Fundamentals of Nanoelectronics

ECE495 - Session 8, Sept 11, 2009

Schrodinger Equation: Finite Difference Method

Ref: Chapter 2.2

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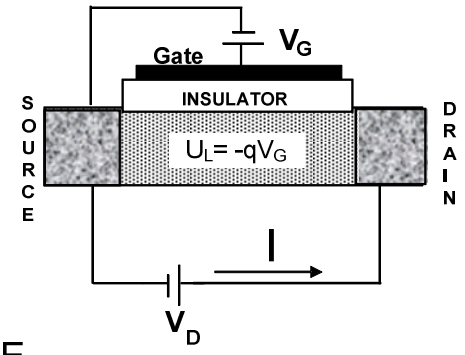
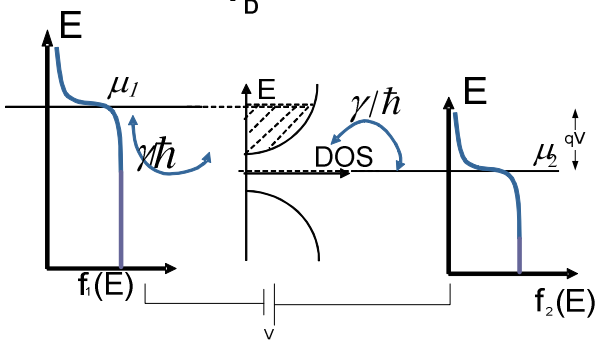
Schrödinger Equation

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



1-D Schrödinger Equation

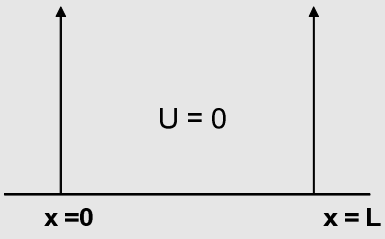
$$E\Psi = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U(\vec{r})\Psi$$ Time independent and 1-D Schrodinger Equation.



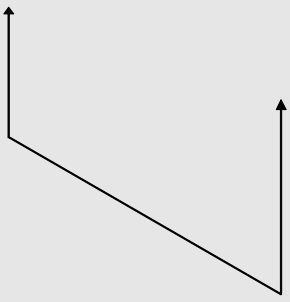
If the potential is independent of x, then the solution to this equation can be written as:

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

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.

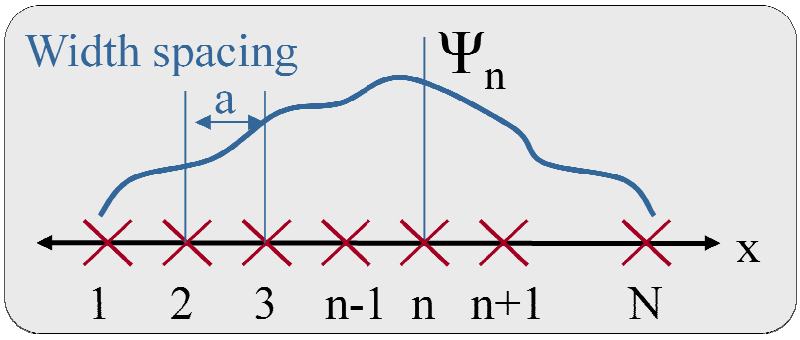


Method

The approach to solve numerically is transforming differential equation to matrix equation.

How can we describe a function as a vector? We set up a lattice of discrete points and record the value of the function at each lattice point. Figure shows the discrete points. As it can be seen corresponding to each lattice point there is a value for the wave function. This can also be viewed as sampling of a continuous function into discrete values. Remember that in order to be able to perform a numerical method we have to a have a finite number of equations so that we can solve them.

First create a lattice for the 1-D problem:



Then, Ψ(x) becomes a column vector telling the value of Ψ at different points.

$$\Psi(x) \rightarrow \begin{bmatrix} \Psi(x_1) \\ \Psi(x_2) \\ \Psi(x_3) \\ \vdots \\ \Psi(x_n) \\ \vdots \\ \Psi(x_N) \end{bmatrix}$$

Then: $E\Psi = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U(\vec{r})\Psi \Rightarrow E\begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_N \end{bmatrix} = \begin{bmatrix} & H & \\ & & \\ & N \times N & \end{bmatrix}\begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_N \end{bmatrix}$

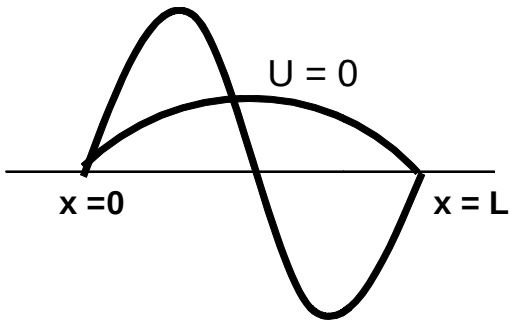
Once one has a matrix equation like above, The eigenvalues of the N by N matrix (H) can be evaluated. There will be N eigenvalues and N eigenvectors.

For large value of N, Matlab can be used to find eigenvalues and eigenvectors:

$[V, D] = eig(H)$ *D* has the eigenvlaues of matrix H as its diagonal elements. *V* has normalized eigenvectors of H as its columns.

Example: Particle in a box

To justify the numerical approach we could test it on an example that we know the answer. Here, this could be particle in a box.



$E\Psi = \underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]}_{Hamiltonian}\Psi$ First try writing the matrix for U(x) and then the matrix for $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$

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:

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

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

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

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

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

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: $E\Psi_n = U(x_n) - t_0(\Psi_{n-1} - 2\Psi_n + \Psi_{n+1})$

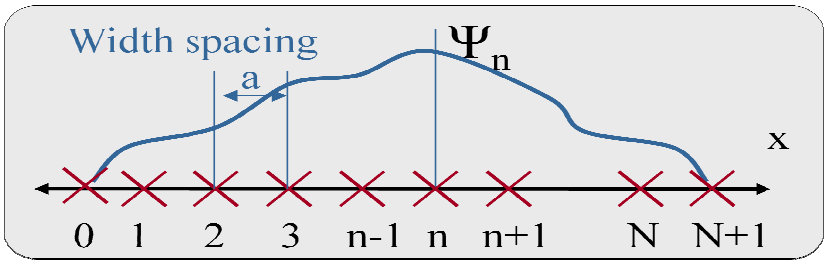
$$E\begin{bmatrix}\Psi_1\\ \Psi_2\\ \vdots\\ \Psi_n\\ \vdots\\ \Psi_N\end{bmatrix}=\begin{bmatrix}2t_0+U(x_1)&-t_0&0&0&0&0\\ -t_0&2t_0+U(x_2)&-t_0&0&0&0\\ 0&-t_0&\ddots&\ddots&0&0\\ 0&0&\ddots&\ddots&\ddots&0\\ 0&0&0&\ddots&\ddots&-t_0\\ 0&0&0&0&-t_0&2t_0+U(x_N)\end{bmatrix}\begin{bmatrix}\Psi_1\\ \Psi_2\\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

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:

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