8.21 The Physics of Energy
Fall 2009

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Quantum Mechanics I

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The QUANTUM WORLD is a STRANGE PLACE!

Position of an object is not well-defined

Objects can tunnel through barriers

Energy, momentum, etc. become discretized

But quantum physics is crucial for energy processes

- Discrete quantum states ⇒ entropy ⇒ thermo ⇒ limits to efficiency
- Nuclear processes: fission + fusion depend on tunneling
- Absorption of light by matter (atmosphere, photovoltaics, etc.): depends on discrete quantum spectrum

This lecture: QM rapid immersion
Classically, particles have position $x$, momentum $p$

In quantum mechanics, particles are described by wavefunctions.

Wavefunction obeys (time-dependent) Schrödinger wave equation:

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

Why do we believe this wacky notion?

- Vast range of experiments over last 100 years
- Foundation of most of modern physics.
2-slit experiment. Shoot particles through one or two slits at screen

Destructive + constructive interference $\Rightarrow$ particles are waves
2-slit experiment. Shoot particles through one or two slits at screen

Destructive + constructive interference $\Rightarrow$ particles are waves
Many phenomena described by waves

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<td>( \frac{\partial}{\partial t} \psi = \frac{i\hbar}{2m} \nabla^2 \psi )</td>
<td>Energy</td>
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Wave equation is linear:

\( \psi_1(x, t) \) and \( \psi_2(x, t) \) solve \( \Rightarrow \) linear combination \( a\psi_1(x, t) + b\psi_2(x, t) \) solves

Exhibit constructive and destructive interference for phases in/out of sync.
Violin string: \( \rho \frac{\partial^2}{\partial t^2} Y(x, t) = T \frac{\partial^2}{\partial x^2} Y(x, t) \)

Solutions: sine modes

\[ Y_n = \cos(n\omega_1 t) \sin(n \cdot \frac{\pi}{L} x) \quad \omega_n = n\omega_1 \]
\[ Y_3 = \cos(3\omega_1 t) \sin(3 \cdot \frac{\pi}{L} x) \quad \omega_3 = 3\omega_1 \]
\[ Y_2 = \cos(2\omega_1 t) \sin(2 \cdot \frac{\pi}{L} x) \quad \omega_2 = 2\omega_1 \]
\[ Y_1 = \cos(\omega_1 t) \sin(\frac{\pi}{L} x) \quad \omega_1 = \frac{\pi}{L} \sqrt{\frac{T}{\rho}} \]

- Modes–higher harmonics \((n = 2, 4, 8, \ldots \text{up by octaves})\)
- \(\omega_n \sim n (2\partial/\partial t’s, 2\partial/\partial x’s)\)
- Pluck string – get superposition (linear combination) of modes

Quantum particle in a 1D box: \( i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) \)

Sine modes again

\[ \psi_n = e^{-iE_n t/\hbar} \sin(n \cdot \frac{\pi}{L} x) \quad E_n = n^2 \hbar \omega_1 \]
\[ \ldots \]
\[ \psi_2 = e^{-iE_2 t/\hbar} \sin(2 \cdot \frac{\pi}{L} x) \quad E_2 = 4\hbar \omega_1 \]
\[ \psi_1 = e^{-iE_1 t/\hbar} \sin(\frac{\pi}{L} x) \quad E_1 = \hbar \omega_1 = \frac{\pi^2 \hbar^2}{2mL^2} \]

- Each mode – state of fixed energy
- \(E_n \sim n^2 (1\partial/\partial t, 2\partial/\partial x’s)\)
- General state – superposition (linear combination) of modes
Quantum wavefunctions are complex – Review of complex numbers

Define $i^2 = -1$

Complex number: $z = x + iy$

Often write $z = re^{i\theta} = r(\cos \theta + i \sin \theta)$

$r = \text{magnitude}, \quad \theta = \text{phase}$

Useful properties of complex numbers:

