Fundamentals of Nanoelectronics

Prof. Supriyo Datta
ECE 453
Purdue University

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Lecture 10: Finite Difference Method 1

Ref. Chapter 2.2

Network for Computational Nanotechnology

NCN nanoHUB online simulations and more

Time Independent Schrödinger Equation

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- Today we want to talk about numerical solutions to Schrödinger equation.
- Consider the time dependent Schrödinger Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + U(x)\Psi$$

- **If** the potential is independent of x, then the solution to this equation can be written as: $\Psi(x,t) = Ae^{-iEt/\hbar}e^{ikx}$
- The only thing that remains to be done is the relationship between E and k called the dispersion relation which can be found by substituting the solution in the equation.
- Generally U(x) is a complicated function and analytical solutions are not achievable. There we have to rely in numerical solutions.
- Notice that as long as U is independent of time, the time portion of the solution above is acceptable. So we can write the solution as: $\Psi(x,t) = Ae^{-iEt/\hbar}\Phi(x) \quad (1)$
- Φ(x) is a complicated function that remains to be found.
- By substituting (1) in the Schrödinger equation we get the time independent Schrödinger equation:

$$i\hbar \frac{-iE}{\hbar} e^{-iEt/\hbar}\Phi(x) = e^{-iEt/\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\Phi}{\partial x^2} + U(x)\Phi\right] \Rightarrow$$

Time Independent Schrödinger Equation: $$E\Phi = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]\Phi$$

Overview - Eigenvalue Problem

- What we want to do next is to solve:

$$E\Phi = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) \right]\Phi$$

- The basic idea for any method of numerical solution to the differential equation is to turn it into a matrix equation. We'll consider the finite difference method here. We'll end up with:

$$E\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} & & \\ & \text{N by N} & \\ & & \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

- What we'll learn for the rest of the class is how the finite difference method turns the differential equation into a matrix equation.
- Once one has a matrix equation like above,

The eigenvalues of the N by N matrix can be evaluated. There will be N eigenvalues and N eigenvectors.

- An example of eigenvalue problem:

$$E\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} \quad (1)$$

- (1)=> $\begin{bmatrix} E-a & -b \\ -c & E-b \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

- To see this write the left hand side of (1) as:

$$\begin{bmatrix} E & 0 \\ 0 & E \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}$$

- And subtract from it the matrix: $\begin{bmatrix} a & b \\ c & d \end{bmatrix}$

Eigenvalue Problem Continued

- From $\begin{bmatrix} E-a & -b \\ -c & E-b \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$
- The eigenvalues can be found using the argument that the matrix on the left must be singular. If it wasn't then multiplying both sides by its inverse would result in a 0 eigenvector which is not the correct answer.
- The matrix won't have an inverse if its determinant is not 0. We have:

$$(E-a)(E-d)-bc=0\ (1) \Rightarrow$$

$$E = E_1, E_2 \ \text{ Eigenvalues}$$

- To see hoe the procedure works, consider a special case: $E\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}$
- From (1)=>

$$(E-0)(E-0)-1\cdot 1=0 \Rightarrow E=+1,-1$$

- Corresponding to each eigenvalue, there is an eigenvector:
- E = +1, then

$$(+1)\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} \Rightarrow \phi_1 = \phi_2 \Rightarrow \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

- E = +1, then

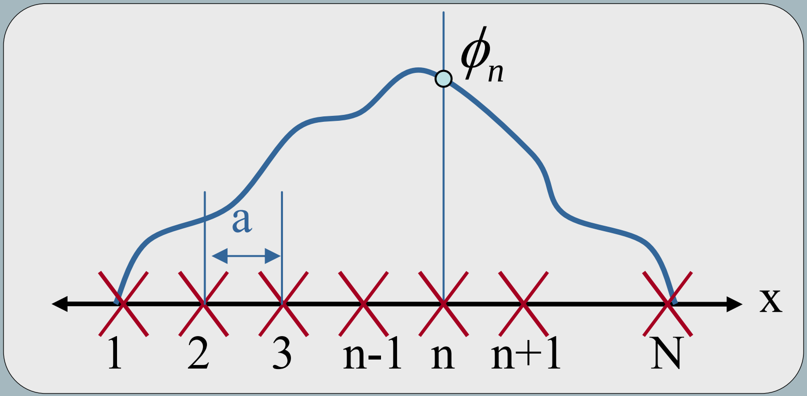
$$(-1)\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} \Rightarrow \phi_1 = \phi_2 \Rightarrow \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

- Notice that if the eigenvectors are multiplied by an arbitrary scalar, the result is still an eigenvector.
- In general for an N by N matrix we'll have N eigenvalues and N corresponding 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.

