ECE 495N

Fundamentals of Nanoelectronics

Fall 2008

Instructor: Supriyo Datta
Purdue University

Lecture: 17
Title: Basis Functions II
Date: October 08, 2008

Video Lectures posted at:
https://www.nanohub.org/resources/5346/

Class notes taken by: Panagopoulos Georgios
Purdue University

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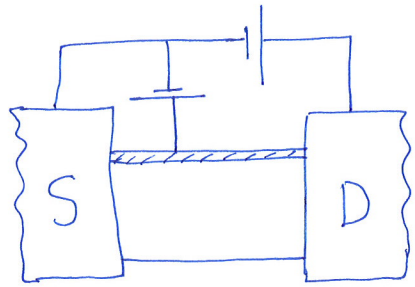
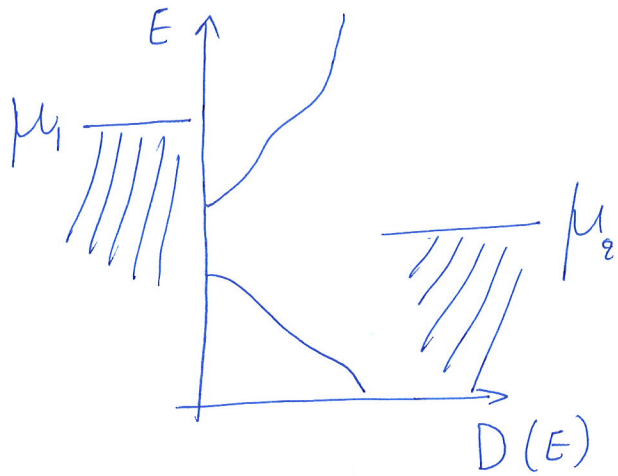
Basis Functions II

Lecture 17

Oct. 08 2008

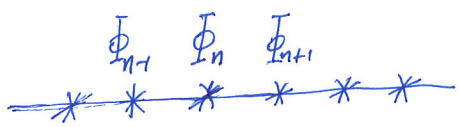


$$E\,\Phi = \underbrace{\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)}_{\equiv H_{op}}\Phi(\vec{r})$$



We Know to solve the Schröndiger Equation for the hydrogen atom and other atoms because the sferical symmetry can reduce it in 1D problem. Then we have the finite difference method to solve it.

$$E[S]\{\Phi\} = [H]\{\Phi\}$$



$$\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & \ddots & \ddots & \\ & & & -1 & 2 \end{bmatrix}$$

We need to find the density of states. But the starting point for this is the Schröndiger Equation

After we can solve this problem using eigenvalues and eigenvectors. But there is a more general method that it's widely used and based on the concept of <u>Basis Functions</u>

these functions are known

$$\Phi(\vec{r}) = \sum_m \phi_m \underbrace{u_m(\vec{r})}_{\text{Basis functions}}$$

$$H_{nm} = \int d\vec{r}\, u_n^* H_{op}\, u_m$$

$$S_{nm} = \int d\vec{r}\, u_n^* u_m$$

Major problem is the time consuming to calculate these integrals.

Gaussian Program → Gaussian Functions

Better Functions

⇓

Less Functions

⇓

Smaller problem to solve

An example is the Fourier Series, but the concept is more general

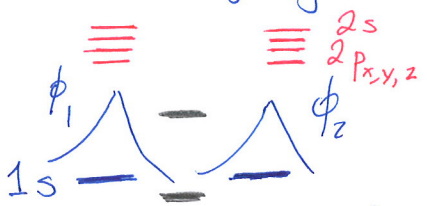
Hydrogen Atom Example
Molecule

H — H

- lattice with 100 points
- 3D structure $100 \times 100 \times 100 = 10^6$
- matrix dimentions $10^6 \times 10^6$

BUT

for one hydrogen atom:



As long as I am interesting for this region of energy and these energies are far away from 2s, 2 $P_{x,y,z}$ then using ϕ_1 and ϕ_2 I am getting good results

I am trying to find a combination of ϕ_1 and ϕ_2

- 2x2 matrix to take very good results
- Very good guess to start
- 10x10 matrix to include 2s and 2 $P_{x,y,z}$

