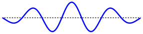
8.21 The Physics of Energy
Fall 2009

8.21 Lecture 6

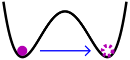
Quantum Mechanics I

September 21, 2009

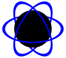
The QUANTUM WORLD is a *STRANGE PLACE!*



Position of an object is not well-defined



Objects can tunnel through barriers



Energy, momentum, etc. become discretized

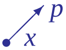
But quantum physics is crucial for energy processes

- 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

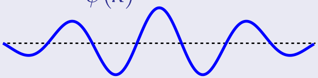
This lecture: QM rapid immersion

Quantum wavefunctions

Classically, particles have position x, momentum p



In quantum mechanics, particles are described by *wavefunctions*



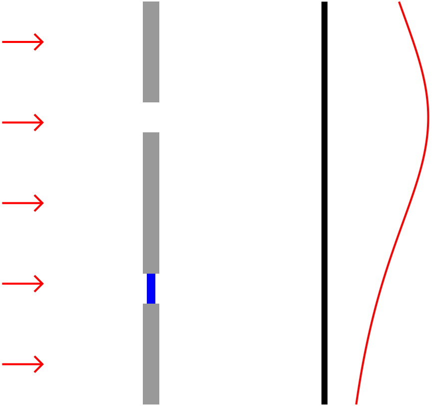
Wavefunction obeys (time-dependent) Schrödinger wave equation

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

Why do we believe this wacky notion?

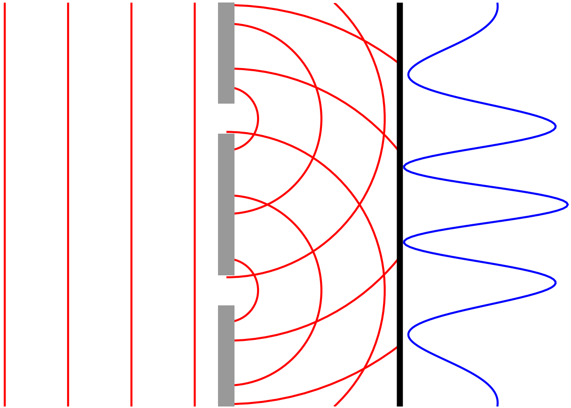
- Vast range of experiments over last 100 years
- Foundation of most of modern physics.

2-slit experiment. Shoot particles through one or two slits at screen



Destructive + constructive interference ⇒ particles are waves

2-slit experiment. Shoot particles through one or two slits at screen



Destructive + constructive interference ⇒ particles are waves

Many phenomena described by waves

		frequency significance
light (EM)	$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{E} = \nabla^2\mathbf{E}$	color
sound (pressure)	$\frac{1}{v_s^2}\frac{\partial^2}{\partial t^2}p = \nabla^2 p$	pitch
QM (wavefunction)	$\frac{\partial}{\partial t}\psi = \frac{i\hbar}{2m}\nabla^2\psi$	energy

Wave equation is linear:

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

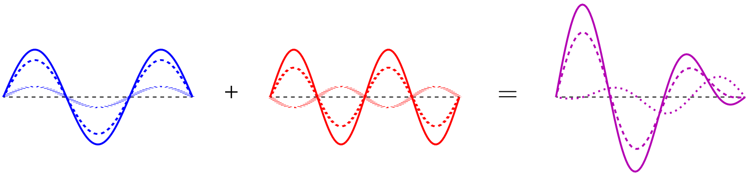
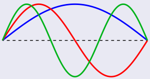


Exhibit constructive and destructive interference for phases in/out of sync.

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

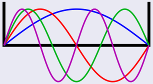


$$Y_n = \cos(n\omega_1 t)\sin(n \cdot \tfrac{\pi}{L} x) \quad \omega_n = n\omega_1$$
$$Y_3 = \cos(3\omega_1 t)\sin(3 \cdot \tfrac{\pi}{L} x) \quad \omega_3 = 3\omega_1$$
$$Y_2 = \cos(2\omega_1 t)\sin(2 \cdot \tfrac{\pi}{L} x) \quad \omega_2 = 2\omega_1$$
$$Y_1 = \cos(\omega_1 t)\sin(\tfrac{\pi}{L} x)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

- Modes–higher harmonics ($n = 2, 4, 8, \ldots$ 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



