

Fundamentals of Nanoelectronics

ECE495 - Session 8, Sept 11, 2009

Schrodinger Equation: Finite Difference Method

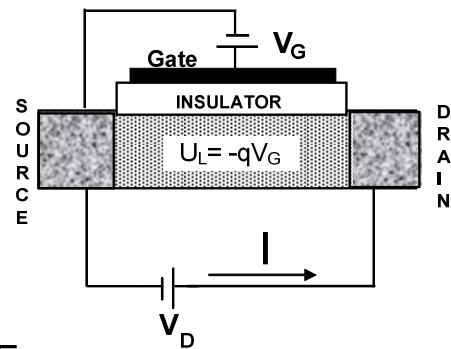
Ref: Chapter 2.2

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Schrödinger Equation

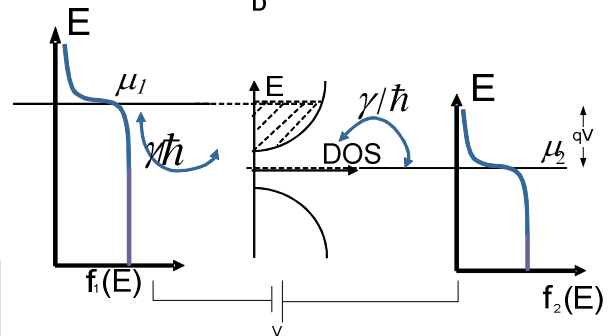
$$E\Psi = \frac{-\hbar^2}{2m} \nabla^2 \Psi + U(\vec{r})\Psi$$



1-D Schrödinger Equation

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

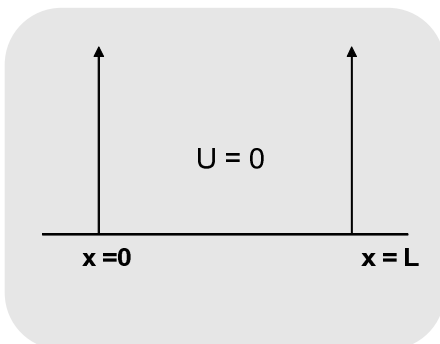
and 1-D Schrodinger Equation.



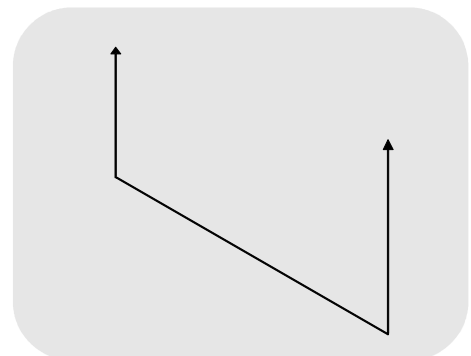
If the potential is independent of x, then the solution to this equation can be written as:

$$\Psi(x,t) = Ae^{-iEt/\hbar} e^{ikx}$$

There is analytical solution for particle in box condition but if we make another type of potential function how should solve Schrödinger Equation? Numerical Solution.



Generally $U(x)$ is a complicated function and analytical solutions are not achievable. Then, we have to rely in numerical solutions.



The total Hamiltonian should be a sum of these two. For now concentrate on the easy part which is $U(x)$.

Consider $E\Psi = [U(x)]\Psi$ Since $U(x)$ is a potential function, on a discrete lattice U would tell us the potential at each lattice point, hence it will be diagonal: $E\Psi_n = U(x_n)\Psi_n$

Writing above as a matrix equation:

$$E \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_N \end{bmatrix} = \begin{bmatrix} H = U(x) \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_N \end{bmatrix} \text{ and } U(x) = \begin{bmatrix} U(x_1) & 0 & \dots & \dots & \dots & 0 \\ 0 & U(x_2) & 0 & \dots & \dots & \vdots \\ \vdots & 0 & \ddots & & & \vdots \\ \vdots & \vdots & & \ddots & & \vdots \\ \vdots & \vdots & & & \ddots & 0 \\ 0 & \dots & \dots & \dots & 0 & U(x_N) \end{bmatrix}$$

Then

$$E \begin{bmatrix} \Psi_1 \\ \vdots \\ \Psi_n \end{bmatrix} = \begin{bmatrix} U(x_1) & & \\ & \ddots & \\ & & U(x_n) \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \vdots \\ \Psi_n \end{bmatrix}$$

