EN 204

Material Science for Energy Applications

Class 3

Shaibal K Sarkar
Department of Energy Science and Engineering
shaibal.sarkar@iitb.ac.in

Brief recap

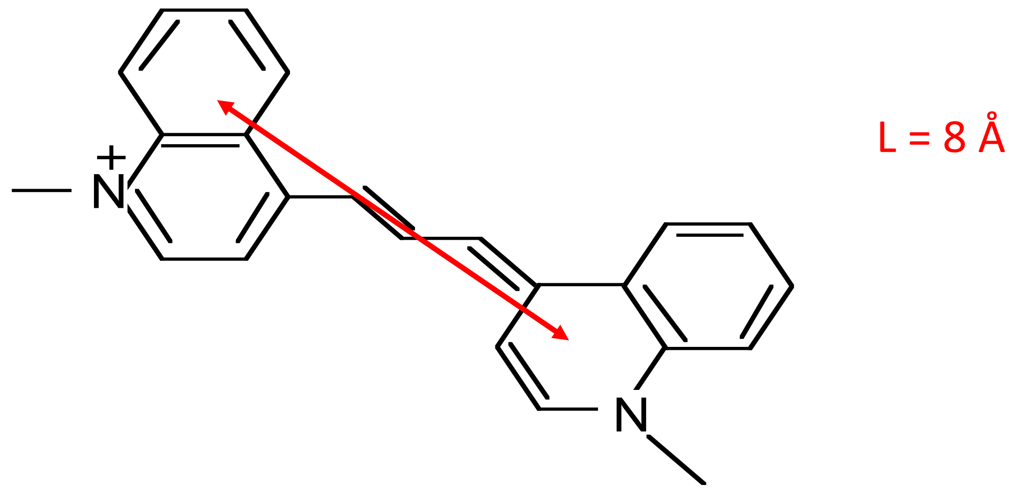
In the last class, we had a brief review of the energy states of any free particle and a bound particle.

We had a classroom quiz and the result is disastrous

Number of students in the class: 27
Quiz result submitted: 17

A real-world example:

Consider the following dye molecule, the length of which can be considered the length of the "box" an electron is limited to:

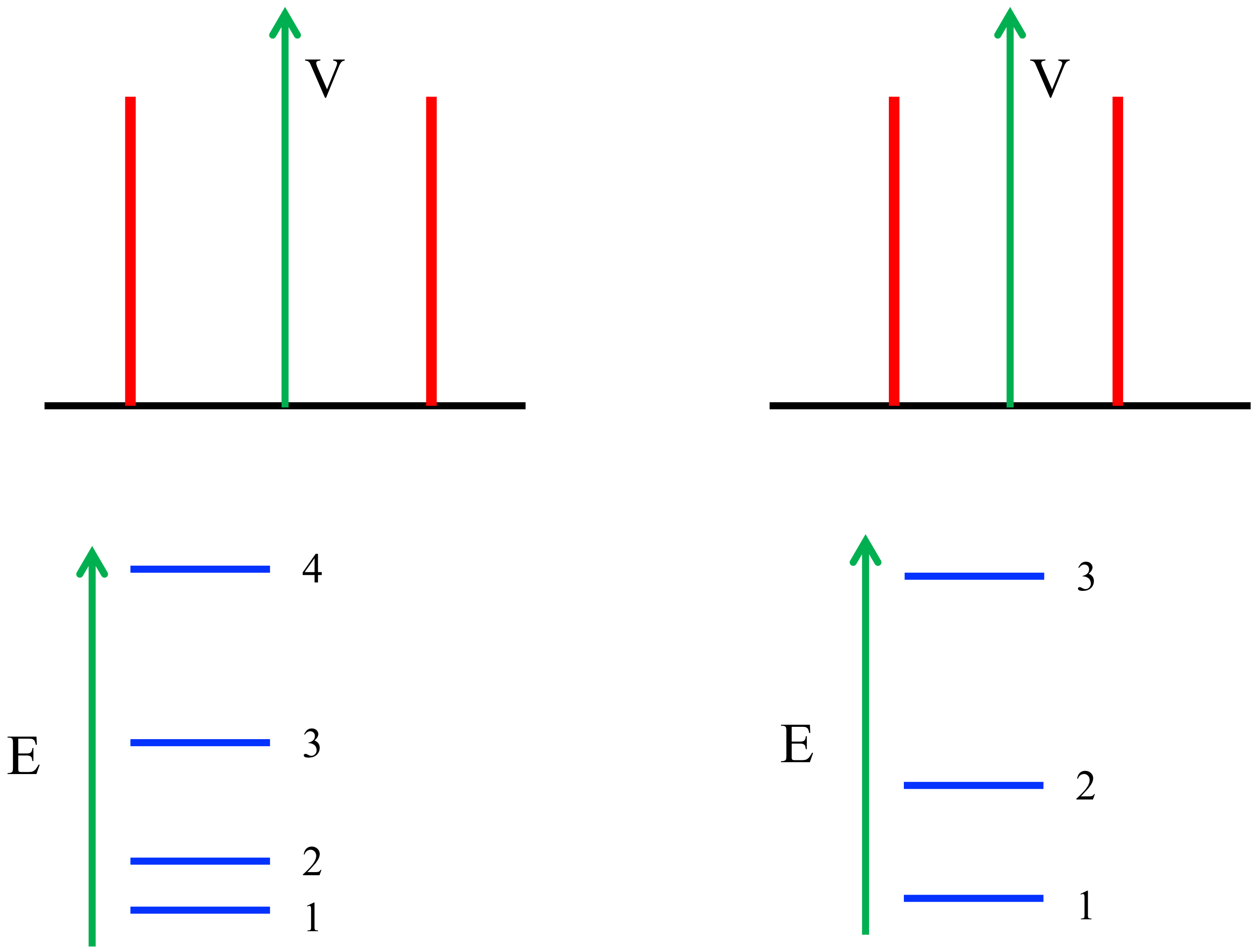


What wavelength of light corresponds to ΔE from n=1 to n=2?

$$\Delta E = \frac{h^2}{8mL^2}\left(n_{final}^2 - n_{initial}^2\right) = \frac{h^2}{8m(8\mathring{A})^2}\left(2^2 - 1\right) = 2.8x10^{-19}J$$

$\lambda \approx 700nm$ (Observed value 680 nm, not bad!)

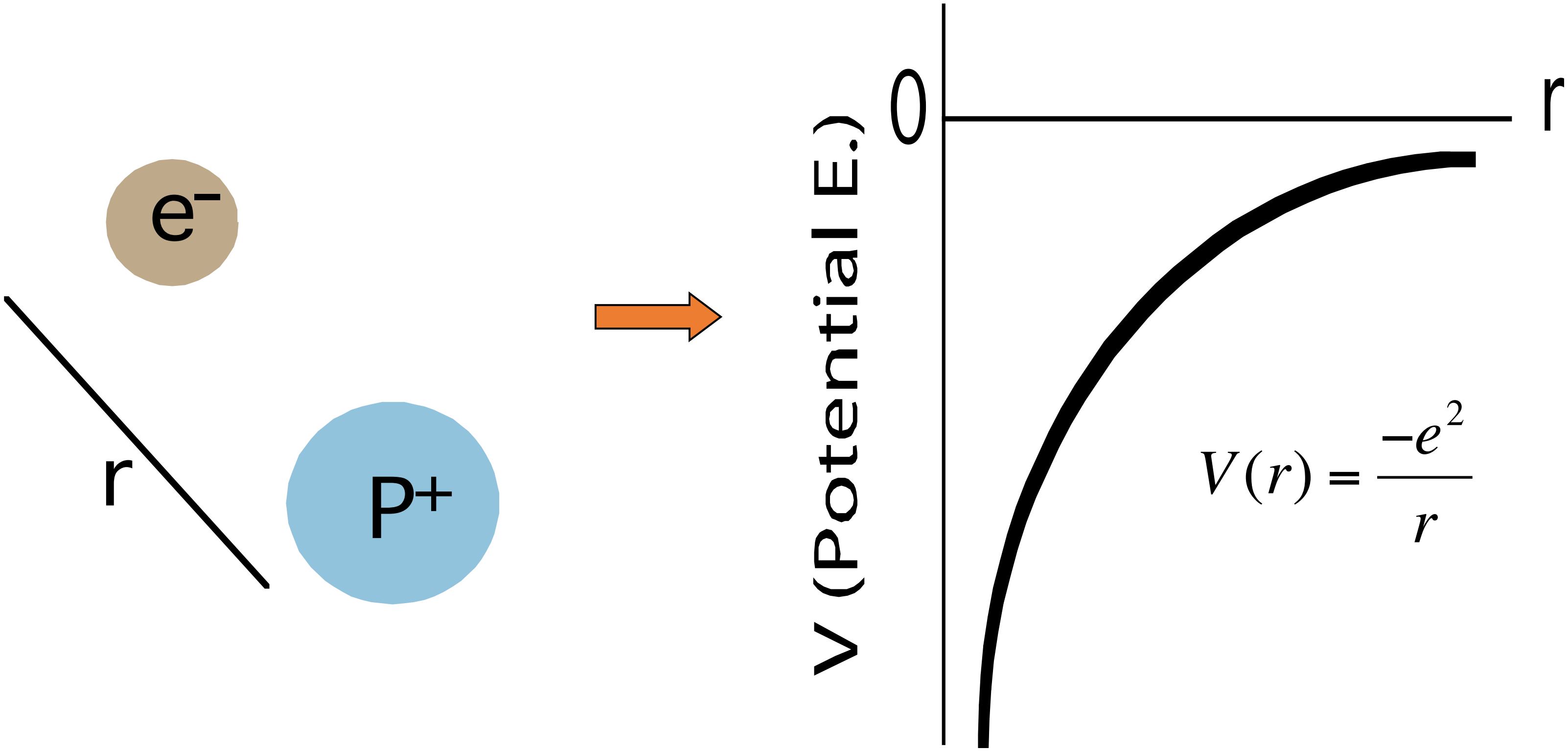
If the length L of the “box” in the particle in a box potential is reduced, what do you expect to happen to the energy levels?