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

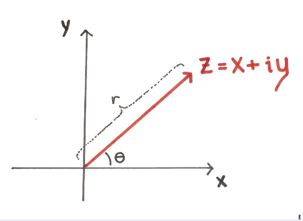
- Each mode – state of fixed energy
- $E_n \sim n^2$ ($1\partial/\partial t$, $2\partial/\partial x$'s)
- General state – superposition (linear combination) of modes

Quantum wavefunctions are complex – Review of complex numbers

Define $i^2 = -1$

Complex number: $z = x + iy$

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

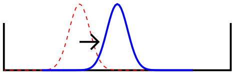
Quantum particle has "energy basis" spatial wavefunctions $\psi_i(\mathbf{x})$
$\psi_i(\mathbf{x})$ have fixed energies E_i

General (time-dependent) state is superposition

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

For macroscopic (classical) systems, combine many quantum states

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



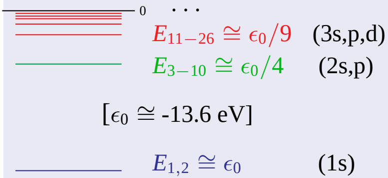
- Wavefunction nonzero through classical barriers $\Rightarrow$ tunneling
- For micro systems (*e.g.* atoms) individual quantum states relevant.

Rules of Quantum Mechanics: 4 Axioms

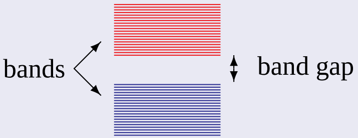
Energy in quantum mechanics

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



Example: semiconductor

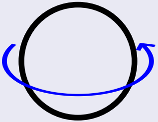


- important for photovoltaics

- Values of E: "spectrum"
- Physicists' job: compute spectrum of physical systems
  — Often deal with ∞ state approximation

Simplest quantum system: "Qubit" = 2-state system (electron spin)

Earth spins



Classically any ω seems ok

$\Rightarrow$ any L, E_{rot}

Electron spins

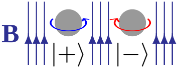
 or 

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

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

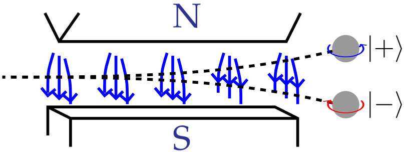
Electron in magnetic field $\mathbf{B} = B\hat{z}$

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



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

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 $|z_1|^2 + |z_2|^2 + \cdots + |z_n|^2 = 1$

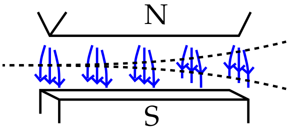
What does a quantum superposition mean?

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

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

Example:

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

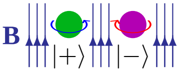


$|+\rangle$, prob = 1/2

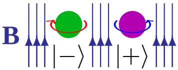
$|-\rangle$, prob = 1/2

⚠ Puzzle: If measurements give random results, how is E conserved?

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



state 1: $|+-\rangle$



state 2: $|-+\rangle$

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

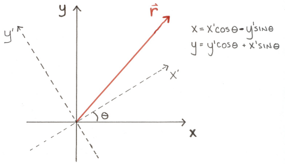
⚠ Matrix notation $|s(t_0)\rangle = \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix}$ $H = \begin{pmatrix} E_1 & 0 & \cdots & 0 \\ 0 & E_2 & & 0 \\ & & \ddots & \\ 0 & 0 & & E_n \end{pmatrix}$

$\Rightarrow$ Schrödinger equation $\frac{\mathrm{d}}{\mathrm{d}t}|s(t)\rangle = -\frac{i}{\hbar}H|s(t)\rangle$

SUMMARY: axioms of quantum mechanics

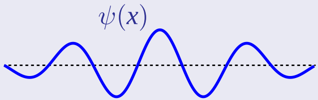
1. Any physical system has a discrete set of E basis states $|s_i\rangle$
2. General state is linear combination $z_1|s_1\rangle + \cdots + z_n|s_n\rangle$
3. Measurement: probability = $|z_i|^2$ that state $\rightarrow |s_i\rangle$
4. Time development linear, $|s_i\rangle \rightarrow e^{-iE_i(t-t_0)/\hbar}|s_i\rangle$

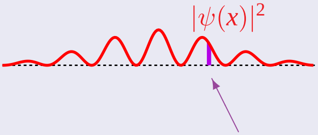
- All of QM, QFT essentially elaboration on principles 1-4 + symmetry, developing tools for calculations in particular cases
- Often work in another basis (not E basis)



- A primary problem: given system, determine spectrum

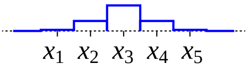
Particle states described by wavefunctions





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

Think of as limit of discrete "position basis"



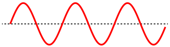
$\longrightarrow$

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

$$\sum_j |\psi_j|^2 = 1 \quad \longrightarrow \quad \int |\psi(x)|^2 dx = 1$$

What are energy basis states ($|s\rangle$'s) for free particle?

