Chemical Engineering 412

Introductory Nuclear Engineering

Lecture 2

Quantum Mechanics I

Relativity

Spiritual Thought

Abraham 3:5

5 And the Lord said unto me: The planet which is the lesser light, lesser than that which is to rule the day, even the night, is above or greater than that upon which thou standest in point of reckoning, for it moveth in order more slow; this is in order because it standeth above the earth upon which thou standest, therefore the reckoning of its time is not so many as to its number of days, and of months, and of years.

Objectives

- Understand Energy/Mass Duality
- Know how to calculate particle/wave properties in classical and quantum conditions
- Understand Schrodinger wave equation
- Know how to use and apply uncertainty principle
- Recognize the reason for quantized energy levels in electrons/nuclei

What $E = mc^2$ means?

Mass and Energy-mathematically equivalent

- Physically equivalent
  - Different manifestations of same thing
  - Adding energy adds mass
    - Higher temperature = more mass
    - Imperceptible at traditional ranges
- Waves - mass, gravitation & momentum
  - Light, electrical waves, kinetic energy, potential energy, and thermal energy
- Mass annihilation – large energy releases
  - Star Trek, not nuclear power

Momentum, KE: Classical & Relativistic

- Classical Mechanics: p = mv
  - $T = \frac{mv^2}{2} = \frac{p^2}{2m} = mc^2 - m_o c^2$
  - $p = \sqrt{2mT}$
- Relativistic Mechanics:
  - $m = \frac{m_0}{\sqrt{1 - v^2/c^2}} \rightarrow m_o{}^2 = m^2 \left(\frac{c^2 - v^2}{c^2}\right)$

Using relativistic mass

$$p^2 \equiv (mv)^2 = \frac{m_0^2 v^2}{1 - \frac{v^2}{c^2}} = \frac{1}{c^2}[(mc^2)^2 - (m_0 c^2)^2] = \frac{1}{c^2}(T^2 + 2Tm_0c^2)$$

Resulting in

$$p = \frac{\sqrt{T^2 + 2Tm_0c^2}}{c} \quad T = c\sqrt{p^2 + m_0^2c^2} - m_0c^2$$

Wave Momentum/Mass

- Waves have mass/momentum ($m=h\nu/c^2$)
- Mass comes only from speed
- $\lambda = \frac{c}{\nu}$
- $E = h\nu$
  - $E = mc^2$
- $p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h\nu}{\lambda}$

Note difference between frequency, given the symbol ν, and velocity, given the similar symbol v. Since light always travels at velocity c, it is rare to have v in an equation about light, though common to have ν in such equations.

Summary

quantity	real (relativistic)	classical
time (t)	$\gamma\ t_0$	t_0
length (ℓ)	ℓ_0/γ	ℓ_0
mass (m)	γm_0	m_0
momentum (p)	$mv = \gamma m_0 v$	$m_0 v$
kinetic energy (T)	$(m - m_0)c^2$ $= (\gamma - 1)m_0 c^2$	$1/2 m_0 v^2$

Lorentz factor $$\gamma = \frac{1}{\sqrt{1 - \left(\frac{v}{c}\right)^2}}$$

Particle Wave Duality (I)

