CHEM F111 : General Chemistry

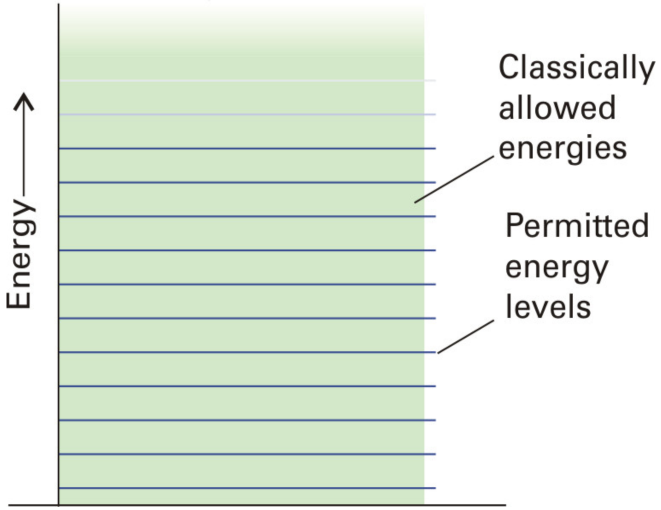
Semester II: AY 2017-18

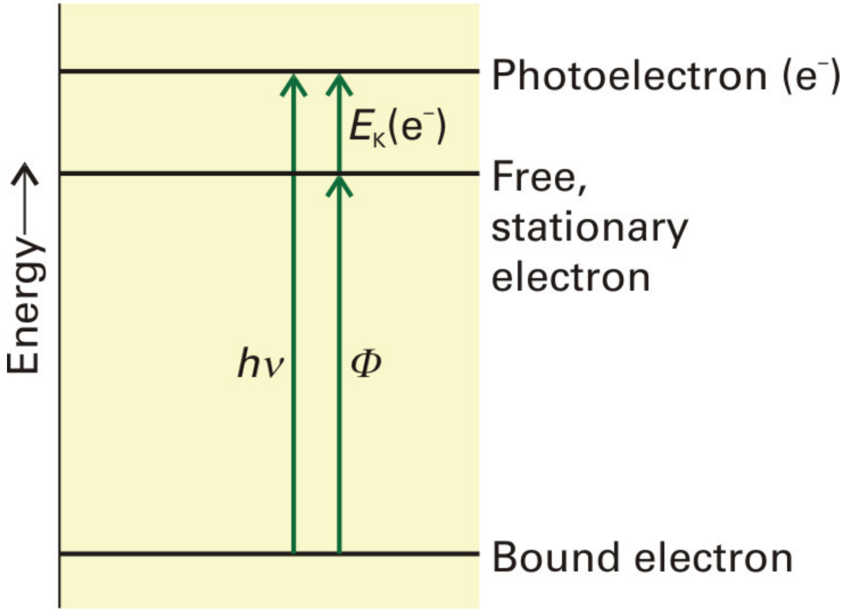
Lecture-03, 12-01-2018

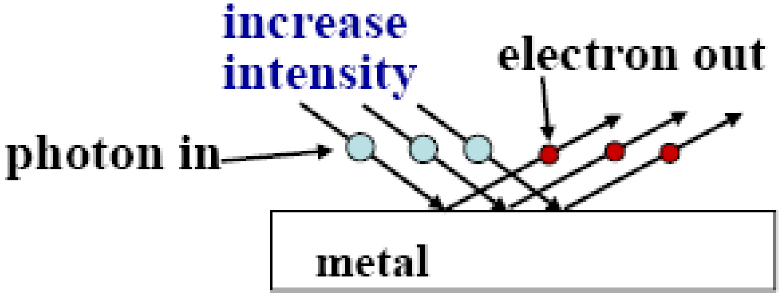
Summary: Lecture-02

Planck's Formula: $\rho(\lambda)d\lambda = (hc/\lambda)(e^{hc/\lambda kT} - 1)^{-1}(8\pi/\lambda^4)d\lambda$