One effect of a "constraining potential" is that the energy of the system becomes **quantized.**

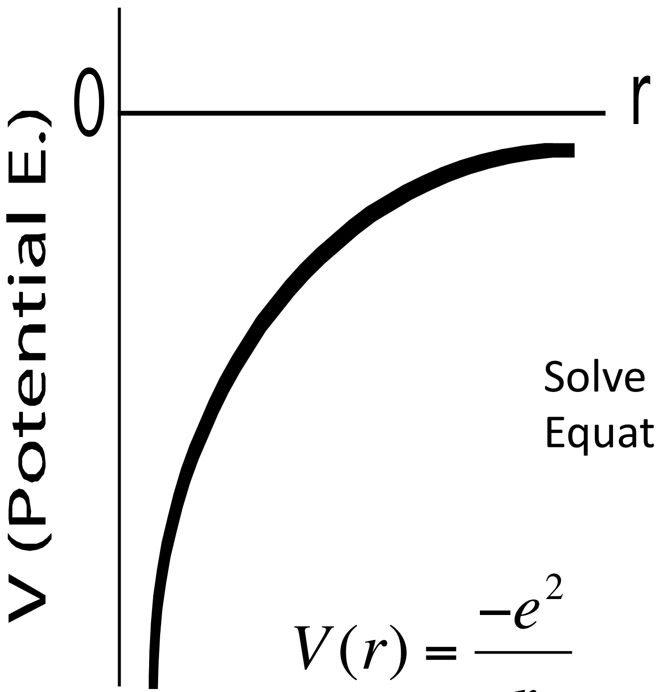
"The Globe is not flat"

Back to the hydrogen atom:



Energy levels of hydrogen atom

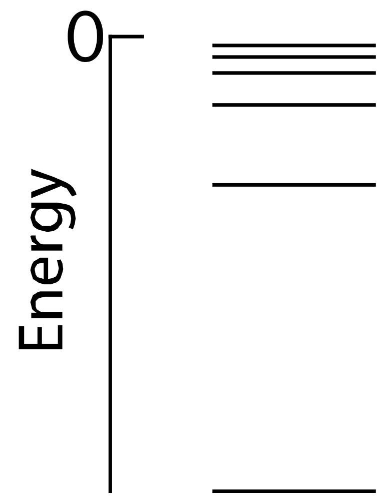
So, for the hydrogen atom, energy becomes quantized due to the presence of a constraining potential.



$$V(r) = \frac{-e^2}{r}$$

Solve the Wave Equation

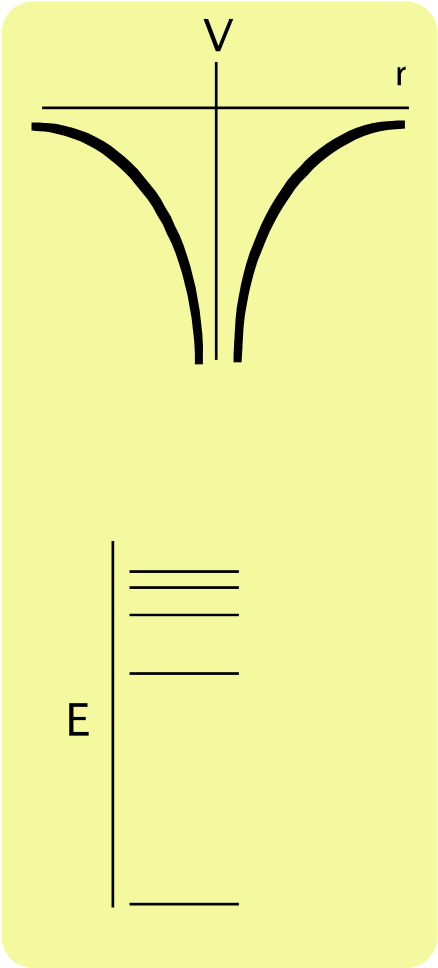
$$E = -2.178x10^{-18} J\left(\frac{Z^2}{n^2}\right)$$



