

# Quantum Transport:

Atom to Transistor

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Lecture 7: Schrödinger Equation: Method of Finite Differences

Ref. Chapter 2.2



Network for Computational Nanotechnology



## Retouch on Concepts

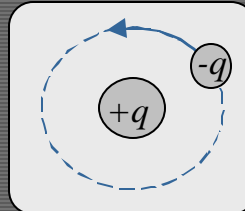
00:00

- Last time, we discussed the Schrödinger Equation:

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

- We began with the simplest case, the Hydrogen atom. It is the simplest because there are no electron-electron interactions
- Experimentally discrete energy levels are observed

### Hydrogen Atom



### Discrete Energy Levels

$$E_n = -E_0/n^2$$

⋮	
n = 4	
—	
n = 3	
—	
n = 2	
—	
n = 1	
—	

## Method of Finite Differences: Lattice Points

03:00

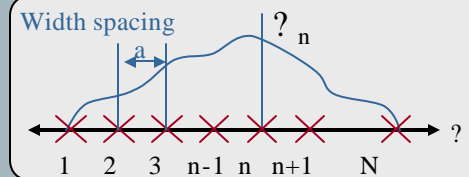
- Today: How to solve the Schrödinger Equation numerically using the method of finite differences.

- Start with the 1-Dimensional Schrödinger equation:

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

- In essence we want to convert the Schrödinger Equation into a matrix equation.

- First create a lattice for the 1-D problem.



- $\psi(x,t)$  therefore becomes a column vector telling the value of  $\psi$  at different points at any given instant of time:

$$\begin{bmatrix} \psi(x_1) \\ \psi(x_2) \\ \psi(x_3) \\ \vdots \\ \psi(x_n) \\ \vdots \\ \psi(x_N) \end{bmatrix}$$

## Method of Finite Differences: Hamiltonian Matrix

07:00

- Similarly, the entire 1-D Schrödinger Equation becomes:

$$i\hbar \frac{d}{dt} \begin{bmatrix} \Psi_1 \\ \vdots \\ \Psi_n \end{bmatrix} = \begin{bmatrix} H \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \vdots \\ \Psi_n \end{bmatrix}$$

- 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

- Formulating Schrödinger's Equation in the following form:

$$\left[ i\hbar \frac{d}{dt} \Psi \right]_{x=x_n} = \left[ \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \Psi \right]_{x=x_n} + [U(x)\Psi(x,t)]_{x=x_n}$$

- The second term on the right side equation can be written down easily and it is  $U(x_n) \times \Psi_n$  for any given point 'n' of the lattice. Note that  $\Psi_n$  only depends on  $\Psi_n$  and this indicates that potential term  $U(x)$  appears on the diagonal of Hamiltonian only.

## Method of Finite Differences: Hamiltonian Matrix

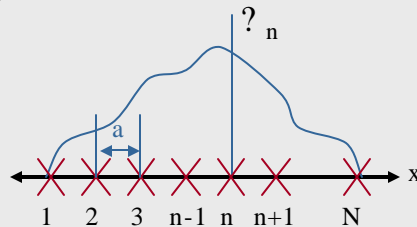
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- Thus:

$$i\hbar \frac{d}{dt} \begin{bmatrix} ?_1 \\ \vdots \\ ?_n \end{bmatrix} = \begin{bmatrix} U(x_1) & & \\ & \ddots & \\ & & U(x_n) \end{bmatrix} \begin{bmatrix} ?_1 \\ \vdots \\ ?_n \end{bmatrix}$$

- Now, how do we write the second derivative at a particular point?

### Points in the Lattice Space



- First try to write  $\left[ \frac{d?}{dx} \right]_{n+1/2}$ ..

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

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

- Then,

$$\begin{aligned} \left[ \frac{d^2?}{dx^2} \right]_n &= \frac{\left[ \frac{d?}{dx} \right]_{n+1/2} - \left[ \frac{d?}{dx} \right]_{n-1/2}}{a} \\ &= \frac{?_{n+1} - 2?_n + ?_{n-1}}{a^2} \end{aligned}$$

Which is the representation of a second derivative in the finite differences method

## Method of Finite Differences: Hamiltonian Matrix

20:52

- Generalizing the numerical expression for the second derivative we get:

$$i\hbar \frac{d}{dt} \psi_n = \frac{-\hbar^2}{2ma^2} [2\psi_n - \psi_{n-1} - \psi_{n+1}] + U(x_n) \psi_n$$

- Let  $t_0 = \hbar^2/2ma^2$  so the Hamiltonian matrix  $i\hbar \frac{\partial}{\partial t} \{\psi\} = [H] \{\psi\}$  now looks like ...

$$i\hbar \frac{d}{dt} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \\ \vdots \\ \psi_N \end{bmatrix} = \begin{bmatrix} 2t_0 + U(x_1) & -t_0 & 0 & 0 & 0 & 0 \\ -t_0 & 2t_0 + U(x_2) & -t_0 & 0 & 0 & 0 \\ 0 & -t_0 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \ddots & \ddots & -t_0 \\ 0 & 0 & 0 & 0 & -t_0 & 2t_0 + U(x_N) \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \\ \vdots \\ \psi_N \end{bmatrix}$$

## Eigen Values Eigen Vectors

27:30

- What about the time derivative

$i\hbar \frac{d}{dt} \Psi(t)$  i.e. How do we calculate  $\Psi(t)$  given some initial state  $\Psi(0)$ ?

