LECTURE # 26

Note Title 3/25/2009

LAST 10 MINUTES
SURVEY ON
<u>INTERNET</u>

Quantum Hall effect
Graphene
Carbon Nanotubes
Excitons and exciton-polaritons
Mesoscopic physics and single electronics
Spectroscopy of quantum dots and quantum wires
Spintronics in metals/semiconductors
Neutron and electron scattering in solids
Solid state devices for quantum information processing
Magnetic properties of solids
Superconductivity

$$H^{TOT} = \sum_i H_i + \frac{1}{2} \sum_{iJ} \frac{e^2}{|\vec{r}_i - \vec{r}_J|}$$

HARTREE-FOCK $\Rightarrow$ ANSATZ FOR $\Psi(r_1 s_1 \ldots r_N s_N)$

$$\Psi^{HF} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(r_1 s_1) & \psi_1(r_2 s_2) & \cdots \\ \psi_2(r_1 s_1) & \cdots & \cdots \\ \vdots & \vdots & \end{vmatrix}$$

ψ_i ARE SINGLE PARTICLE WAVE FUNCTIONS

GOAL: $\rightarrow$ EFFECTIVE SINGLE-PARTICLE SCHR. EQ

FOR ψ_i

$$\langle \Psi^{HF} | H^{TOT} | \Psi^{HF} \rangle = E^{HF}[\{\psi_i^*, \psi_i\}]$$

$$E^{HF} - \mu \left[\sum_i^N |\langle \psi_i | \psi_i \rangle|^2 \right] = \text{CONSTANT}$$

$$\boxed{\frac{\delta E^{HF}}{\delta \psi_i^*} = \mu \psi_i} \rightarrow \text{SCHR. EQ.}$$

Kinetic E

$$\boxed{T[\psi_i] + V^{ION}_{(r)} \psi_i(r) + V^{HARTREE}_{(r)} \psi_i(r) + \underline{\text{EXCHANGE}} = \mu \psi_i}$$

$$V^{HARTREE}_{(r)} = e^2 \int \frac{\rho(r')}{|r - r'|} dr'$$

$$\text{EXCHANGE} = -e^2 \underbrace{\int dr'\, V^{x}(r,r')\, \psi_i(r')}_{\text{NON LOCAL POTENTIAL}}$$

$$V^{x}(r,r') = \sum_{\substack{J\neq i \\ \text{OCCUPIED}}} \frac{\psi_J^*(r')\,\psi_J(r)}{|r-r'|}\,\delta_{s_i,s_J}$$

HARTREE-FOCK FOR FREE ELECTRONS

$$\psi_i(r,s) = \frac{e^{ik\cdot r}}{\sqrt{V}} \times \text{SPIN} \rightarrow \frac{e^{ik\cdot r}}{\sqrt{V}}\alpha(s) \qquad \alpha(s) = \begin{cases} 1 & s=\uparrow \\ 0 & s=\downarrow \end{cases}$$

$$\frac{e^{ik\cdot r}}{\sqrt{S}}\beta(s) \qquad \beta(s) = \begin{cases} 0 & s=\uparrow \\ 1 & s=\downarrow \end{cases}$$

$$\psi_i = \frac{e^{ik\cdot r}}{\sqrt{V}}\alpha$$

$$T[\psi_i] + \cancel{V^{ION}\psi_i + V^{HARTREE}}\psi_i + E_{XCH}[\psi_i] = \underline{\mu}\,\psi_i$$

$V^{ION} \sim$ HOMOGENEOUS + CHARGES

SYSTEM NEUTRAL

$V^{ION} \sim -V^{HARTREE} \Rightarrow E_{XCH}[\psi_i]$ IS THE ONLY IMPORTANT CORRECTION

$$E_{XCH}\left[\psi_i = \frac{e^{ik\cdot r}}{\sqrt{V}}\alpha\right] = -e^2\int dr' \sum_{j\neq i} \delta_{s_i s_j} \frac{\psi_j^*(r')\,\psi_j(r)}{|r-r'|}\psi_i(r')$$