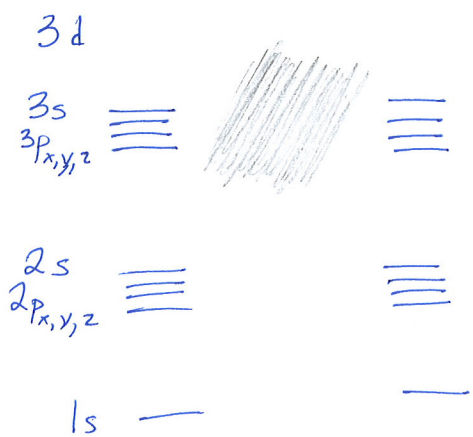
Silicon

^{14}Si

$1s^2$

$2s^2 p^6$

valence electrons $\rightarrow$ $3s^2 p^2$



four basis functions per atom

[H] : 4N x 4N

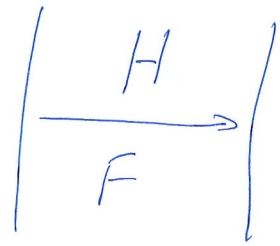
straigt forward to find the eigenvalues of this matrix but takes times

PERIODIC SOLID $\Rightarrow$ BANDSTRUCTURE

analytic solution

Hydrogen Atom – External Force

$$E\Phi = \underbrace{\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)}_{\equiv H_{op} + qF_z \leftarrow z \text{ direction}} \Phi(\vec{r})$$



	1s	2s	$2p_x$	$2p_y$	$2p_z$
1s	E_1				A
2s		E_2			B
$2p_x$			E_2		
$2p_y$				E_2	
$2p_z$	A	B			E_2

$$H_{nm} = \int d\vec{r}\, \overset{1s}{u_n^*} \underbrace{H_{op}\, \overset{1s}{u_m}}_{E_1 u_{1s}}$$

$H_{op}\, u_{1s} = E_1\, u_{1s}$

$H_{op}\, u_{2s} \quad E_2\, u_{2s}$

$$\begin{bmatrix} \text{Hermitian} \\ \text{Matrix} \\ \text{for} \\ H_{op} \\ H_{nm} = H_{mn}^* \end{bmatrix} \begin{Bmatrix} \\ \\ \\ \end{Bmatrix} = E \begin{Bmatrix} \\ \\ \\ \end{Bmatrix}$$

orthogonal eigenvectors

For $E_1 \rightarrow (1\ 0\ 0\ 0\ 0)^T$

$E_2 \rightarrow (0\ 1\ 0\ 0\ 0)^T, (0\ 0\ 1\ 0\ 0)^T, \ldots$

$$H_{nm} = \int d\vec{r}\, u_m^*\, qF_z\, u_n$$

$dx\,dy\,dz$

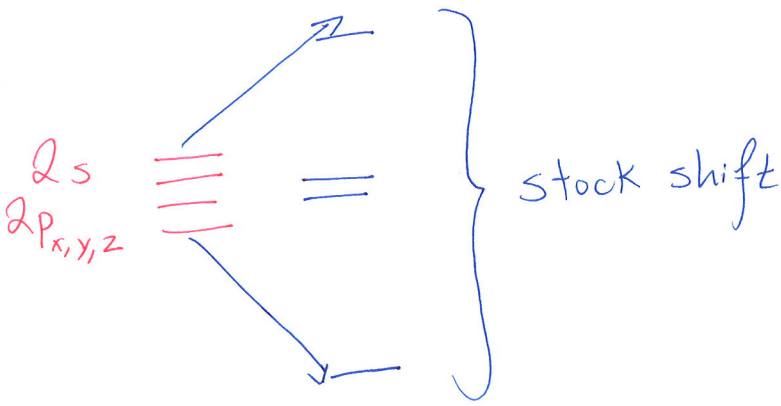
u_m^*: S(x) S(y) S(z)

F_z: S(x) S(y) A(z)

u_n: S(x) S(y) ~~S(z)~~ A(z)

Block Diagonal Matrix

	$2s$	$2p_z$	$2p_x$	$2p_y$
$2s$	E_z	B	0	0
$2p_z$	B	E_z	0	0
$2p_x$	0	0	E_q	0
$2p_y$	0	0	0	E_q



A has small effect is E_1 is very close to E_q or the field is very small