Addition: $(x + iy) + (a + ib) = (x + a) + i(y + b)$

Multiplication: $(x + iy) \times (a + ib) = (xa - yb) + i(ya + xb)$

$(re^{i\theta})(se^{i\psi}) = rse^{i(\theta + \psi)}$

Complex conjugation: $\bar{z} = z^* = x - iy$

Norm: $|z| = \sqrt{x^2 + y^2}, \quad |re^{i\theta}| = r, \quad |z|^2 = z\bar{z} = r^2$
General quantum wavefunction

Quantum particle has “energy basis” spatial wavefunctions $\psi_i(x)$

$\psi_i(x)$ have fixed energies $E_i$

General (time-dependent) state is superposition

$$\psi(x, t) = a_1 e^{-iE_1 t/\hbar} \psi_1(x) + a_2 e^{-iE_2 t/\hbar} \psi_2(x) + \cdots$$

For macroscopic (classical) systems, combine many quantum states

- **Destructive interference** outside small region $\Rightarrow$ classical localization

- Wavefunction nonzero through classical barriers $\Rightarrow$ tunneling

- For micro systems (e.g. atoms) individual quantum states relevant.
Rules of Quantum Mechanics: 4 Axioms

Energy in quantum mechanics

**Axiom 1:** Any finite/physical quantum system has a discrete set of “energy basis states”, which we denote $s_1, s_2, \ldots, s_N$. These states have values of energy $E_1, E_2, \ldots, E_N$.

**Example: hydrogen atom**

\[
\begin{align*}
E_{11 - 26} & \approx \frac{\epsilon_0}{9} \quad (3s, p, d) \\
E_{3 - 10} & \approx \frac{\epsilon_0}{4} \quad (2s, p)
\end{align*}
\]

[$\epsilon_0 \approx -13.6 \text{ eV}$]

\[
\begin{align*}
E_{1,2} & \approx \epsilon_0 \quad (1s)
\end{align*}
\]

- Values of $E$: “spectrum”
- Physicists’ job: compute spectrum of physical systems — Often deal with $\infty$ state approximation

**Example: semiconductor**

- bands
- band gap

- important for photovoltaics
Simplest quantum system: “Qubit” = 2-state system (electron spin)

Earth spins

Classically any $\omega$ seems ok
$\Rightarrow$ any $L, E_{\text{rot}}$

Electron in magnetic field $\mathbf{B} = B\hat{z}$

$$E = -\mathbf{B} \cdot \mu = \tilde{\mu} B L_z$$

$$E_{\pm} = \pm \tilde{\mu} B \hbar / 2$$

Electron spins

or

$$L_z = \pm \frac{1}{2} \hbar$$

- 2 states
- $\hbar \approx 1.0546 \times 10^{-34} \text{ Js}$
  - fundamental quantum unit

Confirmed by experiment
Axiom 2: The state of a quantum system at any point in time is a linear combination ("quantum superposition") of basis states

$$|s\rangle = z_1|s_1\rangle + z_2|s_2\rangle + \cdots + z_n|s_n\rangle$$

- Can think of like a vector: $\mathbf{r} = x\hat{i} + y\hat{j} + z\hat{k}$
- Convention: unit normalization $|z_1|^2 + |z_2|^2 + \cdots + |z_n|^2 = 1$

What does a quantum superposition mean?

Axiom 3: If you measure the system’s energy (assume $E_i$ distinct)

$$\text{probability}(E = E_i) = |z_i|^2,$$ after measurement state $\Rightarrow s_i$

Example:

$$\frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|−\rangle$$

$|+\rangle$, prob = 1/2

$|−\rangle$, prob = 1/2
Puzzle: If measurements give random results, how is $E$ conserved?