Function Becomes a Column Vector

- 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.



- Φ (x,t) therefore becomes a column vector telling the value of Φ at different points. i.e.

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

Writing Potential Function U(x) as a Matrix

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$$E\Phi = \underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) \right]}_{\text{Hamiltonian}} \Phi$$

- Next question is:
- How do we convert the Hamiltonian operator into a matrix?

- 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)… (notice that a term is being neglected in the next equation at this point)

- Consider $E\Phi = \left[U(x)\Phi\right]$
- Since U(x) is a potential function, on a discrete lattice U would tell us the potential at ach lattice point, hence it will be diagonal: $E\phi_n = U(x_n)\phi_n$

- Writing above as a matrix equation:

$$E\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} & & \\ & \text{U(x)} & \\ & & \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

$$U(x) = \begin{bmatrix} U(x_1) & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & U(x_2) & 0 & \cdots & \cdots & \vdots \\ \vdots & 0 & \ddots & & & \vdots \\ \vdots & \vdots & & \ddots & & \vdots \\ \vdots & \vdots & & & \ddots & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & U(x_N) \end{bmatrix}$$

Differential Operator's Discrete Representation 1

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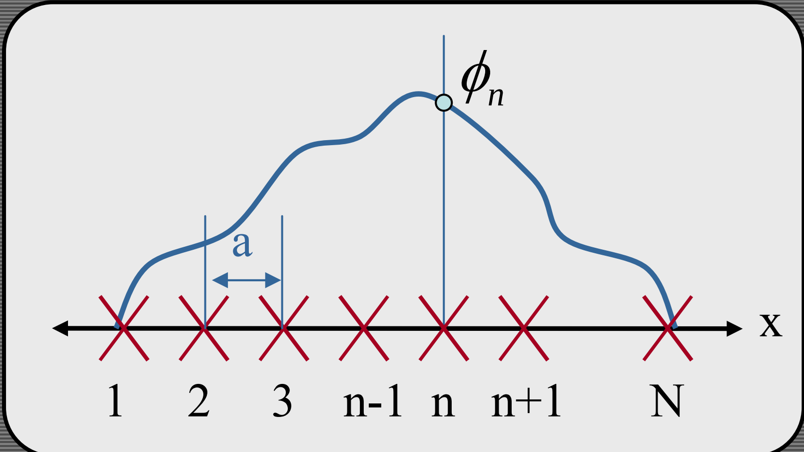


At each particular point the Schrödinger equation (after dropping U) can be written as:

$$\left[E\phi\right]_{x=x_n} = -\frac{\hbar^2}{2m}\left(\frac{d^2\Phi}{dx^2}\right)_{x=x_n}$$

Now start from left and right everything at point n. The constants remain the same. For the wavefunction we right its value at that particular point. We will have:

$$E\phi_n = -\frac{\hbar^2}{2m}\left(\qquad \right)$$

- What goes in the parenthesis is the discrete representation of the differential operator.
- So to turn the differential equation to a difference equation, the most important step is to write the second derivative as a difference expression. Let's state the answer first and then derive it:

$$\frac{d^2\phi_n}{dx^2} = \frac{\phi_{n+1} - 2\phi_n + \phi_{n-1}}{a^2}$$

- Based on what we've done so far, we can write:

$$E\phi_n = U(x_n)\phi_n - t_0\left(\phi_{n-1} - 2\phi_n + \phi_{n+1}\right)$$

$$t_0 \equiv \frac{\hbar^2}{2ma^2}$$

Differential Equation Becomes a Matrix Equation

- Accepting $E\phi_n = -t_0\left(\phi_{n-1} - 2\phi_n + \phi_{n+1}\right) \quad (1)$,how can we write the matrix equation?