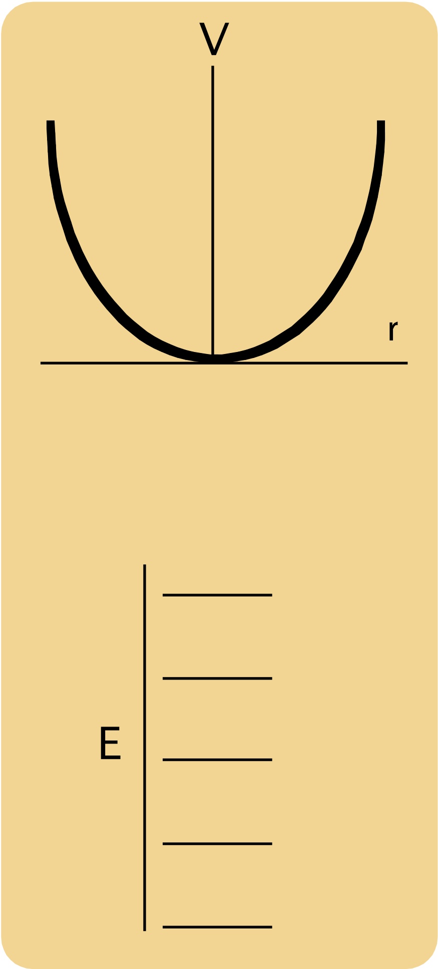
Exact q.m. solution is the Bohr formula!

Distribution of Energy depends on Potential Profile

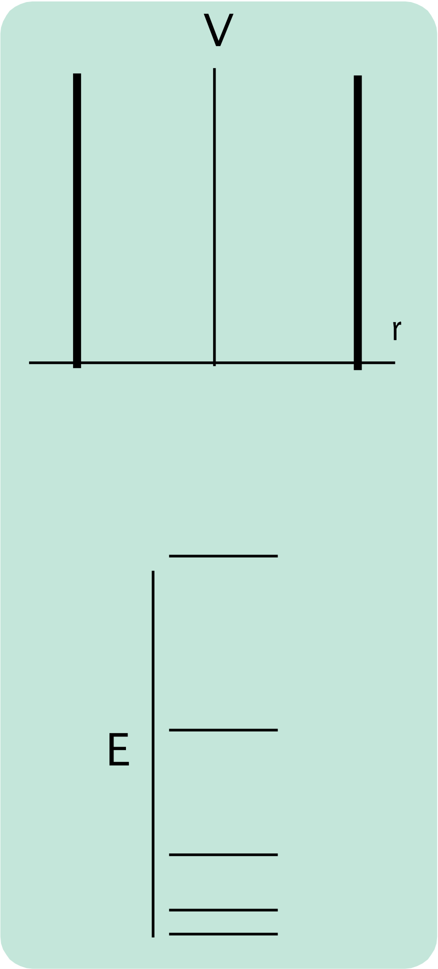
What is the expected distribution of energy levels for the harmonic oscillator?



