

# Fundamentals of Nanoelectronics

ECE495 - Session 9, Sept 14, 2009

## Schrodinger Equation: Separation of Variables

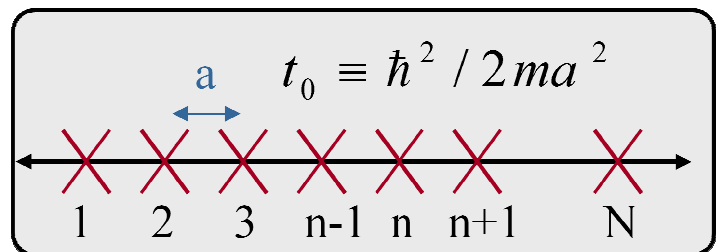
Ref: Chapter 2.2

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### Review

$$E\Psi = \frac{-\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + U(x)\Psi$$



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

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.

We 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. By Matlab on a laptop, it is easy to calculate eigenvalue for up to a 200x200 matrix.

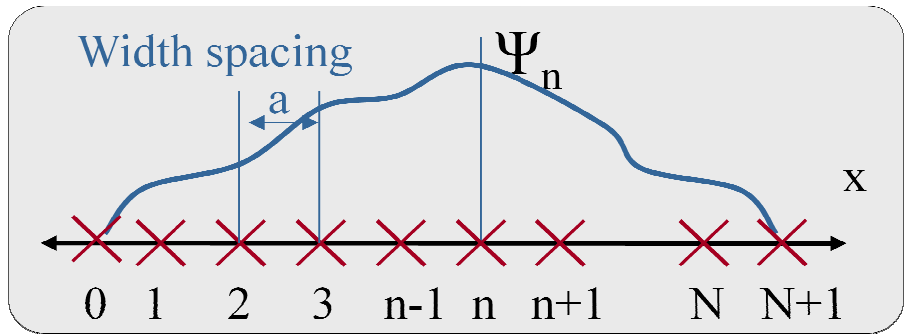
How does the answer look like analytically? For a constant potential, we know the answer analytically and that is a good bench mark for checking the numerical solution. So the analytical eigenvalues for 0 potential are depicted with numerically evaluated eigenvalues.

### Box Boundary Condition

Analytical Solution:  $\sin(kx)$  and  $kL = n\pi$  where  $L = (N+1)a$

The eigenvalues are given by:

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



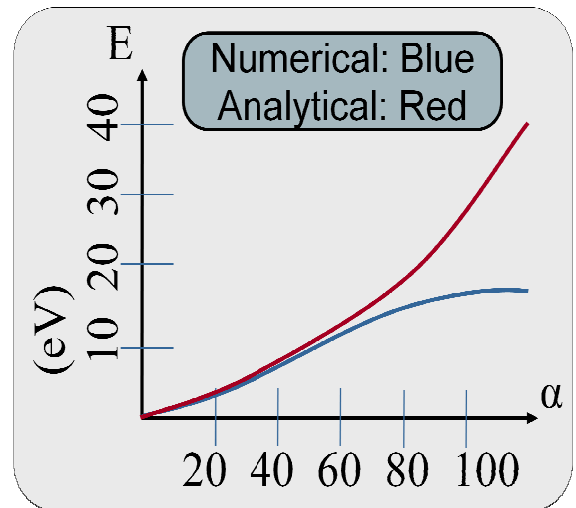
**Periodic Boundary Condition(PBC)**

The solutions are not only  $\sin(kx)$ , it depends on  $\sin(kx)\cos(kx)$  while  $kL=2\pi n$  but it is most common to use  $e^{ikx}, e^{-ikx}$  and it is mathematically more convenient.

The eigenvalues are given by:  $E_n = \frac{\hbar^2}{2m} k_n^2$  based on boundary condition  $e^{ik(x+L)} = e^{ikx}$  then

$$\Rightarrow e^{ikL} = 1 \Rightarrow kL = 2\pi n \Rightarrow k_n = \frac{2\pi}{L} n \text{ (n is an integer)}$$

putting this k in the dispersion relation  $\Rightarrow E = \frac{\hbar^2}{2m} \left(\frac{2\pi}{L}\right)^2 n^2$



In PBC, the points are in pair. These are two degenerate states which have the same energy.

The analytical eigenvalues look like a parabola whereas the numerical ones level off. 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 use the numerical solution.

**2-D Schrödinger Equation**

$$E\Psi = -\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} - \frac{\hbar^2}{2m} \frac{d^2\Psi}{dy^2} + U(x, y)\Psi$$

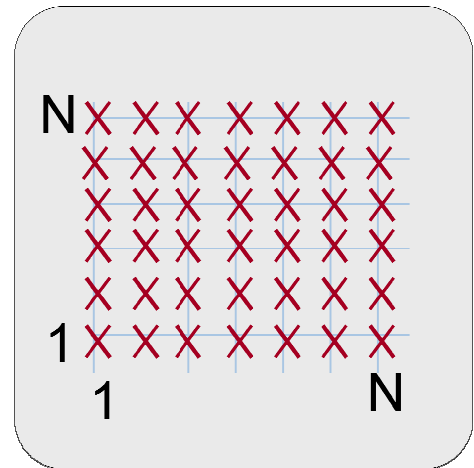
The equation can be read as:

$$E\Psi = \left( -\frac{\hbar^2}{2m} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) + U \right) \Psi . \text{ Now to solve this}$$

equation numerically, we need to make a 2-D lattice. Then we have to turn the equation into a matrix equation.

$$E \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_{10^4} \end{bmatrix} = \begin{bmatrix} & & & \\ & H & & \\ & & & \\ & & & \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_{10^4} \end{bmatrix}$$

$10^4 \times 10^4$



If  $N = 100$ , the lattice points are equal  $10000$  ( $10^4$ ) then the Hamiltonian matrix size will be  $10^4 \times 10^4$ .

This eigenvalue is very hard to calculate. One way to reduce the size of matrix is **separation of variables**.

### Separation of Variables

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:  $\Psi(x, y) = X(x) \times Y(y)$

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

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

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

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 (I) by  $Y(y)$  and (II) 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.

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

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

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$$(E_x + E_y)(XY) = \left( -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) (XY) + (U_x + U_y)(XY) \right) \Rightarrow E = E_x + E_y \text{ and } U = U_x + U_y \Rightarrow$$

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

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:  $10^4 \times 10^4 \Rightarrow 10^2 \times 10^2$  &  $10^2 \times 10^2$

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?

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

## Hydrogen Atom

We can use Separation of variables if the potential can be written as

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

If that is satisfied the one 3 dimensional problem can be written as 3 one dimensional problems which is easier to handle.

What we want to talk is how the energy levels look like for atoms. We start with the simplest of all atoms: **hydrogen atom**.

The potential that the electron sees in the hydrogen atom is  $U(x, y, z) = -\frac{q^2}{4\pi\epsilon_0\sqrt{x^2 + y^2 + z^2}}$

This potential is not separable in Cartesian coordinates but it will be in spherical coordinates which is

$$\text{as: } U(r, \Theta, \Phi) = -\frac{q^2}{4\pi\epsilon_0 r}$$

Then  $E\Psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right) \Psi$  if we assume  $\Psi(r, \theta, \varphi) = \underbrace{f(r)}_{\text{Radial}} \underbrace{Y_l^m(\theta, \varphi)}_{\text{Angular}}$

$$\Rightarrow Ef(r) = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + U(r) + \frac{l(l+1)\hbar^2}{2mr^2} \right) f(r)$$