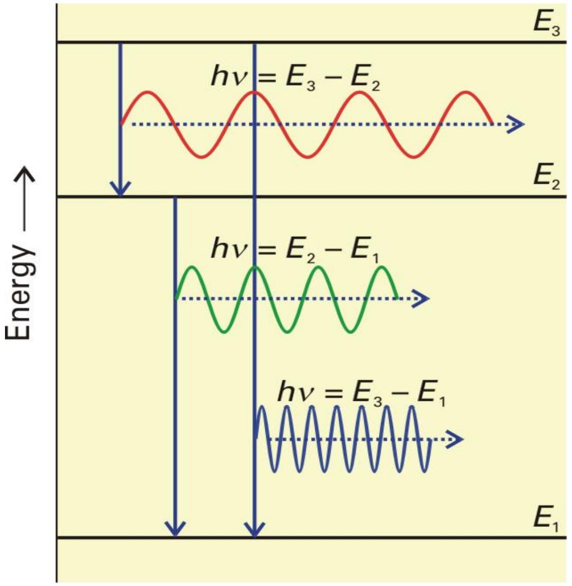
Photoelectric effect: Particle nature of light

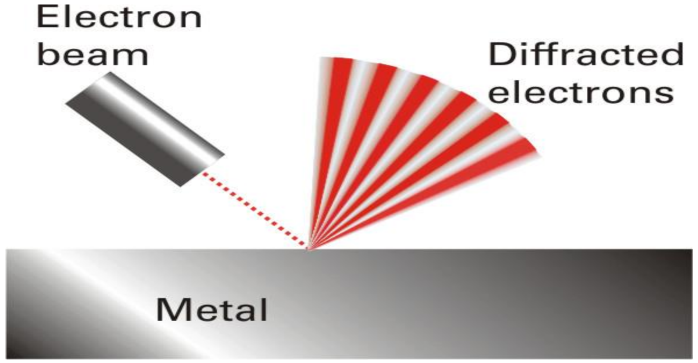






Line spectrum of H-atom



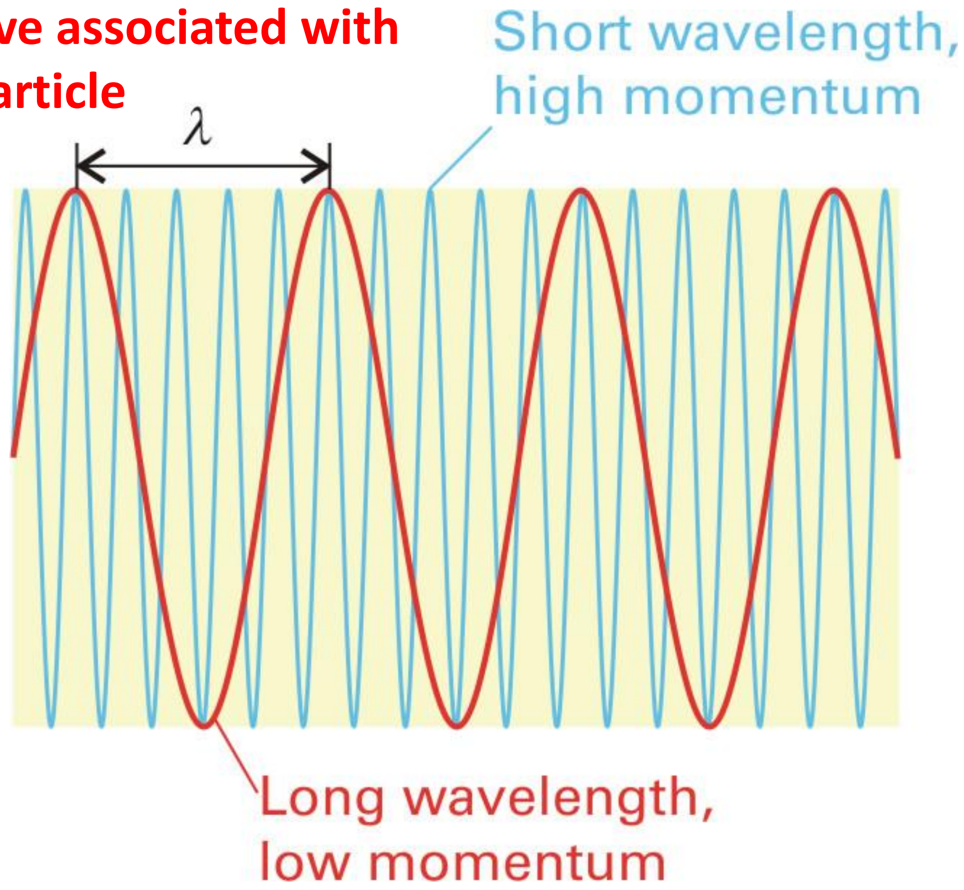


(Detector)

Electron Diffraction:
Wave nature of e-

Summary: Lecture-02

Wave associated with a particle



- Estimate the wavelength of e- that have been accelerated from rest through a potential difference of 40 kV:
  - 6.1×10^{-12} m
- Estimate the wavelength of a tennis ball of mass 57 g travelling at a speed of 80 km h^{-1}:
  - 5.2×10^{-34} m

Classical one dimensional wave equation:

$$\frac{\delta^2\Phi}{\delta x^2} = \frac{1}{v^2}\frac{\delta^2\Phi}{\delta t^2} \quad \text{....Equn. 1}$$

Solution: $\Phi(x,t) = \psi(x)\cos\omega t$

We'll finally obtain: $$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - u(x)]\,\psi(x) = 0$$

Summary: Lecture-02

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - u(x)]\,\psi(x) = 0$$

Equation of state for a particle of mass m moving in a potential field of u(x)

$\psi(x) \Rrightarrow$ measure the spatial amplitude of the matter wave associated with a particle of mass "m"

$\Rrightarrow$ called **wave function** of the particle

Uncertainty Principle – Size does matter

We can not determine simultaneously the exact positon and momenta of a microscopic particle ($\Delta p_x \Delta x \geq \hbar/2$)

