LECTURE #23

Note Title 3/5/2010

MON	MARCH	15	PROBLEMS
WED	"	17	NO CLASS (MARCH MEETING)
FRI	"	19	

CHAP 17

HARTREE

$$\Psi_H(r_1 s_1, \ldots r_N, s_N) = \psi_1(r_1 s_1) \times \psi_2(r_2, s_2) \cdots \times \psi_N(r_N s_N)$$

ANSATZ

$$\langle \Psi_H | H_{TOT} | \Psi_H \rangle = E_{TOT}\left[\{ \psi_i^*, \psi_i \} \right]$$

FUNCTIONAL DEPENDENCE

$$N = \sum_i \int dr_i \, |\psi_i(r_i)|^2$$

LAGRANGE MULTIPLIER

$$F = E_{TOT} - \mu N$$

$$\frac{\delta F[\{\psi_i^*, \psi_i\}]}{\delta \psi_j^*} = 0 \Rightarrow \boxed{\frac{\delta E_{TOT}[\{\psi_i^* \psi_i\}]}{\partial \psi_j^*} = \mu \psi_j}$$

PLAYS THE ROLE OF SINGLE ELECTRON QUASI-PARTICLE ENERGY.

$$\Psi_{HF}(r_1 s_1, \dots r_N s_N) = \frac{DET}{\sqrt{N!}} \begin{bmatrix} \psi_1(r_1 s_1) & \psi_1(r_2 s_2) & \cdots & \psi_1(r_N s_N) \\ \psi_2(r_1 s_1) & \psi_2(r_2 s_2) & \cdots & \\ \vdots & \vdots & & \end{bmatrix}$$

$$\langle \Psi_{HF} | H_{TOT} | \Psi_{HF} \rangle = E_{TOT}^{HF}[\{\psi_i^* \psi_i\}]$$

$$\underbrace{\frac{\delta E^{HF}_{TOT}[\{\psi_i^* \psi_i\}]}{\delta \psi_J^*}} = \mu \psi_J$$

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + V^{ION}\right)\psi_J + \left(e^2 \int dr' \, \sum_i{}' \frac{|\psi_i(r')|^2}{|r-r'|}\right)\psi_J(r)$$

$V^{HARTREE}(r)$ $\rho(r')$ $\psi_J(r)$

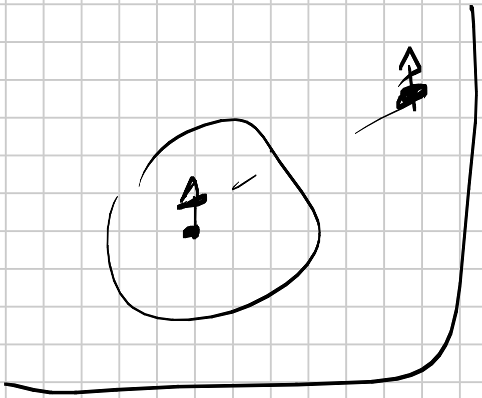
$$\underbrace{- e^2 \int dr' \, \sum_i{}' \frac{\psi_i^*(r')\,\psi_J(r')\,\psi_i(r)}{|r-r'|} \, \delta_{s_i, s_J}} = \mu \psi_J(r)$$

r r'

EXCHANGE- POTENTIAL

$$\int dr' \, V_X(r, r') \, \psi_J(r')$$

NON LOCAL POTENTIAL AND SPIN DEPENDENT POTENTIAL



HARTREE – FOCK FOR FREE ELECTRONS

$$\psi_k(r,s) = \frac{e^{ikr}}{\sqrt{V}}\,\alpha(s) \qquad \alpha(s) = \begin{cases} 1 & s = +\frac{1}{2} \\ 0 & s = -\frac{1}{2} \end{cases}$$

$$\psi_k \qquad \frac{e^{ikr}}{\sqrt{V}}\,\beta(s) \qquad \beta(s) = \begin{cases} 1 & s = \downarrow \\ 0 & s = \uparrow \end{cases}$$

$$T\psi_i + \underbrace{\left(\cancel{V_{ION}} + \cancel{V_{HARTREE}}\right)}\psi_i + E_x[\psi_i] = \mu\,\psi_i$$