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



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

- Matches experimental observation (Davisson-Germer, 1927):

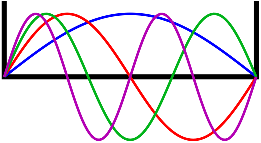
de Broglie wavelength of matter $\lambda = h/p$ ($e^{ipx/\hbar} = e^{2\pi i x/\lambda}$)

- 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



$E_6 = 36\epsilon$

$E_5 = 25\epsilon$

$E_4 = 16\epsilon$

$E_3 = 9\epsilon$

$E_2 = 4\epsilon$

$E_1 = \epsilon$

Spectrum ($\epsilon = \hbar^2\pi^2 n^2/2mL^2$)

Time-independent Schrödinger equation:

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

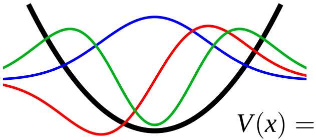
Boundary Conditions: $\psi(0) = \psi(L) = 0$

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

Energy basis states $|n\rangle$: $\psi_n = \sin \pi n x/L$

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

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: $[\omega = \sqrt{k/m}]$

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

$\vdots$

$E_5 = 5\frac{1}{2}\hbar\omega$

$E_4 = 4\frac{1}{2}\hbar\omega$

$E_3 = 3\frac{1}{2}\hbar\omega$

$E_2 = 2\frac{1}{2}\hbar\omega$

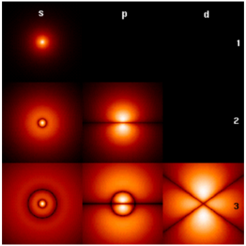
$E_1 = 1\frac{1}{2}\hbar\omega$

$E_0 = \frac{1}{2}\hbar\omega$

Spectrum ($E_n = (n + 1/2)\hbar\omega$)

[Analytic solution; many approaches, one in notes]

Hydrogen-like atom (now in 3D, assume $m_p \gg m_e$)



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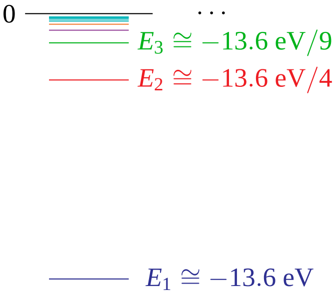


$$H\psi(x) = \left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r}\right]\psi(x) = E\psi(x)$$

Solutions:

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

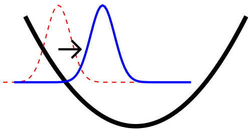
where Bohr radius is $a_0 = \frac{\hbar^2}{me^2} 4\pi\epsilon_0 \approx 0.52 Å$

Spectrum

$(E_n = \frac{-e^2}{4\pi\epsilon_0 a_0 n^2} \cong \frac{-13.6 \text{ eV}}{n^2})$

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

$$\begin{aligned}
\langle x \rangle_{\psi(t)} &= \int dx\; x|\psi(x,t)|^2 \\
\langle p \rangle_{\psi(t)} &= \sum_p \bar{\psi}_p \psi_p p = -i\hbar \int dx\; \bar{\psi}(x,t) \frac{\partial}{\partial x} \psi(x,t)\,.
\end{aligned}$$

Can show

$$\begin{aligned}
\frac{d}{dt} \langle x \rangle_{\psi(t)} &= \frac{1}{m} \langle p \rangle_{\psi(t)} \\
m \frac{d^2}{dt^2} \langle x \rangle_{\psi(t)} &= \frac{d}{dt} \langle p \rangle_{\psi(t)} = -\langle \frac{\partial}{\partial x} V(x) \rangle_{\psi(t)}
\end{aligned}$$

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: $E_n = \hbar^2\pi^2 n^2/2mL^2, n = 1, 2, \ldots$

- 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)