Now, how do we write the second derivative at a particular point? $E\Psi = -\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2}$

At each particular point the Schrödinger equation (after dropping U) can be written as:

$$E\Psi_n = -\frac{\hbar^2}{2m} \left(\frac{d^2\Psi}{dx^2} \right)_n$$

First try to write $\left[\frac{d\Psi}{dx} \right]$: $\left[\frac{d\Psi}{dx} \right]_{n+1/2} = \frac{\Psi_{n+1} - \Psi_n}{a}$ and $\left[\frac{d\Psi}{dx} \right]_{n-1/2} = \frac{\Psi_n - \Psi_{n-1}}{a}$

$$\left[\frac{d^2\Psi}{dx^2} \right]_n = \frac{\left[\frac{d\Psi}{dx} \right]_{n+1/2} - \left[\frac{d\Psi}{dx} \right]_{n-1/2}}{a} \Rightarrow \left[\frac{d^2\Psi}{dx^2} \right]_n = \frac{\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}}{a^2}$$

$$\Rightarrow E\Psi_n = -t_0 [2\Psi_n - \Psi_{n-1} - \Psi_{n+1}] \text{ and } t_0 \equiv \frac{\hbar^2}{2ma^2}$$

$$E \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_n \\ \vdots \\ \Psi_N \end{bmatrix} = t_0 \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \ddots & \ddots & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_n \\ \vdots \\ \Psi_N \end{bmatrix}$$

Tri-diagonal Matrix

If we'd want to also include the potential to the matrix we can add its corresponding values to the diagonal elements: $E\Psi_n = U(x_n) - t_0(\Psi_{n-1} - 2\Psi_n + \Psi_{n+1})$

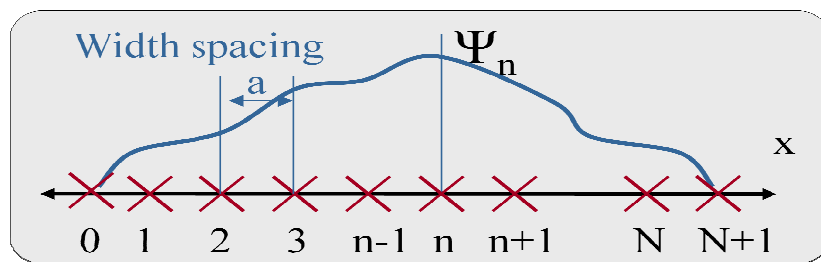
$$E \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_n \\ \vdots \\ \Psi_N \end{bmatrix} = \begin{bmatrix} 2t_0 + U(x_1) & -t_0 & 0 & 0 & 0 & 0 \\ -t_0 & 2t_0 + U(x_2) & -t_0 & 0 & 0 & 0 \\ 0 & -t_0 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \ddots & \ddots & -t_0 \\ 0 & 0 & 0 & 0 & -t_0 & 2t_0 + U(x_N) \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_n \\ \vdots \\ \Psi_N \end{bmatrix}$$

Boundary Conditions

What do we do when we get near a boundary?

$$E \Psi_1 = (-t_0 \Psi_0) + (2t_0 + U_1) \Psi_1 - t_0 \Psi_2$$

Dropping the two terms is equivalent to setting the wavefunction to 0 at the two ends: $\Psi_0 = 0$ and $\Psi_{n+1} = 0$. This would be appropriate for the particle in a box. Problem where the wavefunction is not allowed to penetrate outside the box.



For periodic boundary conditions, such as a particle on a ring, we let $\Psi_0 = \Psi_N$ and $\Psi_{N+1} = \Psi_1$. This is easy to solve mathematically and due to that is used widely. Its real application is Carbon Nanotube. Unlike the infinite-wall scenario, periodic boundary conditions have a slightly different Hamiltonian matrix:

$$\Psi_0 \equiv \Psi_N \Rightarrow [H] = \begin{bmatrix} 2t_0 + U(x_1) & -t_0 & \cdots & \cdots & \cdots & -t_0 \\ -t_0 & 2t_0 + U(x_2) & \cdots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & & & \vdots \\ \vdots & \vdots & & \ddots & & \vdots \\ \vdots & \vdots & & & \ddots & -t_0 \\ -t_0 & \cdots & \cdots & \cdots & -t_0 & 2t_0 + U(x_N) \end{bmatrix}$$