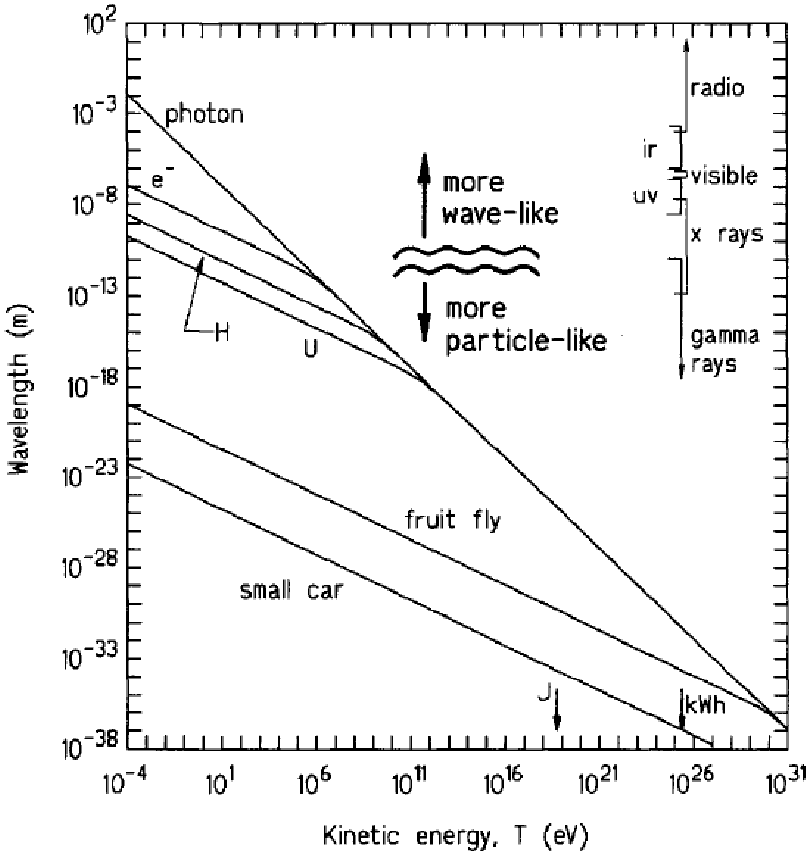
- Waves have particle properties
  - quanta or photons
  - Photoelectric effect, Compton Scattering
- Particles have wave properties
  - De Broglie wave-length
  - Electron scattering
  - $\lambda = \frac{h}{p} = \frac{hc}{\sqrt{T^2+2Tm_oc^2}}$

Particle Wave Duality (II)

- One property (wave or particle) usually dominates
  - Waves:
    - Large wavelengths ($\lambda > 10^{-6}$ m) wave properties
    - Small wavelengths ($\lambda < 10^{-8}$ m) particle properties
  - Particles: $\lambda = \frac{hc}{\sqrt{T^2 + 2Tm_o c^2}}$
    - At very high speed, relativistic behavior
      - $T^2 \gg 2Tm_o c^2$
    - If $\lambda < 10^{-10}$ m, particle behaves as particle

Particle Wave Duality (III)

- Neutron behavior?
  - Low E:
    - $E \sim 10^{-6}$ eV
    - $\lambda = 2.86 \times 10^{-8}$ m
    - comparable to atom spacing
    - scatter off multiple atoms.
  - High E:
    - $E \sim 1$ MeV
    - $\lambda = 2.86 \times 10^{-14}$ m
    - comparable to nucleus size
    - scatter off nucleus.



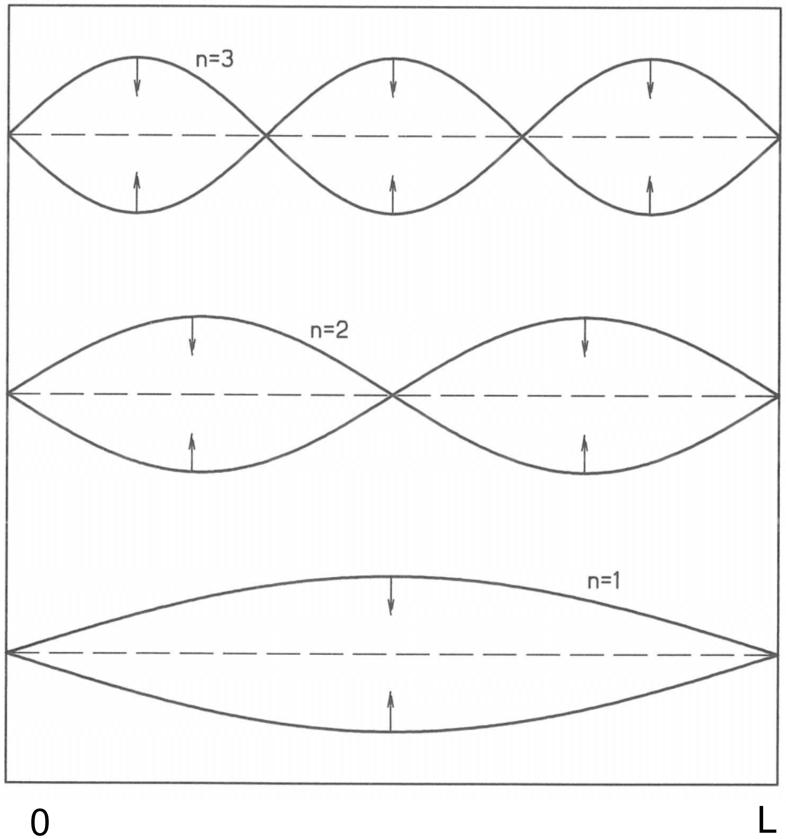
Schrödinger's Wave equation

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = \frac{1}{u^2}\frac{\partial^2 \Psi(x,t)}{\partial t^2}$$

