

Fundamentals of Nanoelectronics

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Lecture 11: Finite Difference Method
Ref. Chapter 2.2

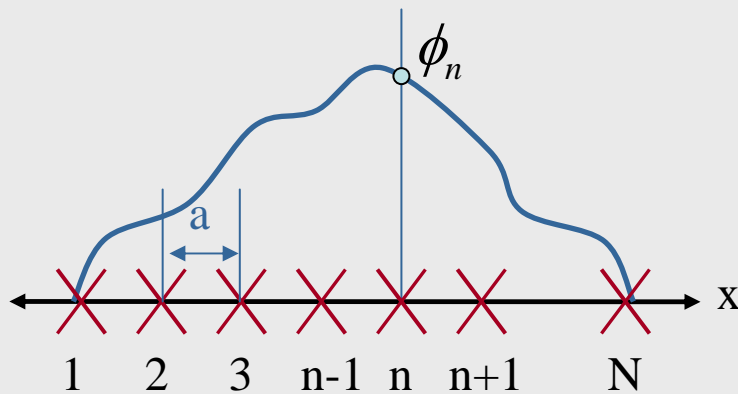


Network for Computational Nanotechnology



Time Independent Schrödinger Equation and Discretization

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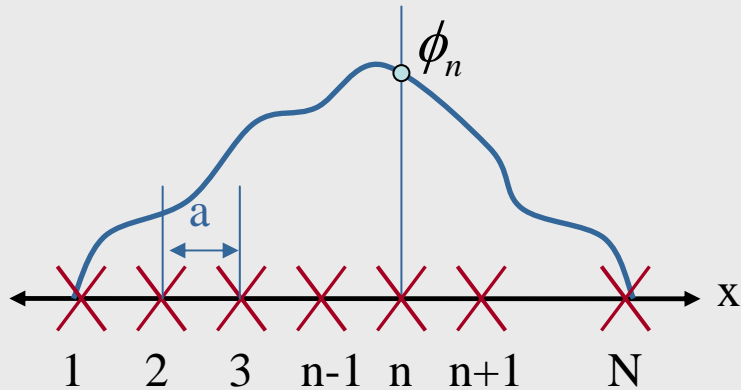


$$E\Phi = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right] \Phi$$

$$E \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

- As it was mentioned before all numerical methods for solving differential equations involve some scheme to convert the original equation into a matrix equation. What we do here is to discretize the lattice and then we write the second derivative as a difference equation.
- Figure on the left 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 have a finite number of equations so that we can solve them.
- To make things easier, for now we set $U(x)=0$. Note that the matrix for U can be written down easily and it can later be added to the matrix that represents the differential operator which we now we'll try to find...

From Derivatives to Differences 1



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

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

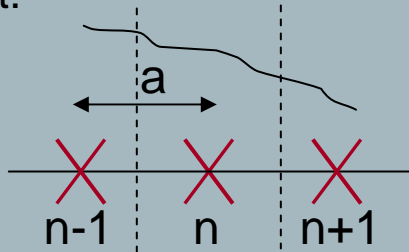
$$[E\phi]_{x=x_n} = -\frac{\hbar^2}{2m} \left(\frac{d^2\Phi}{dx^2} \right)_{x=x_n}$$

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:

- What goes in the parenthesis is the discrete representation of the differential operator.
- So to turn this differential equation to a difference equation, the most important step is to write the second derivative as a difference expression. We start with the difference equation for the first derivative...

From Derivatives to Differences 2

Consider the lattice in the vicinity of the n th point.



In order to right the derivative of the function at n we need to know its values close to n .

This can be done by calculating the amount by which the value of wave function changes as moving from one lattice point to another. This gives us the first derivative. The second derivative is of course the difference of the first derivatives.

