

Fundamentals of Nanoelectronics

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Lecture 12: Separation of Variables

Ref. Chapter 2.2 & 2.3



Network for Computational Nanotechnology



Schrödinger equation (Matrix Form)

00:07

- Remember time independent Schrödinger equation:

$$E\Phi = \left(-\frac{\hbar^2}{2m} \nabla^2 + U \right) \Phi$$

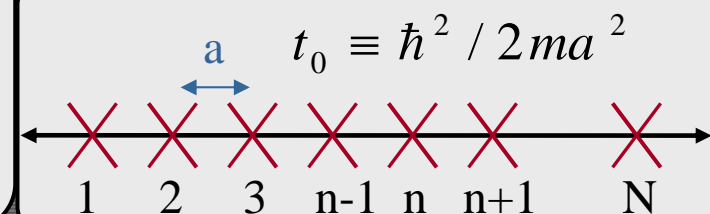
- In one dimension (say in x) if we neglect the potential U, we'll have:

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

- Using finite difference method, we have this matrix equation:

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

- But is there any difference between the solutions of the matrix equation and the analytical solution? In particular how do the eigenvalues of the two methods compare to each other?
- The answer depends on the range of energy which is considered. For low energies the two answers match well whereas for high energies the two deviate from each other and of course it is the numerical answer obtained from the matrix on the left that is not quite right. Let's discuss this more in depth: (See next page)



Numerical vs. Analytical eigenvalues

05:49

- You can set up a matrix and ask Matlab to find the eigenvalues. The number of eigenvalues will be the same as the number of rows (or columns) of the matrix. For a 100 by 100 matrix, we get 100 eigenvalues. Plotting them versus energy gives us the figure below.
- How does the answer look like analytically? For a constant potential, we know the answer analytically and that is a good bench mark for checking the numerical solution. So what are the analytical eigenvalues for 0 potential?

- Schrödinger equation reads: $E\Phi = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \Phi$ The solutions to this equation are the plane waves: $\exp(ikx)$

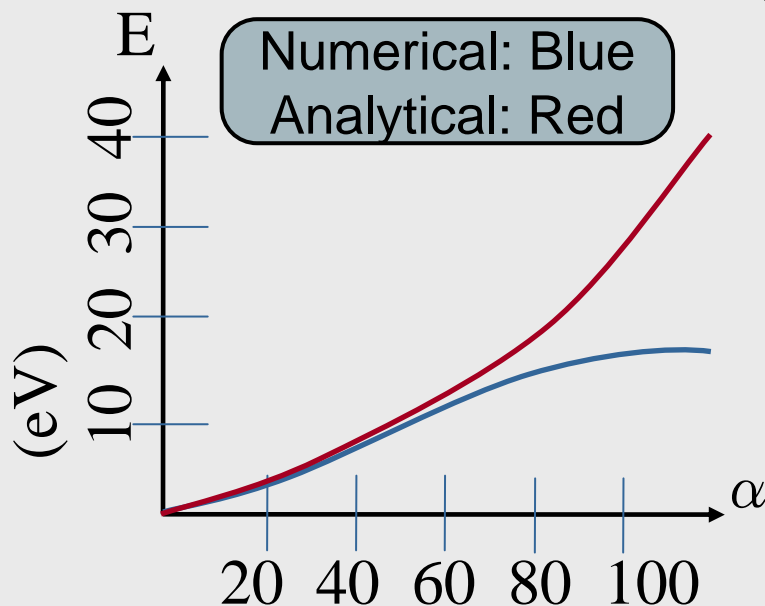
The eigenvalues are given by: $E = \hbar^2 k^2 / 2m$

Periodic boundary conditions require the solutions at the beginning and the end of the lattice to match:

$$e^{ik(x+L)} = e^{ikx} \Rightarrow e^{ikL} = 1 \Rightarrow kL = 2\pi\nu \\ \Rightarrow k = \nu \frac{2\pi}{L} \quad (\nu \text{ is an integer})$$

Putting this k in the eigenvalue equation $\Rightarrow E = \frac{\hbar^2}{2m} \left(\frac{2\pi}{L} \right)^2 \nu^2$

The analytical eigenvalues look like a parabola whereas the numerical ones level off. Why do the answers match at low energies but not high energies?