$$\Psi(0,t) = \Psi(L,t) = 0$$

$Note: Solution\ is\ separable\ in\ x\ and\ t$

Also, $t_c = \frac{1}{v}, \frac{n\pi u t_c}{L} = 2\pi$



$$\Psi(x,t) = A\sin\left(\frac{n\pi x}{L}\right) B\sin\left(\frac{n\pi u t}{L}\right) \quad n = 1, 2, 3, \ldots$$

Wave Equation Solution

$$v = \frac{nu}{2L}, \qquad \mathrm{u} = \lambda v$$

$$\Psi(x,t) = \psi(x)T(t)$$

$$\Psi(x,t) = \psi(x)\sin(2\pi v t) \quad n = 1, 2, 3, \ldots$$

Plug this expression into the wave equation:

$$\frac{d^2\psi(x)}{dx^2} + \frac{4\pi^2 v^2}{u^2}\psi(x) = 0 \; or \; \frac{d^2\psi(x)}{dx^2} + \frac{4\pi^2}{\lambda^2}\psi(x) = 0$$

$$\nabla^2\psi(x,y,z) + \frac{4\pi^2}{\lambda^2}\psi(x,y,z) = 0$$

Apply to bound electron (only one)

- Assume:
  - Nucleus produces electric field on electron, V(x, y, z)
  - Electron has rest mass m (=m_o)
  - Electron kinetic energy = T
  - Electron total energy = E
  - Electron potential energy = V
  - *T=E-V;* $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mT}} = \frac{h}{\sqrt{2m(E-V)}}$

$$-\frac{h^2}{8\pi^2 m}\nabla^2\psi(x,y,z) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$$

Observations on Results

- Only two possible solutions
  1. $\psi(x,y,z)$=0 (trivial)
  2. If E has discrete values; E=E_n, n=0,1,2,3…
     - E_n is eigenvalue, $\psi_n(x,y,z)$ is Eigenfunction
- I.E. electron can only have discrete energy levels – verified
- ψ_n is called a "wave function"
  - Complex quantity, extends over all space
  - Relative amplitude of the particle wave
  - If ψ_n' is a solution, so is ψ_n=ψ_n'A
  - A is selected so that $\iiint \psi_n(x,y,z)\psi_n^*(x,y,z)dV = 1$