Example: 2 separated electrons in B field, total $E = 0$

\[
\begin{align*}
\text{state 1: } & |+\rangle |-\rangle \\
\text{state 2: } & |\rangle |+\rangle
\end{align*}
\]

Both states: $E = E_+ + E_- = 0$

Assume system in state $\frac{1}{\sqrt{2}} |+\rangle - \frac{1}{\sqrt{2}} |\rangle$

Measure spin of first particle

50%: Particle 1 in state $|\rangle$: system in state 1, $E_1 = E_+$, $E_2 = E_-$

50%: Particle 1 in state $|\rangle$: system in state 2, $E_1 = E_-$, $E_2 = E_+$

BUT TOTAL ENERGY IS CONSERVED!
Time Dependence

Axiom 4: If at time $t_0$ a state $|s(t_0)\rangle$ has definite energy $E$ then at time $t$ the state is

$$|s(t)\rangle = e^{-iE(t-t_0)/\hbar}|s(t_0)\rangle$$

Time evolution is linear in $|s\rangle$, so if

$$|s(t_0)\rangle = z_1|s_1\rangle + \cdots + z_n|s_n\rangle$$

then

$$|s(t)\rangle = z_1 e^{-iE_1(t-t_0)/\hbar}|s_1\rangle + \cdots + z_n e^{-iE_n(t-t_0)/\hbar}|s_n\rangle$$

Note: only phase changes for definite $E$ state!

$$\frac{d}{dt}|s(t)\rangle = -\frac{i}{\hbar}E|s(t)\rangle$$

⚠️ Matrix notation

$$|s(t_0)\rangle = \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix} \quad H = \begin{pmatrix} E_1 & 0 & \cdots & 0 \\ 0 & E_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & E_n \end{pmatrix}$$

⇒ Schrödinger equation

$$\frac{d}{dt}|s(t)\rangle = -\frac{i}{\hbar}H|s(t)\rangle$$
SUMMARY: axioms of quantum mechanics

1. Any physical system has a discrete set of E basis states $|s_i\rangle$
2. General state is linear combination $z_1|s_1\rangle + \cdots + z_n|s_n\rangle$
3. Measurement: probability $= |z_i|^2$ that state $\rightarrow |s_i\rangle$
4. Time development linear, $|s_i\rangle \rightarrow e^{-iE_i(t-t_0)/\hbar}|s_i\rangle$

- All of QM, QFT essentially elaboration on principles 1-4 + symmetry, developing tools for calculations in particular cases
- Often work in another basis (not E basis)
- A primary problem: given system, determine spectrum
Particle states described by wavefunctions

Like superposition of states in fixed positions, $|\psi(x)|^2 = \text{prob. @ } x$

Think of as limit of discrete “position basis”

$|\psi\rangle = \sum_j \psi_j |x_j\rangle \rightarrow \psi(x)$

$\sum_j |\psi_j|^2 = 1 \rightarrow \int |\psi(x)|^2 dx = 1$
What are energy basis states (|s⟩’s) for free particle?

Translate ⇒ same Energy: \( \psi(x + \delta) = e^{i\theta\delta} \psi(x) \)

- Plane wave states \( \psi_p(x) = e^{ipx/\hbar} \quad p = \text{momentum!} \)

- Matches experimental observation (Davisson-Germer, 1927):
  de Broglie wavelength of matter \( \lambda = h/p \ (e^{ipx/\hbar} = e^{2\pi ix/\lambda}) \)

- Energy: \( E = \frac{p^2}{2m} \) Schrödinger equation:

\[
E_p \psi_p(x) = \frac{p^2}{2m} \psi_p(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_p(x) = H \psi_p(x)
\]

Time-dependent Schrödinger eq.: \( i\hbar \frac{\partial}{\partial t} \psi(x, t) = H \psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) \)
Back to particle in a (1D) box

Time-independent Schrödinger equation:

\[ H \psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) = E \psi(x) \]

Boundary Conditions: \( \psi(0) = \psi(L) = 0 \)

Solution: Combination of \( e^{ipx/\hbar}, e^{-ipx/\hbar} \)

Energy basis states \( |n\rangle \): \( \psi_n = \sin \frac{\pi nx}{L} \)

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

Spectrum (\( \epsilon = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \))

\[ E_1 = \epsilon \]
\[ E_2 = 4\epsilon \]
\[ E_3 = 9\epsilon \]
\[ E_4 = 16\epsilon \]
\[ E_5 = 25\epsilon \]
\[ E_6 = 36\epsilon \]
Even more useful model: 1D Simple Harmonic Oscillator (SHO)