Hydrogen Atom



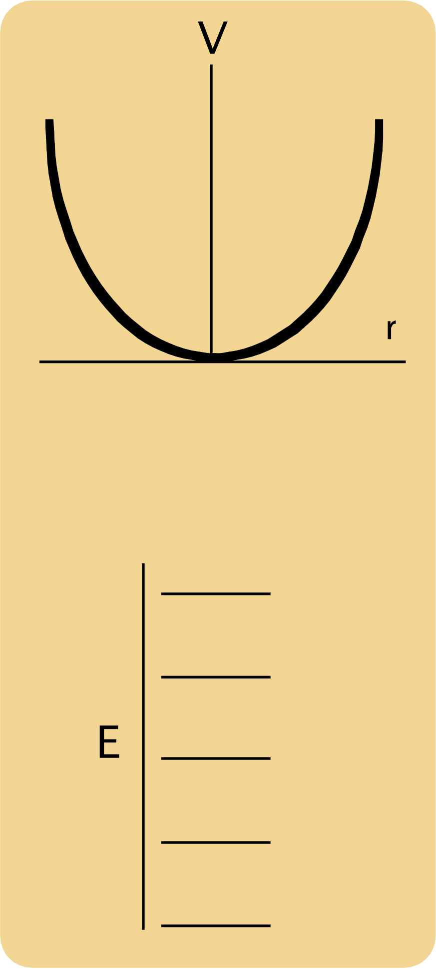
Harmonic Oscillator



Particle in a Box

What is the expected distribution of energy levels for the harmonic oscillator?

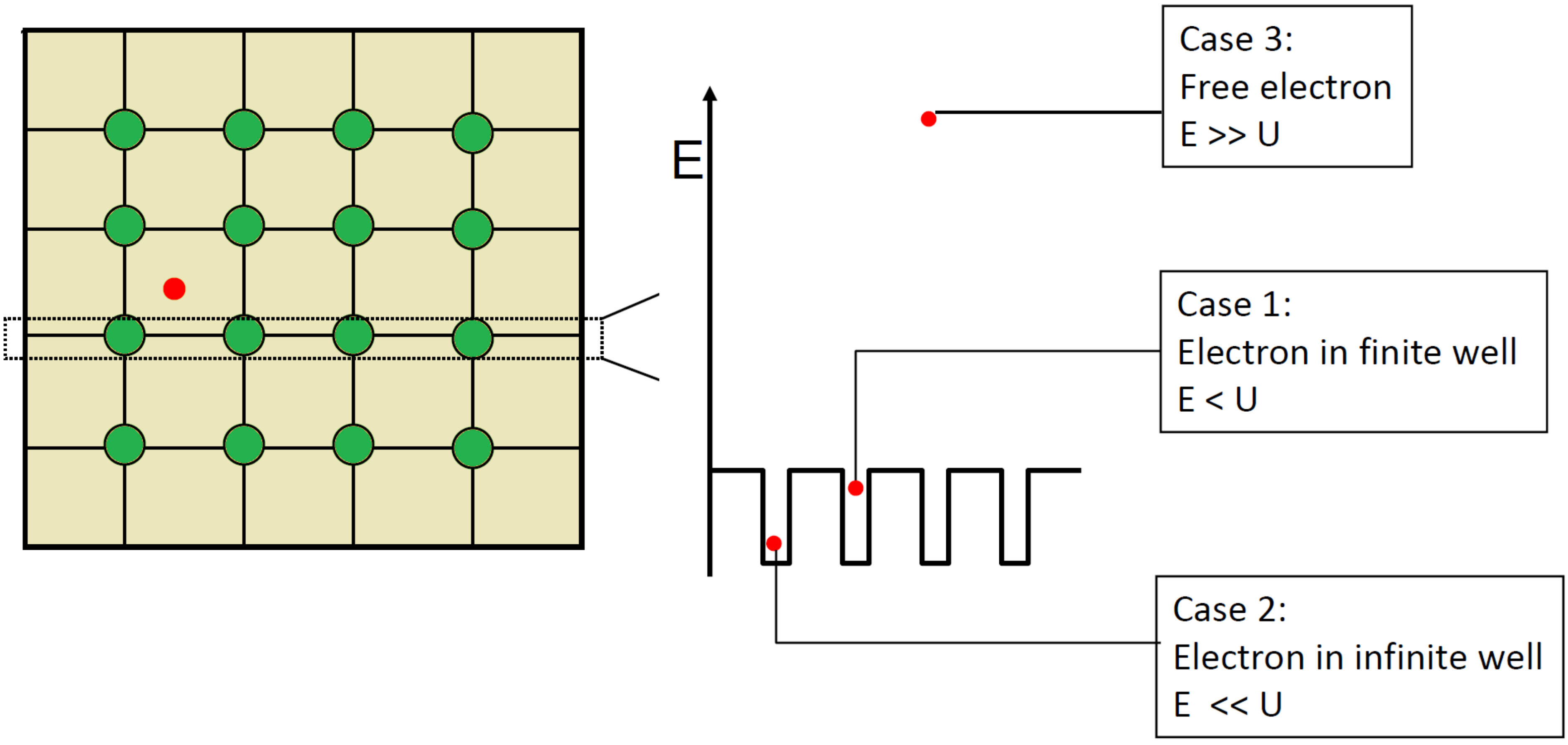
Assignment : Solve it !