PLANE WAVES

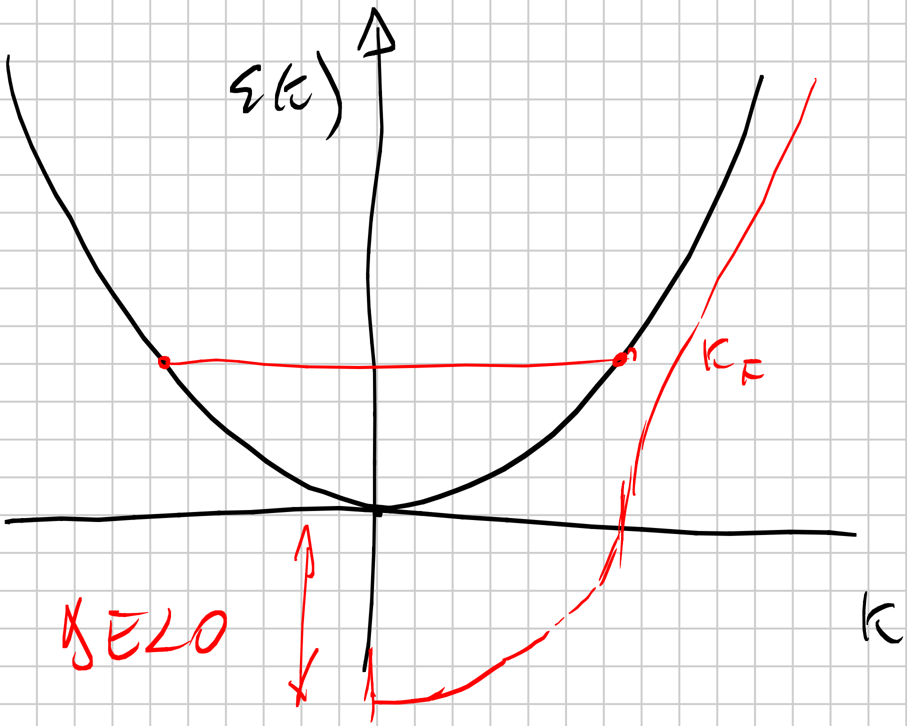
$$E_x\left[\psi_i = \frac{e^{ikr}}{\sqrt{V}}\alpha\right] = -e^2 \int dr' \sum_{J \to k'}{}' \frac{\psi_J^*(r')\,\psi_J(r)}{|r-r'|}\,\psi_i(r') =$$

$$= -\frac{e^2}{V^{3/2}} \int dr' \sum_{k'<k_F} \frac{e^{-ik'\cdot r'}\, e^{ik'\cdot r}}{|r-r'|} \underbrace{e^{ik\cdot r'}\, e^{ik\cdot r}}\, e^{-ik\cdot r}$$

$$= -\frac{1}{V} \sum_{k'<k_F} \underbrace{\int dr' \frac{e^2}{|r-r'|} e^{i(k-k')\cdot(r-r')}}_{\tilde{V}_{COULOMB}(k-k')} \cdot \frac{e^{ikr}}{\sqrt{V}}$$

$$\frac{1}{V} \sum_{k<k_F} \to \int_{|k|<k_F} \frac{d^3k}{(2\pi)^3}$$

$$\varepsilon^{HF}(k) = \frac{\hbar^2 k^2}{2m} - \int_{|k'|<|k_F|} \frac{d^3k'}{(2\pi)^3} \tilde{V}_{COULOMB}(k-k') = \frac{\hbar^2 k^2}{2m} - F(k)$$



ε(k)
k
k_F
δE<0