Quantum Mechanics

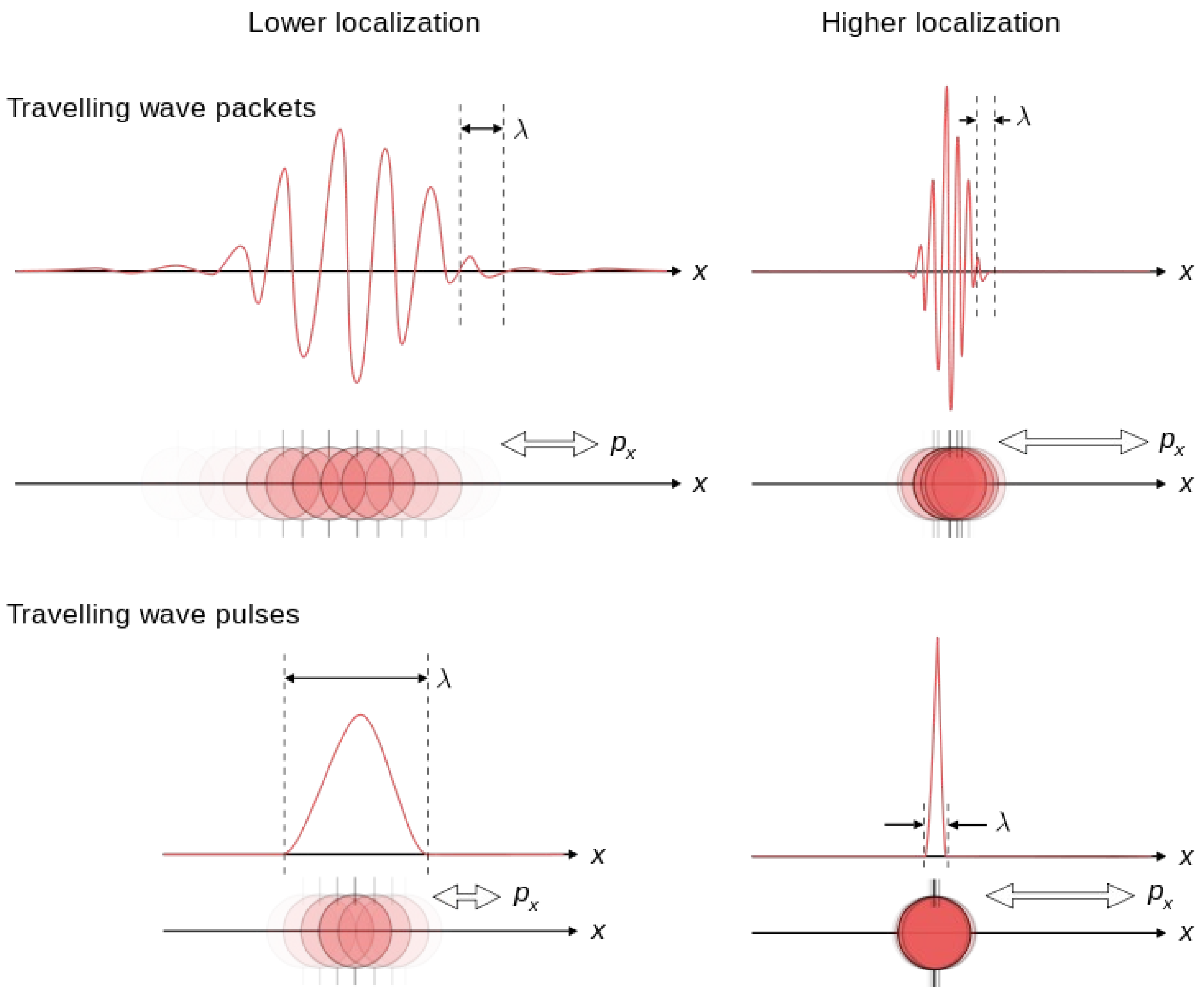
- Particle energy exists in discrete quantities.
- Changes occur over discrete intervals.
- Responsible for maintaining atomic structure (classical model would decay rapidly).
- Electron energy states described by orbitals and are statistical rather than deterministic. These are described by quantum states or numbers.
- Schrödinger's wave equation describes energy levels

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r})\Psi(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) \qquad \hbar=\frac{h}{2\pi}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})+V(\vec{r})\psi(\vec{r})=E\psi(\vec{r})$$

steady-state

Particle-wave Duality



Uncertainty Principle

$$\Delta x \Delta p \geq \frac{h}{4\pi} = \frac{\hbar}{2}$$

$$\Delta t \Delta E \geq \frac{h}{4\pi} = \frac{\hbar}{2}$$

- Position and momentum are fundamentally linked
  - Cannot determine both with arbitrary accuracy.
- Analogously, energy and time are linked
  - Energy of Particle
  - Time a particle remains in a given energy state

Quantum Mechanics (cont'd)

- Quantum particles can penetrate energy barriers that would normally be impenetrable in classical mechanics.
- There is inherent uncertainty in pairs of properties for quantum particles.
  - momentum-position
  - energy-time

Particle in a 1D Box

- Assume:
  - Zero potential in Box, Infinite Potential Outside
  - $\psi(x)$= 0 at x=0 and x=a
  - $\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2 mE}{h^2}\psi(x) = 0$
  - $\mathrm{k} = \frac{8\pi^2 mE}{h^2}$

$$\psi(x) = Asin(kx) + Bcos(kx)$$

$$\psi(x) = 0 = Asin(0) + Bcos(0) = B$$

$$\psi(x) = 0 = Asin(ka)$$

$$k = \frac{n\pi}{a}, n = 1, 2, 3 \ldots; \;\; \psi(x) = Asin\left(\frac{n\pi x}{a}\right)$$