Harmonic Oscillator

Let us come back to the real-life scenario

The Simplest Model to describe electron in solid



Recap of Schrödinger Equation

The time-independent Schrödinger Equation…

$$\frac{d^2\psi}{dx^2} + \frac{2m_0}{\hbar^2}(E-U)\psi = 0$$

If E >U, then ....

$$k \equiv \frac{\sqrt{2m_0[E-U]}}{\hbar} \qquad \frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \boxed{\psi(x) = A\sin(kx) + B\cos(kx)}$$

$$\equiv A_+e^{ikx} + A_-e^{-ikx}$$

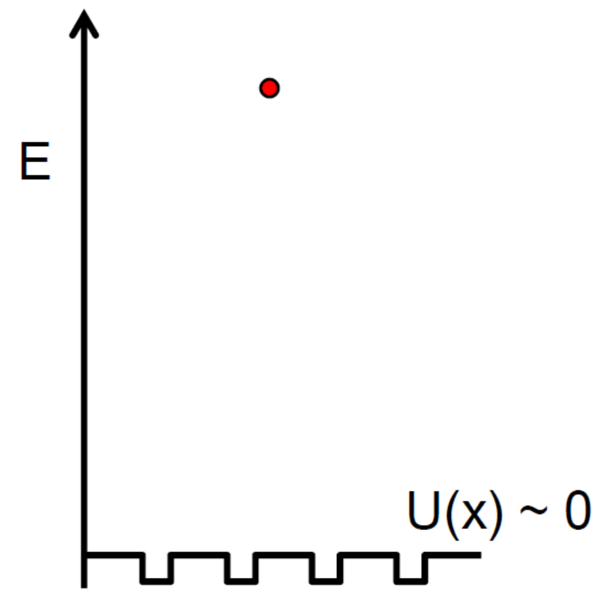
If U>E, then ....

$$\alpha \equiv \frac{\sqrt{2m_0[U-E]}}{\hbar} \qquad \frac{d^2\psi}{dx^2} - \alpha^2\psi = 0 \qquad \boxed{\psi(x) = De^{-\alpha x} + Ee^{+\alpha x}}$$

Case 3: Free Electron, E>>U

$$\frac{d^2\psi}{dx^2}+k^2\psi=0 \qquad k\equiv\frac{\sqrt{2m_0[E-U]}}{\hbar}$$

Particle with E>>U



1) Solution $$\psi(x)=A\,sin(kx)+B\,cos(kx)$$
$$\equiv A_+e^{ikx}+A_-e^{-ikx}$$

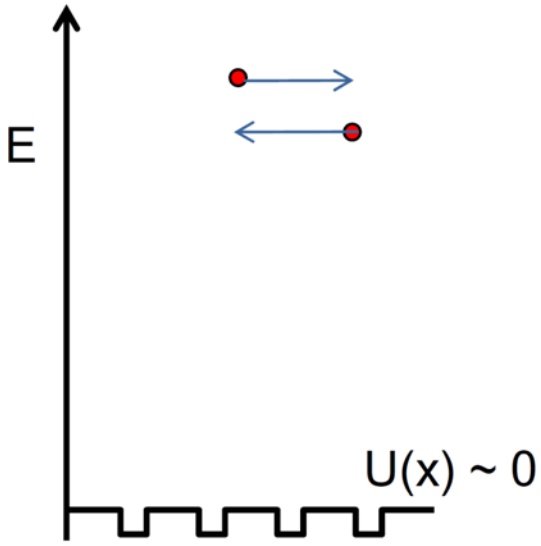
2) Boundary condition $\psi(x)=A_+e^{ikx}$ positive going wave

$=A_-e^{-ikx}$ negative going wave

Case 3: Free Electron, E>>U

$$\psi(x) = A\,sin(kx) + B\,cos(kx)$$
$$\equiv A_+ e^{ikx} + A_- e^{-ikx}$$

$$\psi(x) = A_+ e^{ikx} \quad \text{positive going wave}$$
$$= A_- e^{-ikx} \quad \text{negative going wave}$$



Probability: $|\psi|^2 = \psi\psi^* = |A_+|^2 \; or \; |A_-|^2$

Momentum: $p = \int_0^\infty \Psi^* \left[\frac{\hbar}{i}\frac{d}{dx}\right] \Psi \; dx = \hbar k \text{ or } -\hbar k$

Case 2: Bound Electron, E<<U

Electron in an infinite Quantum well

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad k \equiv \frac{\sqrt{2m_0[E-U]}}{\hbar}$$