$$E\begin{Bmatrix} \phi_1 \\ \phi_2 \\ . \\ . \\ . \\ \phi_N \end{Bmatrix} = \begin{bmatrix} 2t_0 & -t_0 & 0 & \cdots & \cdots & ? \\ -t_0 & 2t_0 & -t_0 & 0 & \cdots & \vdots \\ 0 & -t_0 & \ddots & \ddots & & \vdots \\ \vdots & 0 & \ddots & \ddots & & \vdots \\ \vdots & \vdots & & & \ddots & -t_0 \\ ? & \cdots & \cdots & \cdots & -t_0 & 2t_0 \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \\ . \\ . \\ . \\ \phi_N \end{Bmatrix}$$

- This will be a tridiagonal matrix:
- To see this consider for example one of the equations from the series of equations in (1):

$$E\phi_2 = -t_0\left(\phi_1 - 2\phi_2 + \phi_3\right)$$

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

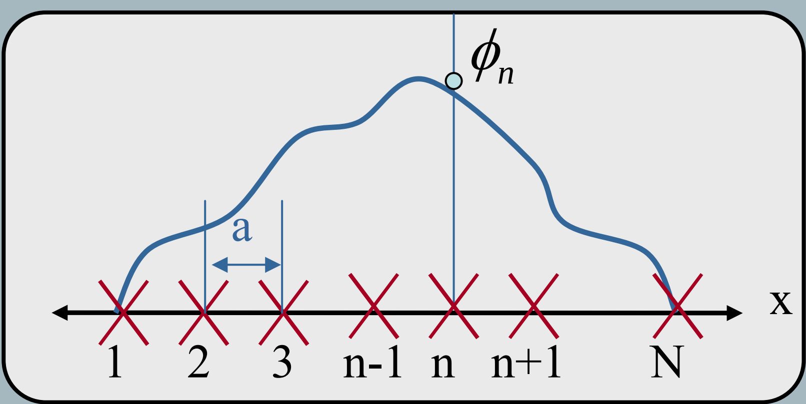
$$E\begin{Bmatrix} \phi_1 \\ \phi_2 \\ . \\ . \\ . \\ \phi_N \end{Bmatrix} = \begin{bmatrix} 2t_0 + U(x_1) & -t_0 & \cdots & \cdots & \cdots & ? \\ -t_0 & 2t_0 + U(x_2) & \cdots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & & & \vdots \\ \vdots & \vdots & & \ddots & & \vdots \\ \vdots & \vdots & & & \ddots & -t_0 \\ ? & \cdots & \cdots & \cdots & -t_0 & 2t_0 + U(x_N) \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \\ . \\ . \\ . \\ \phi_N \end{Bmatrix}$$

Boundary Conditions

- How do we determine the far elements on the anti-diagonal? In other words how do we handle the boundaries?

$$E\begin{Bmatrix}\phi_1\\ \phi_2\\ .\\ .\\ .\\ \phi_N\end{Bmatrix}=\begin{bmatrix}2t_0+U(x_1) & -t_0 & \cdots & \cdots & \cdots & ?\\ -t_0 & 2t_0+U(x_2) & \cdots & \cdots & \cdots & \vdots\\ \vdots & \vdots & \ddots & & & \vdots\\ \vdots & \vdots & & \ddots & & \vdots\\ \vdots & \vdots & & & \ddots & -t_0\\ ? & \cdots & \cdots & \cdots & -t_0 & 2t_0+U(x_N)\end{bmatrix}\begin{Bmatrix}\phi_1\\ \phi_2\\ .\\ .\\ .\\ \phi_N\end{Bmatrix}$$

$$E\phi_n=U(x_n)\phi_n-t_0\left(\phi_{n-1}-2\phi_n+\phi_{n+1}\right)$$



- Dropping the two terms is equivalent to setting wavefunction to 0 at the two ends: $\phi_0=\phi_{N+1}=0$
- This would be appropriate for the particle in a problem where the wavefunction is not allowed penetrate outside the box.
- Next day we'll start with the finite difference