ECE 495N

Fundamentals of Nanoelectronics

Fall 2008

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Lecture: 8
Title: Schrödinger's Equation
Date: September 12, 2008

Video Lectures posted at:
https://www.nanohub.org/resources/5346/

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Schrödinger Equation

Lecture 8

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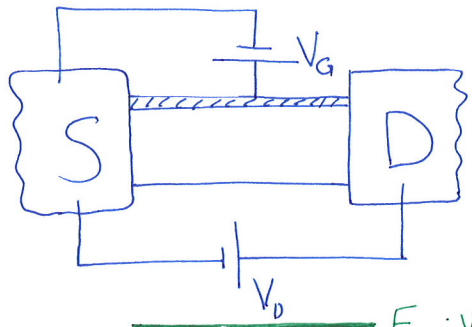
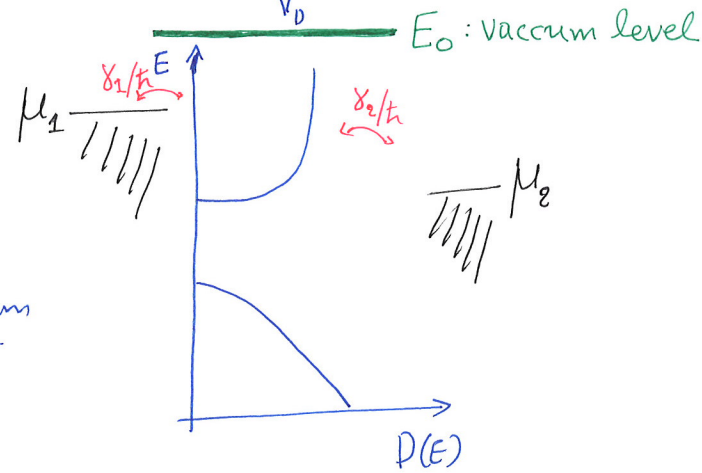
$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2\psi + U(r)\psi\right)$$

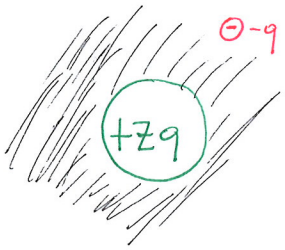
$$\psi(\vec{r},t) = \Phi(\vec{r})\, e^{-iEt/\hbar}$$

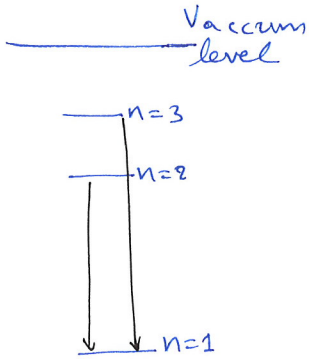
$$\boxed{E\Phi(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2\Phi + U(\vec{r})\Phi}$$





$$U(r) = -\frac{Zq^2}{4\pi\epsilon_0 r}$$





$$\Psi^*\Psi = \Phi^*\Phi(\vec{r})$$

Schrödinger time independent equation can give non-trivial solution only for specific values of E. This in not obvious. Hence we have discrete values. This is a property of waves.

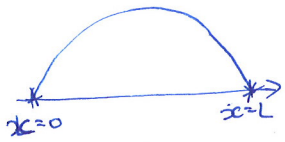
For a classical wave: (analogy)

$$\frac{d^2 f}{dx^2} = -\frac{\omega^2}{v^2} f$$

$$\boxed{e^{ikx}} \Rightarrow -k^2 f = -\frac{\omega^2}{v^2} f$$

$$\Rightarrow \boxed{k^2 = \frac{\omega^2}{v^2}} \leftarrow \text{dispersion relation}$$

$\boxed{e^{-ikx}}$ is also a solution



$\sin kx$

$k_n L = n\pi$

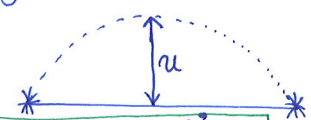
$$\Rightarrow \boxed{k_n = \frac{n\pi}{L}}$$

and $\omega_n = v k_n$

NOTE

In acoustics a wave is described by:

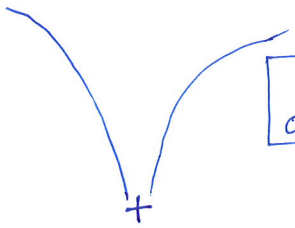
$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \quad \Big\| \quad u(x,t) = e^{-i\omega t} f(x)$$



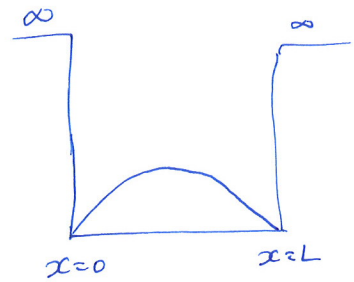
$$\boxed{-\omega^2 f = v^2 \frac{\partial^2 f}{\partial x^2}}$$

Now returning back to the Schrödinger Equation we have

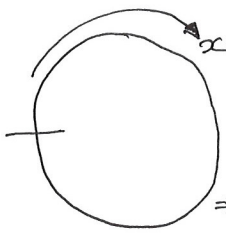
$$E_n = \frac{\hbar^2 k_n^2}{2m} \quad \underline{\text{and}} \quad \boxed{k_n L = n\pi}$$ ← box boundary condition $\boxed{\text{BBC}}$



$\boxed{\text{H atom}}$



$\boxed{\text{particle in a infinite box}}$



solution

$$\boxed{e^{ikx}} = e^{ik(x+L)}$$

$$\Rightarrow e^{ikL} = 1$$

$$\Rightarrow kL = n2\pi$$

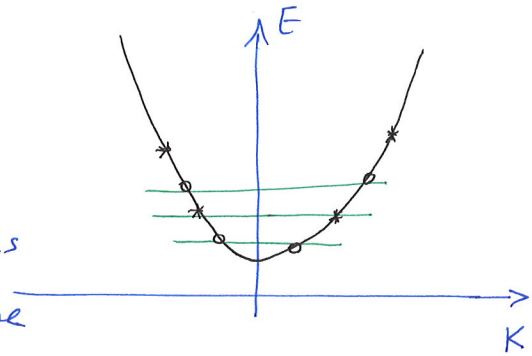
$$\Rightarrow \boxed{k_n = \frac{n2\pi}{L}}$$

periodic boundary condition $\boxed{\text{PBC}}$

solution → $\boxed{\sin kx}$ fits at $x=0$ and with the condition $k_n L = n\pi$ fits the condition at $x=L$

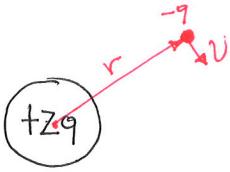
The E-k relationship is the same for both cases, since it comes from the same equation:

$$E = \frac{\hbar^2 k^2}{2m}$$



e^{ikx} and e^{-ikx} are different solutions but $\sin kx$ and $\sin(-kx)$ are the same

Bohr's approach



$$\frac{mv^2}{\cancel{r}} = \frac{Zq^2}{4\pi\epsilon_0 r^{\cancel{2}}} \Rightarrow r = \frac{Zq^2}{4\pi\epsilon_0 (mv^2)}$$

electron's energy → $$E_q = \underbrace{-\frac{Zq^2}{4\pi\epsilon_0 r}}_{\text{potential}} + \underbrace{\frac{1}{2}mv^2}_{\text{kinetic}} = \boxed{-\frac{1}{2}\frac{Zq^2}{4\pi\epsilon_0 r} = E_q}$$

Also (boundary condition): $2\pi r = n\frac{\hbar}{mv} \Rightarrow \boxed{r_n = \frac{n\hbar}{mv}} \Rightarrow mv = \frac{n\hbar}{r}$

BUT $$r = \frac{Zq^2 m}{4\pi\epsilon_0 m^2 v^2} = \frac{Zq^2 m r^2}{4\pi\epsilon_0 n^2\hbar^2} \Rightarrow r_n = \frac{n^2}{Z}\frac{4\pi\epsilon_0\hbar^2}{q^2 m}$$ ← Bohr's radius a_0