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

\[ H\psi(x) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} kx^2 \right] \psi(x) = E\psi(x) \]

Boundary Conditions: \( \psi(|x| \to \infty) = 0 \)

Solution: \( [\omega = \sqrt{k/m}] \)

\[ |0\rangle : \quad \psi_0 = C_0 e^{-\frac{m\omega}{2\hbar} x^2} \]
\[ |1\rangle : \quad \psi_1 = C_1 xe^{-\frac{m\omega}{2\hbar} x^2} \]
\[ |2\rangle : \quad \psi_2 = C_2 \left( \frac{2m\omega}{\hbar} x^2 - 1 \right) e^{-\frac{m\omega}{2\hbar} x^2} \]
\[ \cdots \]

[Analytic solution; many approaches, one in notes]

\[ E_0 = \frac{1}{2} \hbar\omega \]
\[ E_1 = 1\frac{1}{2} \hbar\omega \]
\[ E_2 = 2\frac{1}{2} \hbar\omega \]
\[ E_3 = 3\frac{1}{2} \hbar\omega \]
\[ E_4 = 4\frac{1}{2} \hbar\omega \]
\[ E_5 = 5\frac{1}{2} \hbar\omega \]

Spectrum \( E_n = (n + 1/2) \hbar\omega \)
Hydrogen-like atom (now in 3D, assume $m_p \gg m_e$)

$$H\psi(x) = \left[ -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \right] \psi(x) = E\psi(x)$$

Solutions:

$$\psi_{1s} = C_{1s} \times (a_0)^{-3/2} e^{-r/a_0}$$
$$\psi_{2s} = C_{2s} \times (a_0)^{-3/2} e^{-r/a_0} \left( 1 - \frac{r}{2a_0} \right)$$
$$\psi_{2p} = C_{2p} \times (a_0)^{-3/2} e^{-r/a_0} \left( \frac{x, y, z}{r} \right)$$

... where Bohr radius is $a_0 = \frac{\hbar^2}{me^2}4\pi\epsilon_0 \approx 0.52\text{Å}$

$$E_1 \approx -13.6 \text{ eV}$$

Spectrum

$$E_n = \frac{-e^2}{4\pi\epsilon_0 a_0 n^2} \approx \frac{-13.6 \text{ eV}}{n^2}$$
How does quantum state ⇒ classical physics?

Consider particle in potential

Sum of energy basis states ⇒ “localized wave packet”

Time evolution under Schrödinger equation \( \dot{\psi}(t) = \frac{-i}{\hbar} H \psi(t) \)

⇒ Packet follows classical laws

Define

\[
\langle x \rangle_{\psi(t)} = \int dx \ x |\psi(x, t)|^2
\]

\[
\langle p \rangle_{\psi(t)} = \sum_p \bar{\psi}_p \psi_p p = -i\hbar \int dx \ \bar{\psi}(x, t) \frac{\partial}{\partial x} \psi(x, t).
\]

Can show

\[
\frac{d}{dt} \langle x \rangle_{\psi(t)} = \frac{1}{m} \langle p \rangle_{\psi(t)}
\]

\[
m \frac{d^2}{dt^2} \langle x \rangle_{\psi(t)} = \frac{d}{dt} \langle p \rangle_{\psi(t)} = -\langle \frac{\partial}{\partial x} V(x) \rangle_{\psi(t)}
\]
SUMMARY of QM

- Quantum particles described by wavefunction

- Any quantum system: basis of states w/ fixed energy (A1)
  General state linear combination (superposition) of energy basis (A2)

- Quantum particles: for $V = 0$, $e^{ipx/\hbar}$ has momentum $p$, $E = p^2 / 2m$

- Energy basis states with potential $V$ : $H\psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right]\psi = E\psi$

- Box spectrum: $E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}, n = 1, 2, \ldots$

- SHO spectrum: $E_n = (n + 1/2)\hbar\omega, n = 0, 1, \ldots$

- Time-dependent Schrödinger eq. $\dot{\psi}(t) = -\frac{i}{\hbar}H\psi(t)$ [E $\propto$ frequency] (A4)