

ECE 495N

**Fundamentals of
Nanoelectronics**

Fall 2008

**Instructor: Supriyo Datta
Purdue University**

Lecture: 10

Title: Schrödinger's Equation in 3-D

Date: September 17, 2008

Video Lectures posted at:

<https://www.nanohub.org/resources/5346/>

**Class notes taken by: Panagopoulos Georgios
Purdue University**



Schrödinger's Equation in 3-D

Lecture 10

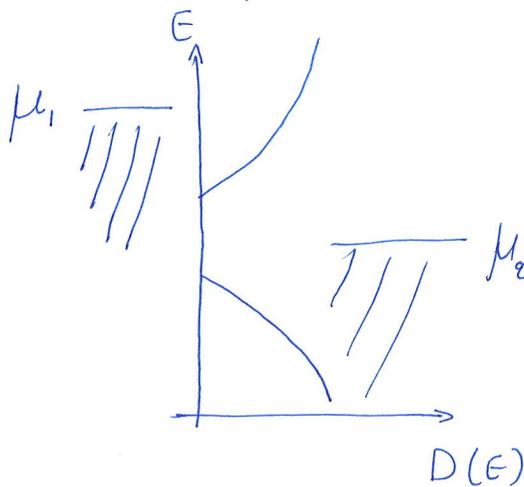
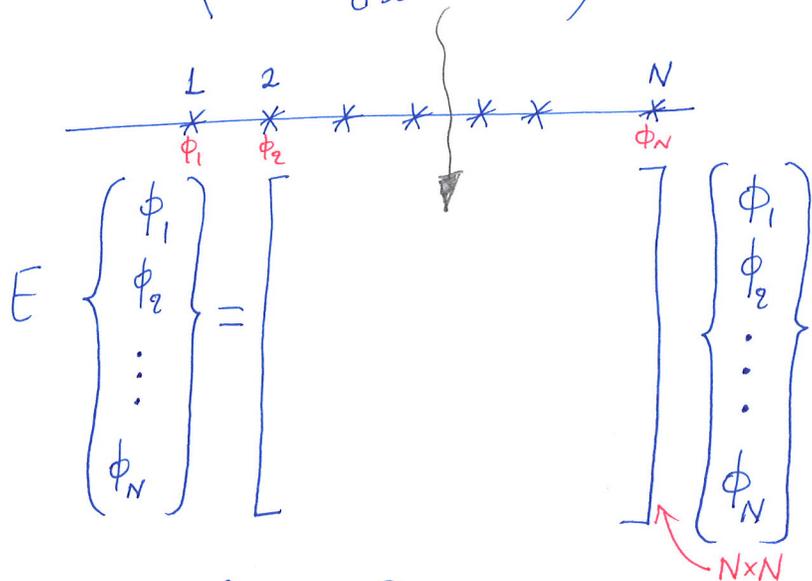
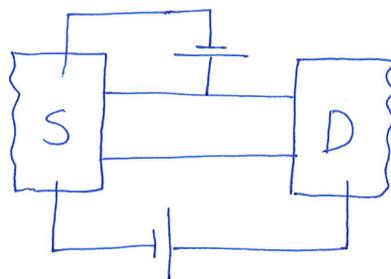
Sept 17 2008

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

Time Independent S.E.

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

1D



$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Laplace Operator

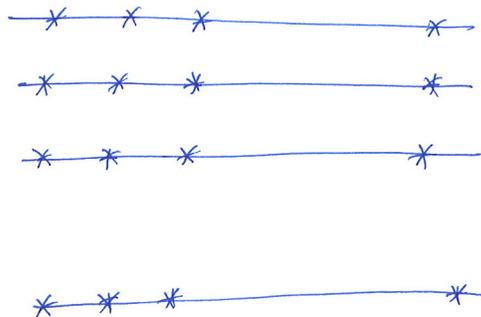
2D Schrödinger Equation

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

$$= \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \mathcal{L}(\theta, \phi)$$

where

$$\mathcal{L}(\theta, \phi) \equiv \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$



