ECE 495N

Fundamentals of Nanoelectronics

Fall 2008

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Lecture: 16
Title: Basis Functions I
Date: October 06, 2008

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

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Basis Functions I

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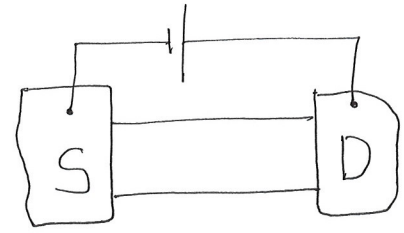
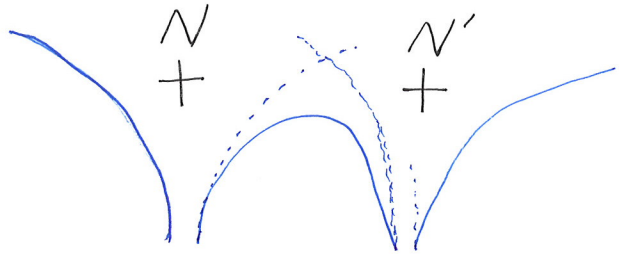
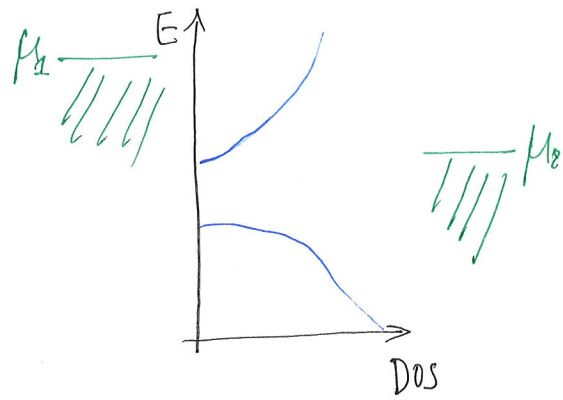
$$E\,\Phi(\vec{r}) = \overbrace{\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)}^{\equiv H_{op}}\Phi(\vec{r})$$







$$U(\vec{r}) = U_N(\vec{r}) + U_{N'}(\vec{r})$$

spherically symmetric around N point

spherically symmetric around N' point

turn to a discreate lattice

$$E\{\phi\} = [H]\{\phi\}$$

very huge matrix ⇒ difficult to solve. SOLUTION?: BASIS FUNCTIONS

Using the method of basis functions the solution is written with this way:

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

coefficients of the corresponding basis function

So finaly we are taking not $E\{\phi\} = [H]\{\phi\}$ but

$$E[S]\{\phi\} = [H]\{\phi\} \Rightarrow E\{\phi\} = \underbrace{[S]^{-1}[H]}_{H'}\{\phi\}$$

$$\Rightarrow E\{\phi\} = [H']\{\phi\}$$

Now we will try to write down expressions for both matrices H and S. The rule for them is:

$$H_{mn} = \int \underbrace{d\vec{r}}_{\equiv dxdydz} \, u_m^* \, H_{op} \, u_n \quad (I) \quad \text{and}$$

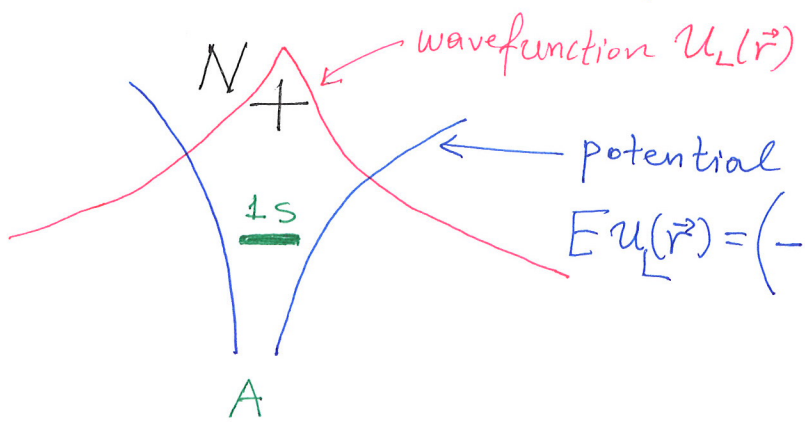
$$S_{mn} = \int d\vec{r} \, u_m^* \, u_n \quad (II)$$

1. <u>first-principles method</u>: starting from S.E. and calculate the integrals (I) and (II)