Information required in classical mechanics to predict the future motion of a particle can not be obtained

Quantum Mechanics 1925 – 1927, The Uncertainty Principle {https://history.aip.org/exhibits/heisenberg/p08.htm}

Approach to quantum mechanics

- Postulate the basic principles.
- Use those postulates and/or experimental observation.
- Propose a function – state or wave function (ψ).
- In general, ψ is a function of space (x, in 1D) and time (t)

ψ ≡ ψ (x, t)

- Wave function contains all the information about a system.

Interested in stationary states: ψ(x)

- Schröndinger equation of mass **m** – rearrange Equn. 4:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+u(x)\,\psi\,(x)=E\,\psi\,(x)$$

Equation of state

Equation of state for a particle of mass m moving in a potential field of u(x)

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - u(x)]\,\psi(x) = 0$$

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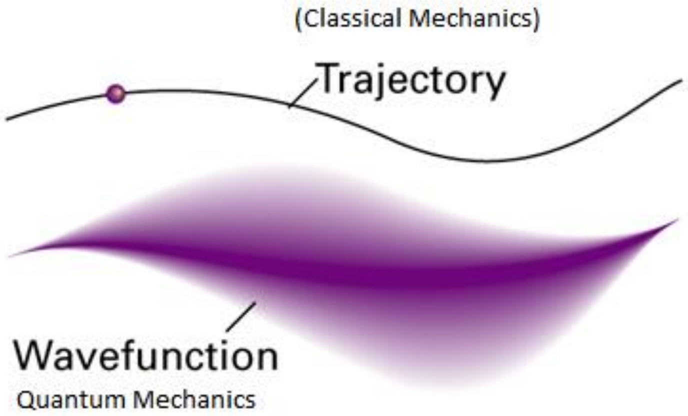
Erwin Schröndinger



Schröndinger Equation

Time independent Schröndinger Equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+u(x)\,\psi\,(x)=E\,\psi\,(x)$$

$\psi(x) \Rrightarrow$ measure the spatial amplitude of the matter wave

$(\text{Amplitude})^2 \Rrightarrow$ Intensity

What do we mean by intensity?