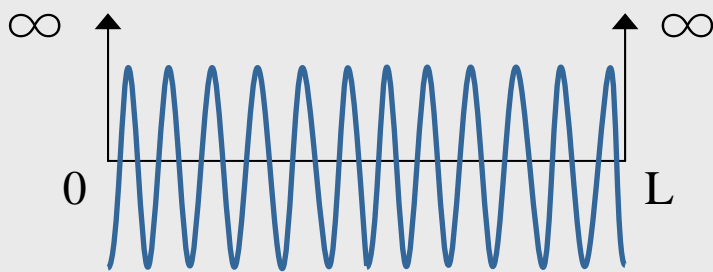


Wavefunction varies rapidly at high energies

12:01

- As it can be seen from the figure, the numerical solution deviates from the analytical one. The reason is that at low energies the wavefunction varies slowly whereas at high energies it changes very fast. If the lattice points are not close enough then the numerical solution fails to capture the whole physics and fails to give the right answer. Therefore we can trust the numerical eigenvalues at low energies and ignore them for higher values of energy.
- It turns out that for current flow the energy range of interest is a small region around the chemical potential. This is why we're ok to use the numerical solution.

High Energy Wave: Infinite Square Well



- Why do the two answers deviate? The reason relies in turning the second order derivative to a difference equation.
$$\frac{d^2\Phi}{dx^2} \Rightarrow \frac{\Phi_{n-1} - 2\Phi_n + \Phi_{n+1}}{a^2}$$
- We will discuss this issue more when we talk about bandstructure.

- How do the boundary conditions affect the results? More specifically what is the difference between the eigenvalues for periodic boundary conditions versus box boundary conditions?
- For periodic boundary conditions we have the solutions:

$$e^{ikx}, e^{-ikx}$$

- Both of these solutions give the same eigenvalue because $-k$ and k give the same energy:

$$E = \hbar^2 k^2 / 2m$$

- The eigenvalues in this case come in pairs: at each energy there are two eigenvalues.

- Using the box boundary conditions, the situation will be different. In that case there will be no pairs but the eigenvalues will be closer together. In this case they will be π/L apart whereas in the previous case they were $2\pi/L$ apart. Why?
- For the solutions we can have any linear combination of exponentials that satisfy box boundary conditions:

$$(e^{ikx} - e^{-ikx}) / 2i = \sin(kx)$$

- The box boundary conditions tell us that the wavefunction has to go to 0 at the ends.

$$\sin(kL) = 0 \Rightarrow kL = \nu\pi$$

- Notice that $-k$ and k values give two wavefunctions that are not linearly independent and hence they are not separate solutions.
- In both cases we have the same number of eigenvalues.

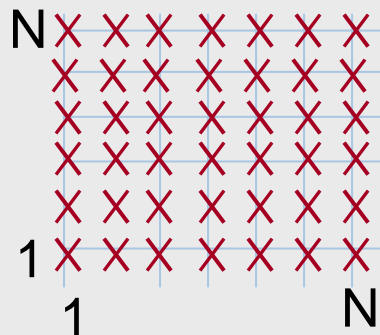
Separation of variables (reasons/conditions)

23:58

- How do we solve Schrödinger equation in two dimensions?
- The equation reads:

$$E\Phi = \left(-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + U \right) \Phi$$

- Just as we set up a lattice in 1 dimension, we can set up a lattice in two dimensions.



- Then we have to turn the equation into a matrix equation.

- The wavefunction vector in the matrix form has the value of the wavefunction at each discrete lattice point. For this lattice we will have N^2 values. This means that the matrix size will be N^2 by N^2 . As N gets large, it will be hard for the computer to calculate its eigenvalues.
- We can see that this makes it hard to solve problems in higher dimensions because of the limited power of computers.
- For higher dimensions we use another method called separation of variables. This method can be used only if the potential satisfies certain conditions. If it is so, then the big problem in higher dimensions can be broken into small problems in lower dimensions.
- How does this method work and what condition should the potential satisfy?

Method of Separation of variables

30:00

- If the potential has the following property:

$$U(x, y) = U_x(x) + U_y(y)$$

- Then separation of variables can be used to give the wavefunction as:

$$\Phi(x, y) = X(x) \times Y(y) \quad (0)$$

- We can find X and Y by solving the following equations:

$$E_x X(x) = \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U_x(x) \right] X(x) \quad (1)$$

$$E_y Y(y) = \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + U_y(y) \right] Y(y) \quad (2)$$

- One thing that we can show easily is that if we combine these two equations we can get back the original 2-D Schrödinger equation.