$$\psi_j \to \frac{e^{ik'\cdot r}}{\sqrt{V}}\alpha$$

$$E_{XCH} = -\frac{e^2}{V^{3/2}}\int dr' \sum_{k'<k_F} \frac{\overset{x}{e^{-i\vec{k}'\cdot\vec{r}'}}\,\overset{y}{e^{ik'\cdot r}}}{|\vec{r}-\vec{r}'|}\underset{x}{e^{ik\cdot r'}} \quad \underbrace{\cdot e^{ik\cdot r}\cdot e^{-ik\cdot r}}_{x}$$

$$E_{XCH} = -\frac{1}{V} \sum_{k' < K_F} \boxed{\int dr' \, \frac{e^2 \, e^{i(\vec{k}-\vec{k}')\cdot(\vec{r}-\vec{r}')}}{|\vec{r}-\vec{r}'|}} \frac{e^{i k \cdot r}}{\sqrt{V}}$$

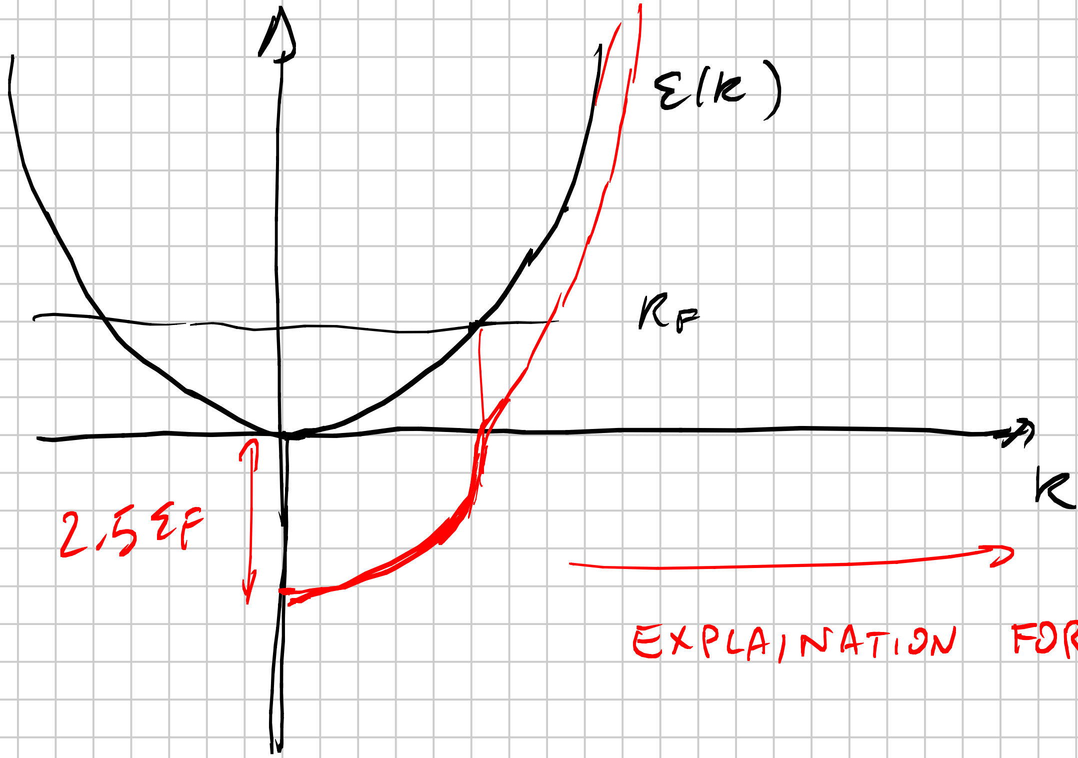
FOURIER TRANSF
OF COULOMB

$$= V_{COULOMB}(\vec{k}-\vec{k}')$$

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

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} - \int_{|k'|<k_F} \frac{d^3k'}{(2\pi)^3} V_{COULOMB}(\vec{k}-\vec{k}')$$

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} - F(k)$$



CAN BE SEEN AS EXPLAINATION FOR THE "STABILITY" OF METALS