ECE 659 Quantum Transport: Atom to Transistor

Lecture 13: Differential to Matrix Equations

Supriyo Datta

Spring 2009

Notes prepared by Samiran Ganguly

$$E = \frac{p^2}{2m} + U(x)$$

Time dependent Schrodinger Equation

$$i\hbar \frac{\partial \psi}{\partial t} = \left[\frac{1}{2m} \left(-i\hbar \frac{\partial}{\partial x} \right)^2 + U \right] \psi$$

Time independent Schrodinger Equation

$$E\phi = H\phi$$

Hamilton's equations

$$p = \hbar k$$

$$\frac{dx}{dt} = \frac{1}{\hbar} \frac{\partial E}{\partial k}$$

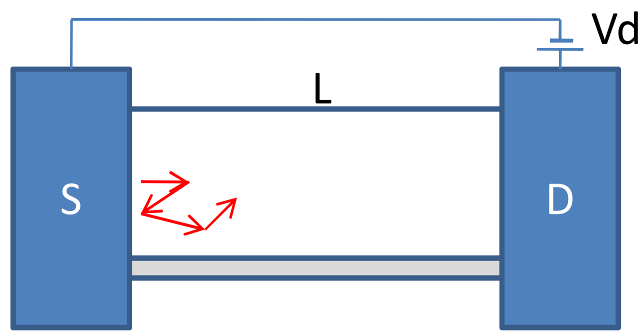
$$\hbar \frac{dk}{dt} = -\frac{\partial E}{\partial x}$$

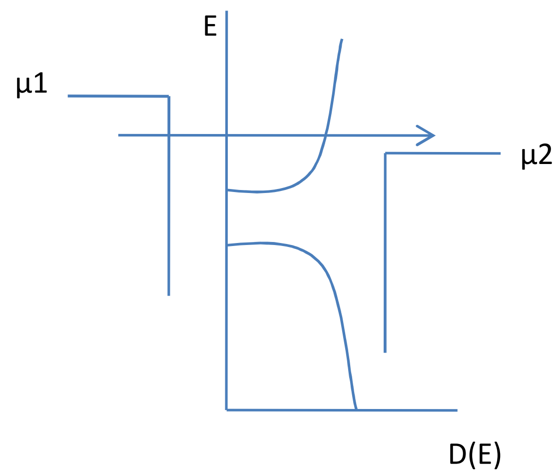
If U is constant then the solution is $\psi \sim e^{ikx} e^{-i\frac{Et}{\hbar}}$

then

$$\frac{\partial \psi}{\partial t} \to -\frac{iE}{\hbar}$$

$$\frac{\partial}{\partial x} \to ik$$





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

Time independent Schrodinger equation with a space dependent potential

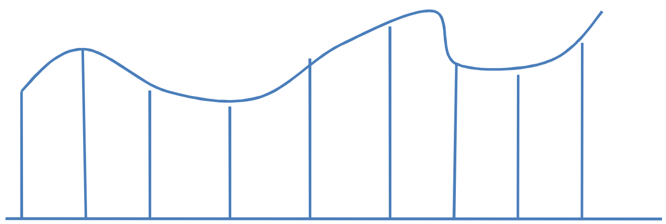
$$E\Phi = H_{op}\Phi$$

In matrix version

$$E\{\phi\} = [H]\{\phi\}$$

Column vector

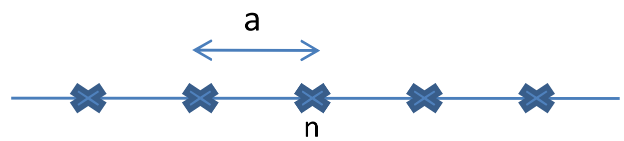
Square matrix



$$\Phi(x) = \sum \phi_m u_m(x)$$

$u_m(x) \rightarrow$ Basis function

$$E\phi_n = \sum_m H_{nm}\phi_m$$



$$E\phi_n = \sum_m H_{nm}\phi_m$$

$$H = \begin{bmatrix} \varepsilon & t & & \\ t & \varepsilon & t & \\ & t & \varepsilon & \ddots \\ & & \ddots & \ddots \end{bmatrix}$$

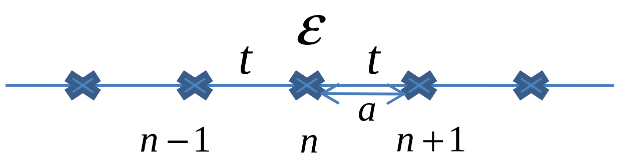
$$E\Phi = -\frac{\hbar^2}{2m}\frac{\partial^2\Phi}{\partial x^2} + U_0\Phi$$

$$E = \frac{\hbar^2 k^2}{2m} + U_0$$

One of the possible solutions $\phi = e^{ikx}$

$$E\phi_n = \sum_n H_{nm}\phi_m$$

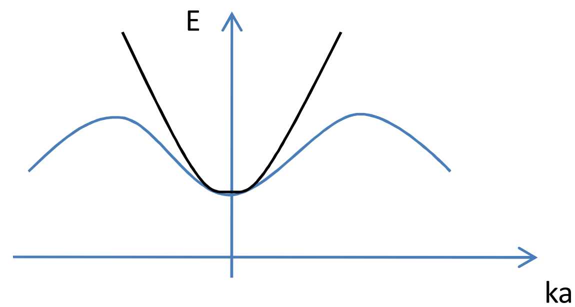
$$= t\phi_{n-1} + \varepsilon\phi_n + t\phi_{n+1}$$



$$E\phi_n = t\phi_{n-1} + \varepsilon\phi_n + t\phi_{n+1}$$
$$E = \varepsilon + 2t\cos ka$$

If we take one more neighbor

$$E = \varepsilon + 2t\cos ka + 2t'\cos 2ka$$



For small ka

$$\cos ka = 1 - \frac{k^2a^2}{2}$$

$$E = \varepsilon + 2t - ta^2k^2$$

$$\varepsilon + 2t = U_0$$

$$-t = \frac{\hbar^2}{2ma^2}$$