1) Solutions: $\psi = A\sin kx + B\cos(kx)$

2) Boundary conditions

$$\psi(x=0) = 0 = A\,sin\,k(0) + B\,cos\,k(0)$$

$$\psi(x=a) = 0 = A\,sin(ka) = A\,sin(n\pi)$$

$$k_n = \frac{n\pi}{a} = \frac{\sqrt{2m_0E_n}}{\hbar} \qquad \boxed{E_n = \frac{\hbar^2 n^2 \pi^2}{2m_0 a^2}}$$

Quick Suggestion: Five Steps for Analytical Solution

$$\frac{d^2\psi}{dx^2}+k^2\psi=0$$

$$\psi(x=-\infty)=0$$
$$\psi(x=+\infty)=0$$

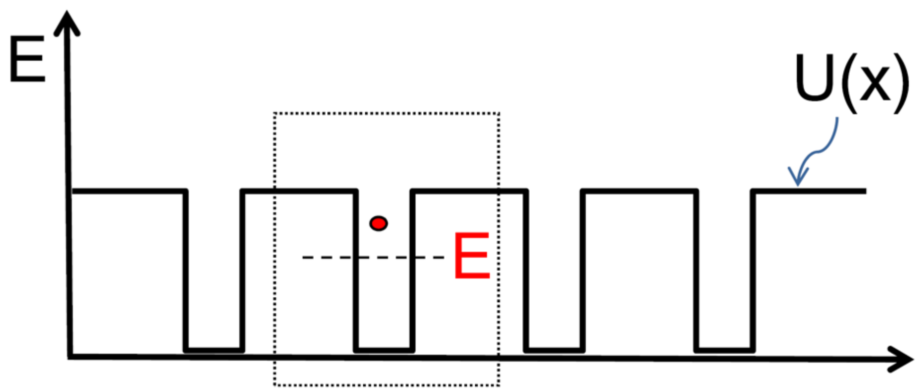
$$\psi\big|_{x={x_B}^-}=\psi\big|_{x={x_B}^+}$$
$$\left.\frac{d\psi}{dx}\right|_{x={x_B}^-}=\left.\frac{d\psi}{dx}\right|_{x={x_B}^+}$$

Det(coefficient matix)=0

$$\int_{-\infty}^{\infty}\left|\psi(x,E)\right|^2dx=1$$

Case 1: Loosely Bound Electron E<U

Electron in a Finite well



$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

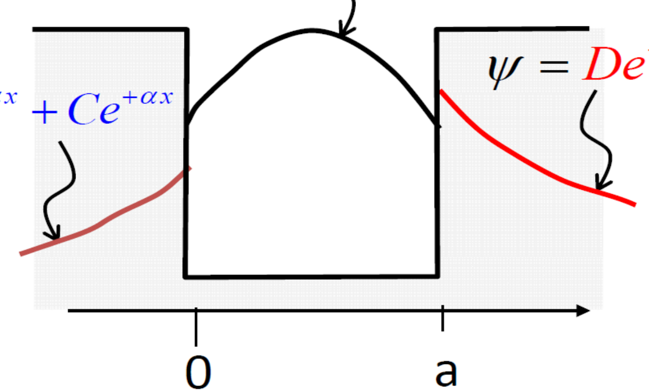
$$\psi(x = -\infty) = 0$$

$$\psi(x = +\infty) = 0$$

$$\psi = A\sin kx + B\cos kx$$

$$\psi = \cancel{M}e^{-\alpha x} + Ce^{+\alpha x}$$

$$\psi = De^{-\alpha x} + \cancel{N}e^{+\alpha x}$$



Case 1: Loosely Bound Electron E<U

Continuity of Wave function

Implementing 3rd step

$$\psi\Big|_{x=x_B^-} = \psi\Big|_{x=x_B^+}$$

$$\left.\frac{d\psi}{dx}\right|_{x=x_B^-} = \left.\frac{d\psi}{dx}\right|_{x=x_B^+}$$