- To show this multiply (1) by Y(y) and (2) by X(x). In both cases we can put X or Y in front of the derivative operator because the derivative is with respect to another variable.

$$E_x XY = \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U_x(x) \right] XY$$

$$+ E_y XY = \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + U_y(y) \right] XY$$

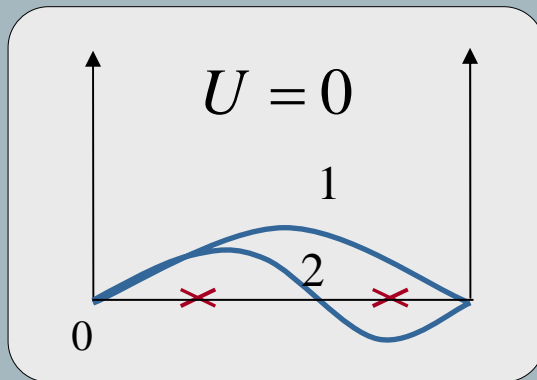
$$E\Phi = \left(-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + U \right) \Phi$$

- From above we can see that: $E = E_x + E_y$
- What we have gained is that if the potential can be separated into two parts the big 2-D problem can be broken into two 1-D problems which are a lot easier to solve.

$$10^4 \text{ by } 10^4 \Rightarrow 10^2 \text{ by } 10^2 \text{ \& } 10^2 \text{ by } 10^2$$

An example: particle in a box problem

36:31

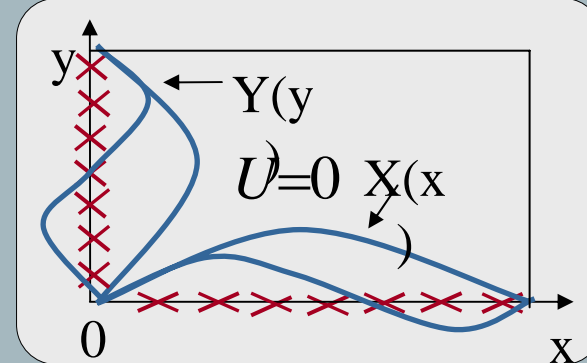


- For particle in a 1-D box we had:

$$k_v L = v\pi$$

$$E_v = \frac{\hbar^2}{2m} \left(\frac{\pi}{L} \right)^2 v^2$$

- How do we solve the problem of a particle in a 2-D box?



- What are the solutions to the problem of a particle in a 2-D box? The eigenvalues become

$$E_{xv} = \frac{\hbar^2}{2m} \left(\frac{\pi}{L} \right)^2 v^2 \quad k_v L = v\pi$$

$$E_{yn} = \frac{\hbar^2}{2m} \left(\frac{\pi}{L} \right)^2 n^2 \quad k_n L = n\pi$$

- We'll have product solutions of $X(x)$ and $Y(y)$ for eigenfunctions: $\Phi(x, y) \propto \sin k_v x \sin k_v y$

- The eigenenergies are

$$E_{v,n} = \frac{\hbar^2 \pi^2}{2mL^2} (v^2 + n^2)$$

Separation of variables

Energy Levels

43:01

- If we had solved the problem directly by setting up lattice with 100 points in each direction, we'd have a 10000 by 10000 matrix, which would give us 10000 eigenvalues. Here we have two lattices each with 100 points. That gives us a total of 200 eigenvalues. So what happened to the 10000?

- To answer this question have a look at:

$$E_{v,n} = \frac{\hbar^2 \pi^2}{2mL^2} (v^2 + n^2)$$

- The point is you can pair a single eigenvalue in the x direction to any of the 100 values in the y direction and vice versa. This gives you a total 10000 eigenvalues.
- It is important to remember that the method of separation of variables could be used only if the potential has the form:

$$U(x, y) = U_x(x) + U_y(y)$$

Energy levels in 2-D

(2,2)	—————	8E ₀
(1,2) or (2,1)	=====	5E ₀
(1,1)	—————	2E ₀

One point to notice is that with the method of separation of variables, one needs two indices to label the energy levels in 2-D and 3 indices to label the energy levels in 3-D:

Energy levels in 3-D

(122,212,221)	—————	9E ₀
(112,211,121)	=====	6E ₀
(1,1,1)	—————	3E ₀