- The amount by which the function changes going from $n-1$ to n divided by the distance between the two points is the first derivative.

$$\left[\frac{d\phi}{dx} \right]_{n+1/2} = \frac{\phi_{n+1} - \phi_n}{a}$$

$$\left[\frac{d\phi}{dx} \right]_{n-1/2} = \frac{\phi_n - \phi_{n-1}}{a}$$

- Notice that the closer the lattice points the better the approximation.
- What do we do now to get the second derivative at n ? Subtract the first derivative at $n-1/2$ from the first derivative at $n+1/2$ and again divide by the distance (a) between them

From Derivatives to Differences 3

- The second derivative is:

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

- Where $\left[\frac{d\phi}{dx} \right]_{n+1/2} = \frac{\phi_{n+1} - \phi_n}{a}$ and

$$\left[\frac{d\phi}{dx} \right]_{n-1/2} = \frac{\phi_n - \phi_{n-1}}{a}$$

- So

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

- And finally our Schrödinger equation becomes:

$$E\phi_n = -\frac{\hbar^2}{2ma^2} (\phi_{n+1} - 2\phi_n + \phi_{n-1})$$

- This was the essence of the finite difference method. The equation above is the Schrödinger equation at a particular point n. There are N of these equations. All together they can be written as a matrix equation. To make things more compact and elegant define:

$$t_0 = \hbar^2 / 2ma^2$$

- and take the negative sign inside to get:

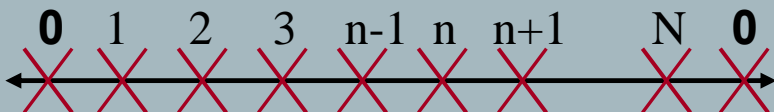
$$E\phi_n = t_0 (2\phi_n - \phi_{n+1} - \phi_{n-1})$$

Boundary Conditions (BC)

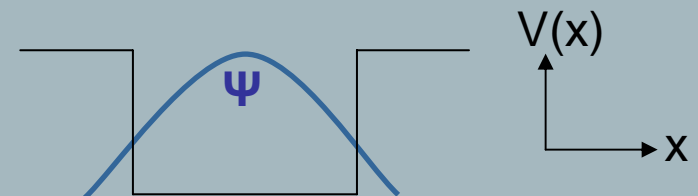
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$$E \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \cdot \\ \cdot \\ \cdot \\ \phi_N \end{Bmatrix} = \begin{bmatrix} 2t_0 & -t_0 & \cdots & \cdots & \cdots & ? \\ -t_0 & 2t_0 & \cdots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & & & \vdots \\ \vdots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

• The easiest boundary condition to implement is to assume that the wavefunction is 0 at the two ends of the 1-D lattice. Notice that the issue of boundary conditions comes in play because we want to have a finite dimensional matrix. So we have to end it somewhere and that brings about boundaries.



• This assumption is an exact one if we were to describe the energy levels of a particle with infinite potential walls. In that case there would be no way for the wavefunction to leak outside of the box. However if the potential walls were not infinite, there would be some leakage. In that case we increase the lattice size to incorporate non-zero values of the wavefunction. One point to notice is that the potential would have 2 different values inside and outside of the box which can easily be entered in the Hamiltonian matrix. (We just add what ever potential we have the diagonal element corresponding to the lattice points.)



- In the following weeks we'll be talking about the energy levels of solids. One very interesting point about metals and semiconductors is that the electronic levels can be obtained from a slightly modified Schrödinger equation.

- The modification is in the value of m .

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

- Whereas the value of m in the equation above is the actual mass of electron, the modified m denoted by m^* is not. It is called the effective mass. It incorporates the potential of the solids who have periodic structure. Using this concept, one can obtain the energy levels of such solids using what's called an effective mass equation without having to enter...

...the value of $U(x)$ which corresponds to the periodic nuclear potentials that exist in a solid.