$$C = B$$

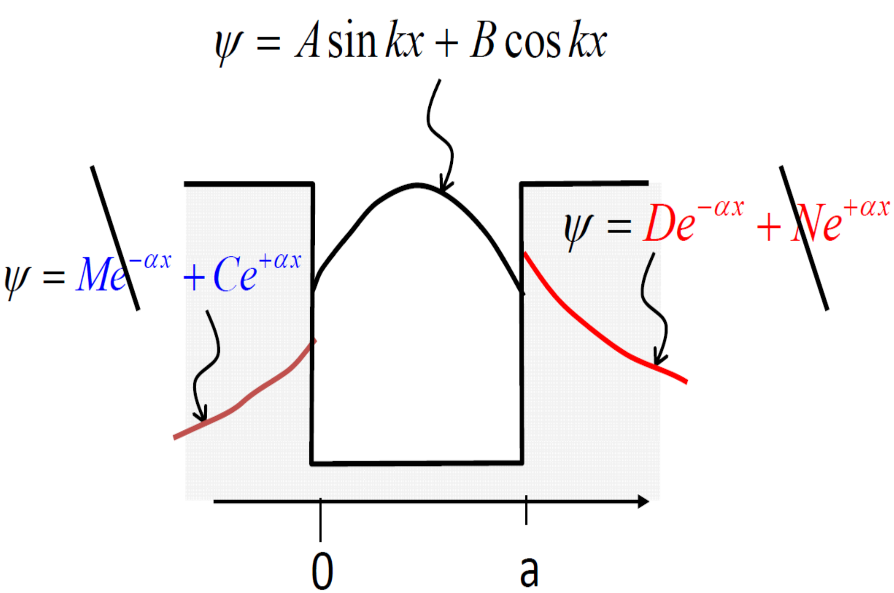
$$\alpha C = -kA$$

$$A\sin(ka) + B\cos(ka) = De^{-\alpha a}$$

$$kA\cos(ka) - kB\sin(ka) = -\alpha De^{-\alpha a}$$

$$\Downarrow$$

$$\begin{pmatrix} 0 & 1 & -1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & -e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & \alpha e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$



Case 1: Loosely Bound Electron E<U

$\triangle$(coefficient matrix)=0

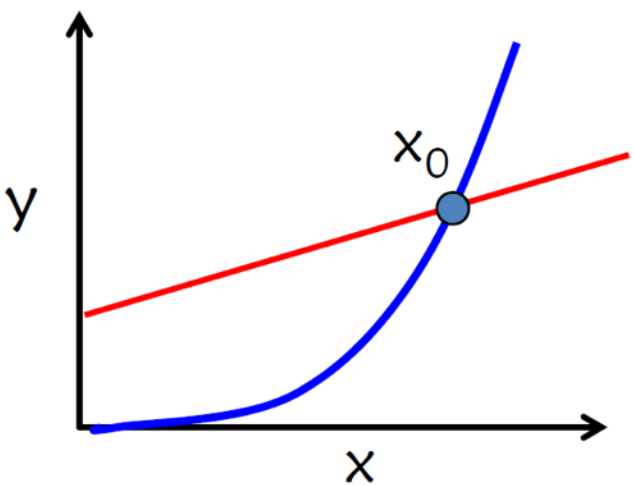
$$\tan(\alpha a\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1} \qquad \xi \equiv \frac{E}{U_0} \quad \alpha \equiv \sqrt{\frac{2mU_0}{\hbar^2}}$$

Only Unknown is E

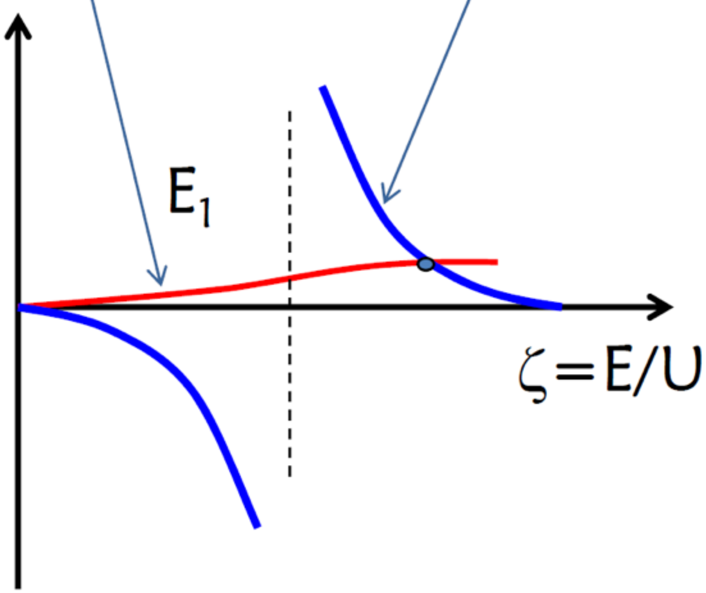
Graphical Solution for bound level

$$x^2 = x + 5$$

$$y_1 = x^2 \quad y_2 = x + 5$$



$$\tan(\alpha_0 a\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$



Graphical Solution for bound level

Finding the Energy State