{\lambda}$
* find the allowed energies $E_n$
* sub $k$ into $\psi(x)$ and normalize to find the amplitude $A$
* Now you know everything about a QM system in this potential, and you can calculate for any expectation value

Infinite square well: $V(0<x<L) = 0$, $V=\infty$ outside

What is probability of finding particle outside?
Inside: SE becomes
$$E \psi = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2}$$

* Solve this simple diffeq, using $E=p^2/2m$,
* $\psi(x) = A \sin kx + B \cos kx$: apply BC to find $A$ and $B$
* Draw wavefunctions, find wavenumbers: $k_n L = \pm n\pi$
* find the allowed energies:
* sub $k$ into $\psi(x)$ and normalize:
* Finally, the wavefunction is

Square well: homework

Repeat the process above, but center the infinite square well of width $L$ about the point $x=0$.
Preview: discuss similarities and differences

Finite square well: $V=0$ inside, $V_0$ outside

Infinite square well application:
Ex.6-2 Electron in a wire (p.256)
\[ \psi'(x) \text{ be continuous at these points. Outside the well, i.e., for } 0 > x > L, \]
6-18 becomes
\[
\frac{\psi''(x)}{k^2} (V_0 - E) \phi(x) = \alpha^2 \phi(x)
\]
where
\[
\alpha^2 = \frac{2m}{k^2} (V_0 - E) > 0
\]

Everywhere: \(\Psi, \Psi', \Psi''\) continuous
Outside: \(\Psi \to 0, \Psi'' \sim \Psi\) because \(E < V_0\) (bound)
Inside: \(\Psi'' \sim -\Psi\) because \(V=0\) (V-E < 0)

Which of these states are allowed?

Outside: \(\Psi \to 0, \Psi'' \sim \Psi\) because \(E < V_0\) (bound)
Inside: \(\Psi'' \sim -\Psi\) because \(V=0\) (V-E < 0)

Finite square well:
- BC: \(\Psi\) is NOT zero at the edges, so wavefunction can spill out of potential
- Wide deep well has many, but finite, states
- Shallow, narrow well has at least one bound state

Summary:
- Time-independent Schrodinger equation has stationary states \(\psi(x)\)
- \(k, \psi(x),\) and \(E\) depend on \(V(x)\) (shape & BC)
- wavefunctions oscillate as \(e^{i\omega t}\)
- wavefunctions can spill out of potential wells and tunnel through barriers