2 <u>semi-empirical approach</u>: deside for each material which are the appropriate parameters finding from experiment. There are two categories:
   (i) parameters for both H and S are given
   (ii) S matrix is ignored, that is $S = I$

$$E\,\Phi(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_N(\vec{r}) + U_{N'}(\vec{r})\right)\Phi(\vec{r})$$

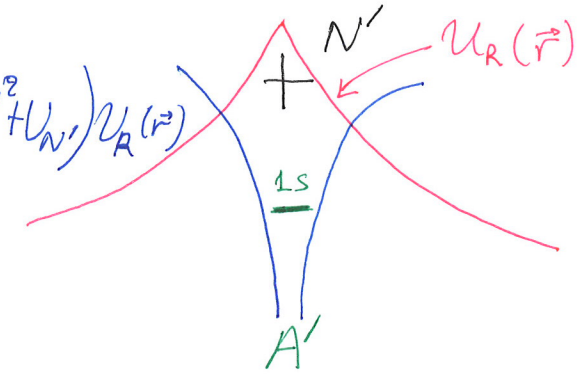
Hydrogen Atom located at A

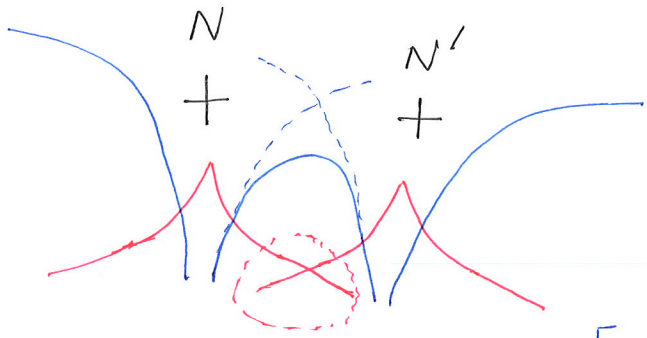


$$E\,u_L(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_N\right)u_L(\vec{r})$$

Hydrogen Atom located at A'

$$E\,u_R(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_{N'}\right)u_R(\vec{r})$$





$$\Phi(\vec{r}) = \phi_1 \overbrace{u_L}^{\text{Left } 1s} + \phi_2 \overbrace{u_R}^{\text{Right } 1s}$$

$$\Downarrow$$

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

— $S_{\underset{11}{22}} = \int d\vec{r}\, u_{\underset{R}{L}}(\vec{r})\, u_{\underset{R}{L}}(\vec{r}) = \underset{=1}{1}$

— $S_{\underset{21}{12}} = \int d\vec{r}\, u_{\underset{R}{L}}(\vec{r})\, u_{\underset{L}{R}}(\vec{r}) = S$

So, $\boxed{S = \begin{bmatrix} 1 & S \\ S & 1 \end{bmatrix}}$

— $H_{\underset{21}{11}} = \int d\vec{r}\, u_{\underset{R}{L}}(\vec{r}) \left[\overbrace{-\frac{\hbar^2}{2m}\nabla^2 + U_N}^{E_1} + U_{N'} \right] u_L(\vec{r})$

$$= \underbrace{\overbrace{\int d\vec{r}\, u_{\underset{R}{L}}(\vec{r})\, E_1\, u_L(\vec{r})}^{E_1 S}}_{= E_1} + \underbrace{\overbrace{\int d\vec{r}\, u_{\underset{R}{L}}(\vec{r})\, U_{N'}\, u_L}^{\equiv b}}_{\equiv \alpha}$$

So, $H = \begin{bmatrix} E_1 + \alpha & E_1 S + b \\ E_1 S + b & E_1 + \alpha \end{bmatrix}$ where $S \equiv \int d\vec{r}\, u_L u_R$

$\alpha \equiv \int d\vec{r}\, u_L U_{N'} u_R$

$b \equiv \int d\vec{r}\, u_R U_{N'} u_L$

$$E\{\phi\} = \begin{bmatrix} 1 & s \\ s & 1 \end{bmatrix}^{-1} \cdot \begin{bmatrix} E_1 + \alpha & E_1 s + b \\ E_1 s + b & E_1 + a \end{bmatrix} \{\phi\}$$

if s is very small then $S \cong I$ and $S^{-1} \cong I$

$E_1 + \dfrac{\alpha + b}{1+s}$, one eigenvalue with eigenvec $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$E_1 + \dfrac{\alpha - b}{1-s}$, second eigenvalue with eigenvector $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

— ← anti-bonding level

E_1 — — E_1

closer

— ← bonding level

NOTE

if $\begin{bmatrix} A & B \\ B & A \end{bmatrix}$ then it has eigenvalues $A+B$ and $A-B$ (with corresponding eigenvectors: $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$)