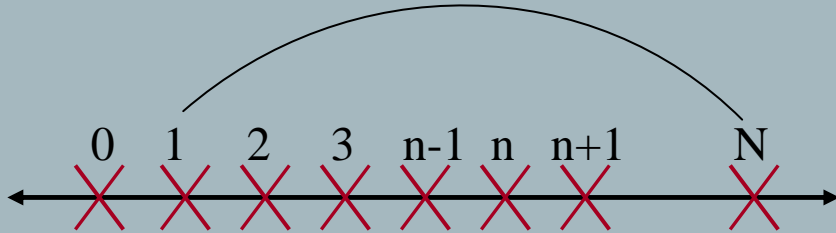
$$E\Phi = \left[-\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} \right] \Phi$$

- What this means is that given a piece of silicon, you could estimate the energy levels by solving a particle in a box problem which leads us to another point and that is the usage of periodic boundary conditions.

- Although the right boundary conditions to be used are infinite wall BCs, the periodic BCs are often used because of 2 reasons: 1. It makes the math easy. 2. When trying to understand the energy levels deep in the middle of a solid, then what happens at the boundaries are not important. But what is periodic BC?

Periodic Boundary Conditions 1

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- The idea is as the name suggests. Considering the above lattice, one thinks of the Nth point as having the exact potential as the 0th point. The N+1 point would have the exact potential as the first point and so on. Notice that we've assumed that the period is N.
- Knowing this, how can we modify the Hamiltonian matrix to obey the boundary conditions?
- Remember that whatever the boundary conditions are, they enter at the points indicated here....

$$H = \begin{bmatrix} & \times \\ \times & \end{bmatrix}$$

- To implement the periodic boundary conditions then like this:
We've assumed the solid to be like a ring meaning the Nth point is the same as the 0th point.
Ordinarily point one is connected to the 0th point described by $-t_0$. But now point 0 is point N.
Indeed what happens is that point N is connected to point 1 via $-t_0$. As the result this value seats in the place of the matrix element that connects N to 1.

$$H = \begin{bmatrix} & -t_0 \\ \times & \end{bmatrix}$$

Equation 1 now becomes:

$$E\phi_1 = 2t_0\phi_1 - t_0\phi_2 - t_0\phi_N$$

How about the other diagonal element?

Periodic Boundary Conditions 2

36:00

- Using the same idea, the other element will also be turn out to be $-t_0$.
- This is consistent with postulates of quantum mechanics: We want the eigen values of the Hamiltonian matrix to be real. For this to happen, the H matrix must be Hermitian. If all the matrix elements are real then being Hermitian comes down to being symmetric. And symmetric means that we have to have $-t_0$ for both of our diagonal elements that describe the boundary conditions:

$$H = \begin{bmatrix} & -t_0 \\ -t_0 & \end{bmatrix}$$

- In general H must be Hermitian. This means that the matrix is the same as its conjugate transpose.
- But why does this periodic boundary condition make things simpler? The answer lies in the properties of the exponential function as a solution of Schrödinger equation:

$$E\Phi = \left[-\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} \right] \Phi$$

- For the box boundary conditions we had to consider the function $\sin(x)$ because the exponential doesn't go to 0 at the ends. However the situation is different for periodic boundary conditions...

- Indeed, the exponential e^{ikx} can be considered as a solution to Schrödinger equation with periodic boundary. The advantage of exponentials is that taking their derivatives is very easy, their magnitude squared is 1, ect.
- Let's see what this Per. BCs means for exponentials:

$$e^{ikx} \Rightarrow e^{ik(x+L)} = e^{ikx}$$

For the equation to hold we have to have:

$$kL = n2\pi \Rightarrow k = n \frac{2\pi}{L}$$

- One last point:
It seems as if with exponentials we have half as much allowed values of k because they are 2π apart whereas for $\sin(x)$ values of k are only π apart.
- This is not true though. Because in the case of $\sin(x)$, the k and $-k$ values produce two wavefunctions that are different just by a constant factor. This means that we don't have two independent functions. For exponentials on the other hand, k and $-k$ values produce two independent solutions.
- Altogether we conclude that the number of k values in both cases are the same. For $\sin(x)$ all k values are positive and π apart. For e^{ikx} are both positive and negative and 2π apart.