- Answer: Find the eigenvalues  $E_a$  and eigenvectors  $\{a\}$  of the matrix  $[H]$ . Such that,  $[H]\{a\} = E_a\{a\}$

- Using the eigenvectors as a basis set, by substitution it can be shown that  $\Psi(t) = \sum_a \{a\} e^{(-iE_a t)/\hbar}$  satisfies the matrix form of the Schrödinger Equation

- And similarly, so does any linear combination of basis functions

$$\{\Psi(t)\} = \sum_a C_a e^{-iE_a t/\hbar} \{a\}$$

- What is not clear, is what the coefficients  $C_a$  are. This depends on the problem

**But first step is to  
find the eigen value  $E_a$   
And the eigen vector  $\{a\}$**

## Boundary Conditions

35:34

- What do we do when we get near a boundary?

• In the case of infinite -wall boundary conditions, such as the infinite square well,

$$-t_0 \psi_0 + (2t_0 + U_1) \psi_1 - t_0 \psi_2$$

is replaced by

$$(2t_0 + U_1) \psi_1 - t_0 \psi_2$$

and

$$-t_0 \psi_{N-1} + (2t_0 + U_N) \psi_N - t_0 \psi_{N+1}$$

by

$$-t_0 \psi_{N-1} + (2t_0 + U_N) \psi_N$$

Meaning,  $\psi_0$  and  $\psi_{N+1}$  are considered equal to zero

- For periodic boundary conditions, such as a particle on a ring, we let  $\psi_0 = \psi_N$  and  $\psi_{N+1} = \psi_1$

- Unlike the infinite-wall scenario, periodic boundary conditions have a slightly different Hamiltonian matrix:

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

- Sub-note: Most Hamiltonians are normally Hermitian:

$$H^\dagger = (H^*)^T = H$$



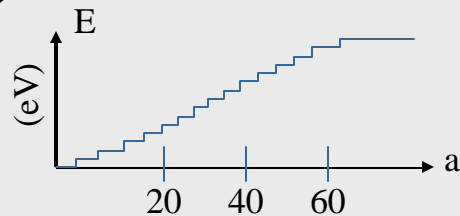
## PERIODIC VS. BOX Boundary Conditions

42:36

- For periodic boundary conditions eigenvalues come in degenerate pairs

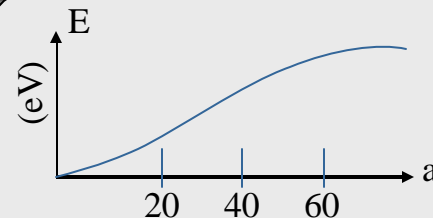
- Whereas for BOX boundary conditions the eigenvalues are non degenerate

### Degenerate Eigenvalues



- This is because the eigenfunctions for the periodic case are:  
 $\sin(k_a x)$  and  $\cos(k_a x)$   
with  $k_a = (a2\pi)/L$ ,  $a = 1, 2, \dots$

### Non-Degenerate Eigenvalues

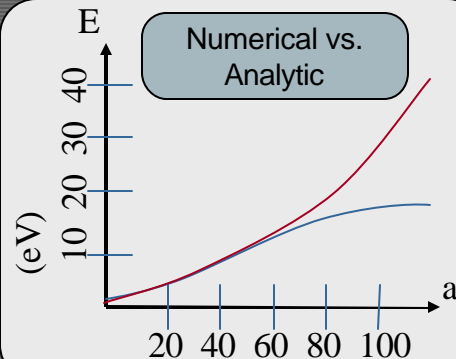


- This is because the eigenfunctions for the this case are:  
 $\sin(k_a x)$   
with  $k_a = (a\pi)/L$ ,  $a = 1, 2, \dots$

## Numerical vs. Analytical Eigenvalues

46:47

- Finally note that numerical analysis yields eigenvalues close to analytical result only for low energies.
- For example a 100 point lattice in the infinite square well yields the following...



• Where the analytical result is given by  $E_a = (\hbar^2 a^2 p^2) / 2mL^2$

- This occurs because at very high energies the wave function oscillates very fast and the wide lattice spacing does not capture the whole story.

High Energy Wave: Infinite Square Well

