

Fundamentals of Nanoelectronics

ECE495 - Session 7, Sept 9, 2009

Schrodinger Equation - Basic Concepts

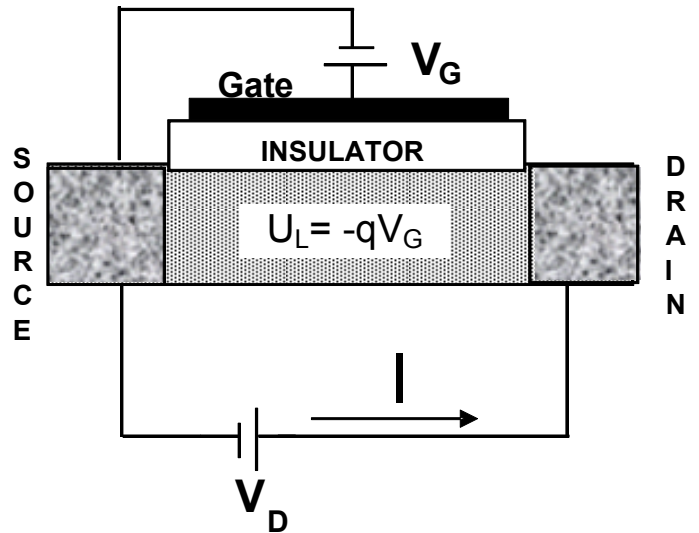
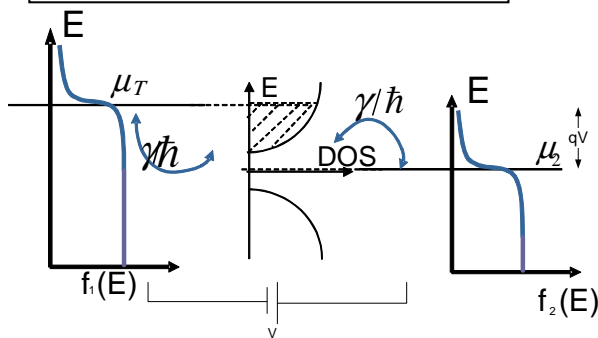
Ref: Chapter 2.1

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Review

During last classes we learned how to calculate current for small device. Given a set of energy levels or Density of States (DOS), we've talked about the I-V characteristics of a device. What we want to understand now is how to model such energy levels / DOS and what is the origination of these states.



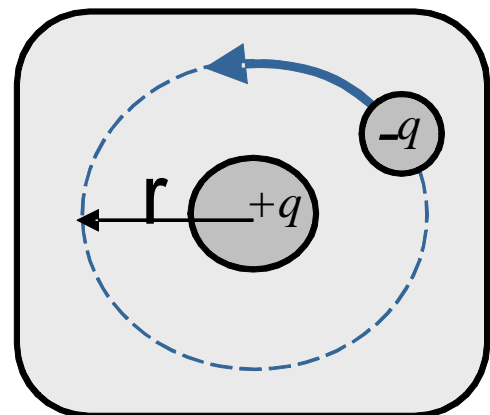
Discrete Energy Spectrum

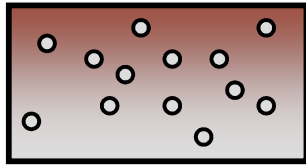
To achieve this, scientists started with the simplest material possible, namely the Hydrogen atom.

$$U = \frac{-q^2}{4\pi\epsilon_0 r} + \frac{1}{2}mv^2$$

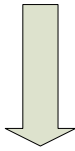
the first part is potential energy

and the second part is kinetic energy.





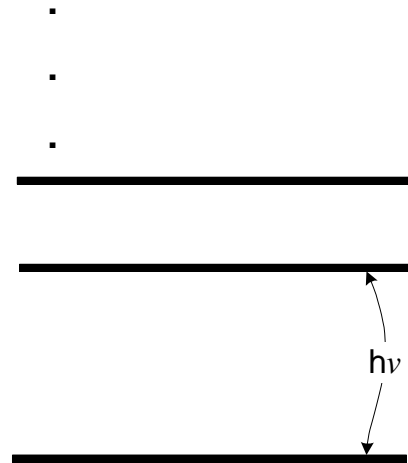
When they heated Hydrogen gas, the results was discrete spectrum!



The results from Hydrogen atoms were discrete frequencies.



Original motivation for creating the Schrödinger Equation comes from discrete photon emission energy bands that were observed when Hydrogen-like atoms were heated. These energy levels could not be explained using classical physics.



Schrödinger Equation

$$E\Psi = \frac{-\hbar^2}{2m} \nabla^2\Psi + U(\vec{r})\Psi \quad \text{and} \quad U = \frac{-q^2}{4\pi\epsilon_0 r}$$

There is only analytical solution for hydrogen atom and for all other atoms they solve it numerically. And Schrodinger showed its analytical solution for Hydrogen.

How does the Schrödinger Equation lead to discrete energy levels?