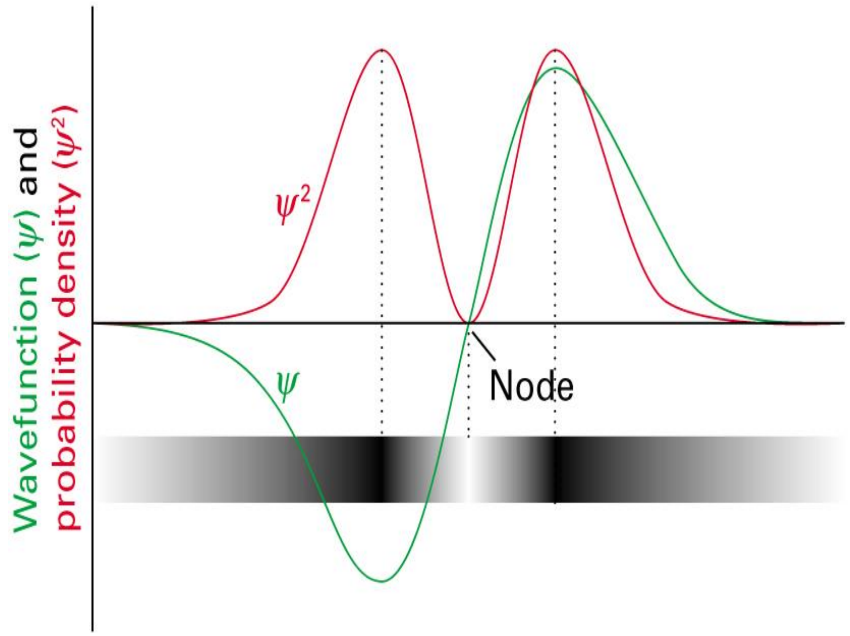
The Born Interpretation

Intensity ⇛ (Amplitude)^2 $\{|\psi\ (x)|^2\}$ ⇛ Probability density

For our discussion in one dimension:

Probability that the particle is located in space in the region of x to x + dx

$\{\psi\ (x)$ **is also known as "probability amplitude function"}**



$$P = \int_a^b \Psi\Psi^* \, dV = \int_a^b |\Psi|^2 \, dV$$

Ψ^* **complex conjugate of** Ψ

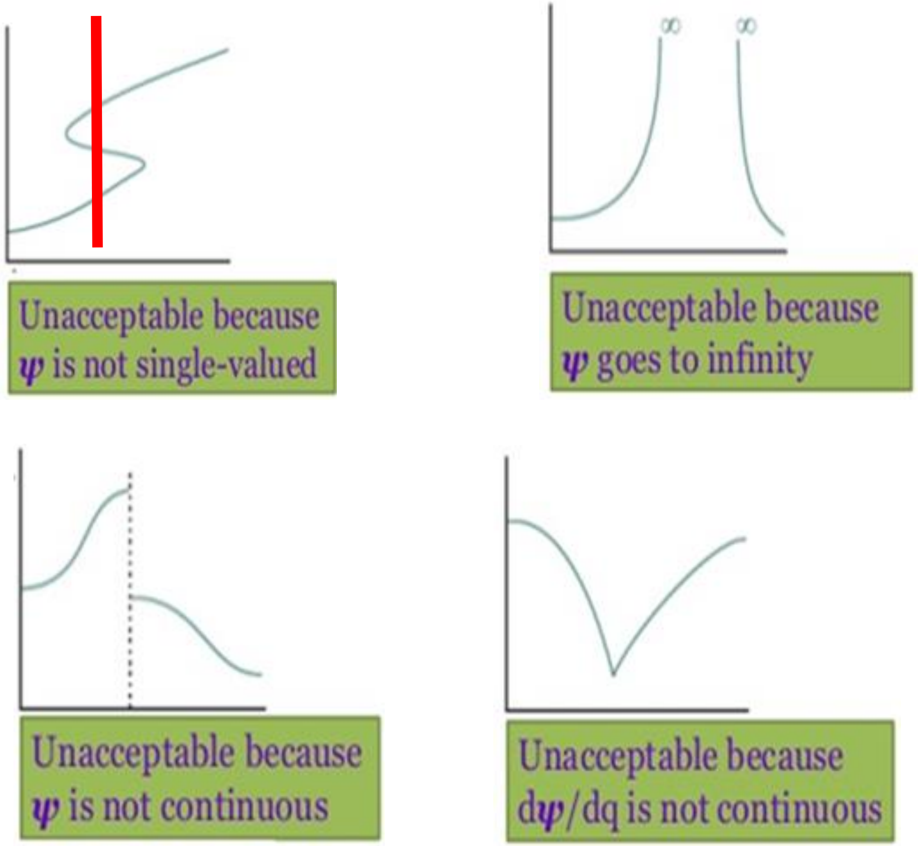
Solution of Schröndinger Equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + u(x)\,\psi\,(x) = E\,\psi\,(x)$$

Well behaved ψ for a physical system

Four conditions are put forward to make probability functions, which are solution of Schröndinger equations, consistent with a reasonable picture of nature. Born conditions act as boundary condition to the solution of Schröndinger differential equation.

- Ψ must be single-valued.
- Ψ must be finite everywhere.
- Ψ must be continuous.
- $\frac{d\psi}{dx}$ must be continuous.



Normalization of wavefunction is a consequence of Born Interpretation.

$$\int_{-\infty}^{\infty} [N\Psi(x)]\,[N\,\Psi(x)]dx = 1$$

Postulates of Quantum Mechanics

Postulate 1:

The state of a quantum-mechanical system is completely specified by a function ψ(r, t) that depends on the coordinates of the particle and on the time. This function is called the wave function or the sate function, has the important property that ψ*(r, t) ψ(r, t) *d*x *d*y *d*z is the probability that the particle lies in the volume element *d*x *d*y *d*z, located at a point r, at the time t.

(We'll work only with stationary states)

Postulate 2:

To every observable in classical mechanics there corresponds an operator in quantum mechanics.

Postulates of Quantum Mechanics

Observables in Quantum mechanics:

Apply the operator on the state function of the systems – outcome will be observable {Measurement technique}.

Observable	Operator
Position	$\hat{x}$
Momentum	$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$
Energy	$E = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

Postulates of Quantum Mechanics

Postulate 3:

Quantum Mechanical operators are **special in nature**. In any measurement of the observable associated with the operator $\hat{A}$, the only values that will be ever observed are the eigenvalues a, which satisfy the eigen value equation:

$$\hat{A}\,\psi = a\,\psi$$

In general, an operator will have a set of eigen functions and eigenvalues, and we'll indicate this by:

$$\hat{A}\,\psi_n = an\,\psi_n$$

eigenvalues

eigen functions

Eigen value equation

a) Show e^{ax} is an eigenfunction of $\frac{d}{dx}$. Determine the eigen value.

b) Show that e^{ax^2} is not an eigenfunction of $\frac{d}{dx}$

Work out: Show that e^{ax} is an eigenfunction of the operator $\widehat{D}^n$ ($\widehat{D} = \frac{d}{dx}$). What is the eigen value?