Matrix size: $N^2 \times N^2 \rightarrow$ It's going up very fast

Suppose that the potential $U(x, y)$ can be written as

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

Separation of Variables

then

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

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

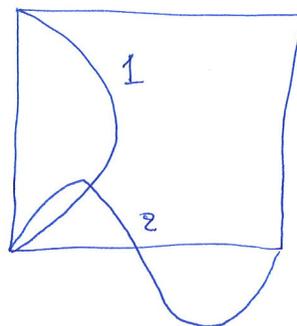
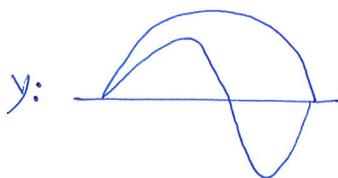
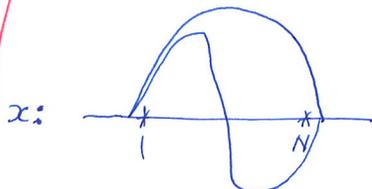
and $\phi(x, y) = f(x) \cdot g(y)$ will be the solution of the initial problem

$$(1) \xrightarrow{g(y)} E_x f(x) g(y) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U_x(x) \right] f(x) g(y) \quad (3)$$

$$(2) \xrightarrow{f(x)} E_y f(x) g(y) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dy^2} + U_y(y) \right] f(x) g(y) \quad (4)$$

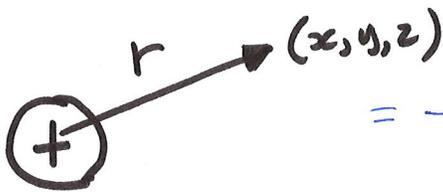
$$(3) + (4) \Rightarrow (E_x + E_y) f \cdot g = \left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) + \underbrace{U_x(x) + U_y(y)}_{U(x, y)} \right] f \cdot g$$

$$E = E_x + E_y$$



Hydrogen Atom

$$U = - \frac{Z q^2}{4\pi\epsilon_0 r} \quad \frac{H}{Z=1} = - \frac{q^2}{4\pi\epsilon_0 r}$$



$$= - \frac{q^2}{4\pi\epsilon_0} \frac{1}{\sqrt{x^2 + y^2 + z^2}}$$

It's impossible to write this function as $f(x) + g(y) + h(z)$
THAT'S A PROBLEM

Solution: spherical coordinates (spherical symmetry of the problem)

$$L(\theta, \phi) Y_l^m(\theta, \phi) = -l(l+1) Y_l^m(\theta, \phi)$$

-l, ..., +l

0, 1, 2, ...

$$Y_0^0 = 1$$

$$Y_1^0 = \cos\theta$$

$$L(\theta, \phi) \cos\theta = \frac{1}{\sin\theta} \frac{d}{d\theta} \left[\sin\theta \frac{d}{d\theta} \cos\theta \right] = \frac{1}{\cancel{\sin\theta}} \left(-2 \cancel{\sin\theta} \cos\theta \right)$$

$$= -2 \cos\theta = -1(1+1) \cos\theta$$

$$\Phi(\vec{r}) = f(r) \cdot Y_l^m(\theta, \phi)$$

$\left. \begin{array}{l} r, \theta, \phi \\ x, y, z \end{array} \right\}$

If we now substitute to the Schrodinger Equation then:

$$E f(r) Y_l^m(\theta, \phi) = - \frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) f(r) Y_l^m - \frac{\hbar^2}{2mr^2} L Y_l^m + U(r) Y_l^m$$

$$\Leftrightarrow E f(r) Y_{\ell}^m(\theta, \phi) = -\frac{\hbar^2}{2m} \left(\frac{g^2}{dr^2} + \frac{2}{r} \frac{g}{dr} \right) f(r) Y_{\ell}^m + \frac{\hbar^2}{2mr^2} f(r) \ell(\ell+1) Y_{\ell}^m + f(r) U(r) Y_{\ell}^m$$

$$E f(r) = -\frac{\hbar^2}{2m} \left(\frac{g^2}{dr^2} + \frac{2}{r} \frac{g}{dr} \right) f(r) + \left[\frac{\ell(\ell+1)\hbar^2}{2mr^2} + U(r) \right] f(r)$$

$\underbrace{\frac{\hbar^2}{4\pi\epsilon_0 r}}_{\text{Coulomb potential}}$

This is the equation that we have to solve for the radial part. This also can be simplified a little more. This equation is exactly the same as this:

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

but we have the additional term $\frac{2}{r} \cdot \frac{g}{dr}$ inside the operator.

$$f(r) = \frac{g(r)}{r} \quad \leftarrow \text{If } f(r) \text{ satisfies this equation the } g(r) \text{ will satisfy}$$

$$\Rightarrow E g(r) = \left[-\frac{\hbar^2}{2m} \frac{d}{dr^2} + U(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2} \right] g(r)$$

The last equation does not have the first derivative and it's look to the Schrodinger equation (1D)

Finally the solutions will have the form:

$$\Phi(\vec{r}) = \frac{g(r)}{r} \cdot Y_{\ell}^m(\theta, \phi)$$

and we can use it for every atom in the Periodic Table, not only for the hydrogen atom.