Vibrating String

The general one-dimensional wave equation is:

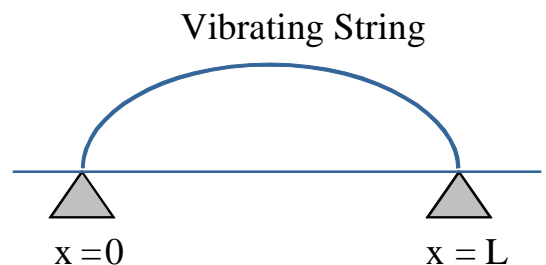
$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$

v is speed and u describes

displacement which is a function of time and position.

$$u \sim e^{-i\omega t} \Rightarrow u(x,t) = \tilde{u}(x)e^{-i\omega t}$$

$$\Leftrightarrow (-i\omega)^2 \tilde{u}(x)e^{-i\omega t} = v^2 \frac{\partial^2}{\partial x^2} (\tilde{u}(x)e^{-i\omega t})$$



$$\Rightarrow -\omega^2 \tilde{u}(x) = v^2 \frac{\partial^2}{\partial u^2} \tilde{u}(x) \quad \text{This is time independent version}$$

There are two types of solution for this equation:

1. Ae^{ikx} or $Ae^{ikx} + Be^{-ikx}$
2. $A \cos kx + B \sin kx$

If we use first type solution

$$-\omega^2 \tilde{u}(x) = v^2 \frac{\partial^2}{\partial u^2} \tilde{u}(x) \Rightarrow$$

$$-\omega^2 = v^2 (ik)^2 \Rightarrow \omega^2 = v^2 k^2 \Rightarrow k^2 = \frac{\omega^2}{v^2} \Rightarrow k = \frac{\omega}{v} \quad (I)$$

For boundary conditions ($x = 0$ and $x = L$) we will use the second type solution:

$$\tilde{u}(x) = A \cos kx + B \sin kx \quad \text{and at } x = 0 \tilde{u}(x) = 0 \text{ then } A = 0 \Rightarrow \tilde{u}(x) = B \sin kx$$

$$\text{at } x = L \tilde{u}(x) = 0 \text{ then } B \sin kx = 0 \Rightarrow kL = \pi n \Rightarrow k = \frac{\pi n}{L} \quad (II)$$

(I) & (II) $\Rightarrow \omega = kv = \frac{n\pi v}{L} = n \frac{\pi v}{L}$ n is an integer value and the $\frac{\pi v}{L}$ is fixed then the ω will get only discrete values.

$$f = \frac{\omega}{2\pi} = \frac{nv}{2L}$$

1-D Schrödinger Equation

$$E\Psi = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + U(\vec{r})\Psi \quad \text{Time independent and 1-D Schrodinger Equation.}$$

$$i\hbar \frac{\partial \Phi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Phi}{\partial x^2} + U(\vec{r})\Phi \quad \text{Time dependent and 1-D Schrodinger Equation.}$$

To achieve first from second equation we should use this equation: $\Phi(x, t) = \Psi(x)e^{-iEt/\hbar}$

The only difference between the 1-D Schrodinger eq. and guitar string eq. is the $U(x)$ and this makes the eq. solving hard because it is a function of x .

There are some assumptions to reduce the complexity and then solve the Schrodinger eq. like assuming the particle in the box. While it is quantum analogue of a 1-dimensional vibrating string. (the particle in a box (or infinite square well)).

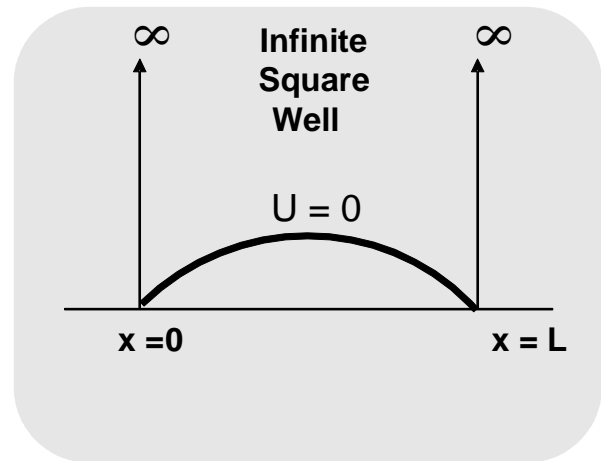
$$\text{Then the 1-dimensional Schrödinger Equation is: } i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

Now Schrödinger equation is like guitar string equation.

$$\Phi(x, t) = e^{\pm ikx} e^{-iEt/\hbar} \quad \therefore E = \frac{\hbar^2 k^2}{2m} \equiv \omega = kV$$

$$atx = 0 \rightarrow \Psi(x) = B \sin(kx) \Rightarrow k = \frac{n\pi}{L}$$

$$\Rightarrow E_n = \frac{\hbar^2}{2m} \frac{\pi^2}{L^2} n^2 \equiv \omega_n = n \frac{\pi V}{L}$$



The last equations are called "**Dispersion relation**". Because it makes relation between time dependent part (ω or E) and position dependent part (k).