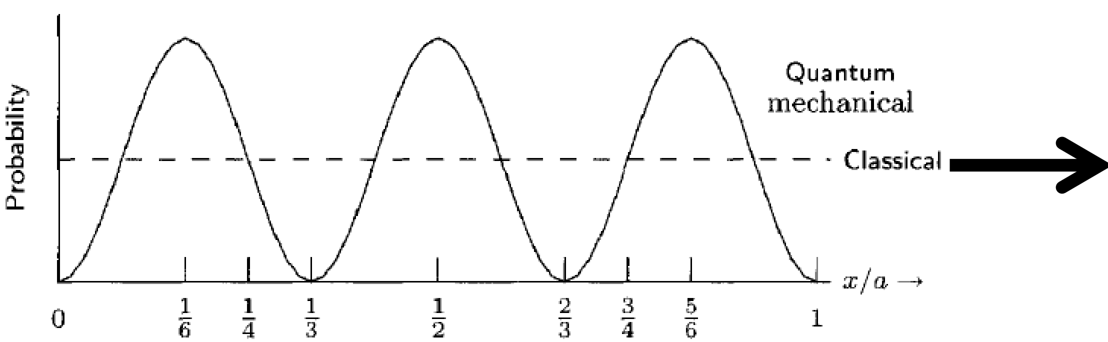
Particle in a 1D Box (continued)

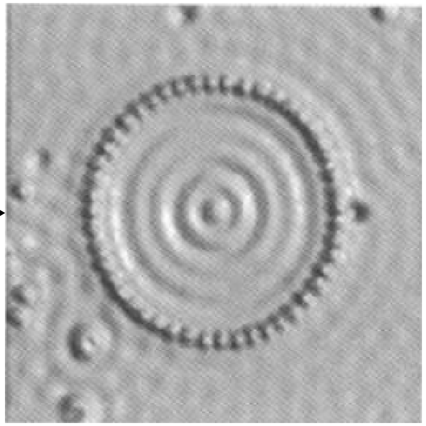
- $\mathrm{E} = \frac{h^2 k_n}{8\pi^2 m} = \frac{h^2 n^2}{8ma^2}$

$$\int_0^a |\psi_n(x)|^2\, dx = A \int_0^a sin\left(\frac{n\pi x}{a}\right) dx = 1$$

$$\psi(x) = \sqrt{\frac{2}{a}} sin \frac{n\pi x}{a}, n = 0,1,2,3 \ldots$$

$$|\psi(x)|^2 dx = \frac{2}{a} sin^2 \frac{n\pi x}{a} dx$$





Hydrogen atom electron

- Fully 3D (spherical) model a.k.a. box
- V(r) = -e^2/r

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{8\pi^2\mu}{h^2}\left[E-V(r)\right]\psi=0,$$

$$\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$$

$$\frac{d^2\Phi(\phi)}{d\phi^2}=-m^2\Phi(\phi).$$

$$\frac{1}{\sin\theta}\frac{d^2\Theta(\theta)}{d\theta^2}-\frac{m^2}{\sin^2\theta}\Theta(\theta)+\beta\Theta(\theta)=0$$

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{dR(r)}{dr}\right]+-\frac{\beta}{r^2}R(r)+\frac{8\pi^2\mu}{h^2}\left[E-V(r)\right]R(r)=0$$

Hydrogen Solution

- Solution to $\frac{d^2\Phi(\phi)}{d\phi^2} = -m^2\Phi(\phi).$
  - $\Phi(\phi) = A sin(m\phi) + B cos(m\phi)$
  - Solutions only exist if:
    - m, l, and n are constrained
    - m is integer, m = 0,$\pm$1 ,$\pm$2 ,$\pm$3… - azmuthal
    - β = l(l+1) – angular momentum
    - $E_n = \frac{2\pi^2 \mu e^2}{h^2 n^2}, n = 1, 2, 3$ – principal
- These define electron clouds!
  - m has 2l+1 values
  - l can't be greater than n-1
  - $m_s = \pm 1/2$ – added if S.E. is relativistically evaluated

Balmer series from hydrogen