LECTURE # 29

Note Title 4/1/2009

~~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

INTRODUCTION TO DENSITY FUNCTIONAL THEORY

HARTREE - FOCK

$E^{HF}[\{\psi_i \psi_i^*\}]$ → FUNCTIONAL

$$\frac{\delta E^{HF}}{\delta \psi_i^*} = \mu \psi_i \Rightarrow$$ EFFECTIVE 1 PARTICLE SCHR EQ

HARTREE + EXCHANGE

DENSITY FUNCTIONAL :

$E[n(r)]$ TOT ENERGY AS FUNCTIONAL OF

$n(r)$ (ELECTONIC DENSITY)

$\frac{\delta E[n(r)]}{\delta n}$ → VARIATION ON $n(r)$

N ELECTRONS

$$H^{TOT} = T + V^{ION} + H^{(2)}$$

$$T = \sum_{i}^{N} \frac{p_i^2}{2m}$$

$$H^{(2)} = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|}$$

ALWAYS THE SAME FOR ATOMS, MOLECULES, CRYSTALS

- ALL PROPERTIES OF N-ELECTRON SYSTEMS ARE UNIQUELY DETERMINED BY $V^{ION} = v(r)$
- ANY OBSERVABLE $O[v(r)]$ IS A FUNCTIONAL OF $v(r)$
- IN PARTICULAR, TOTAL DENSITY

$$\hat{\rho} = \sum_i \delta(r - r_i)$$

$$\langle \Psi^{MANY-BODY} | \hat{\rho} | \Psi^{MANY-BODY} \rangle = n(r)$$

$n[v(u)]$: DENSITY IS A FUNCTIONAL OF $v(u)$

DENSITY FUNCTIONAL THEORY BASED ON

(I) HOHENBERG - KOHN THEOREM:

$v(n)$ IS UNIQUELY DETERMINED BY $n(u)$ i.e. $v[n(u)]$

REDUCTIO AD ABSURDUM:

IF STATEMENT OF THEOREM IS NOT TRUE THEN

$\exists\, v(n)$ AND $v'(u)$ THAT WILL GIVE THE SAME $n(u)$

$v(u) \neq v'(u)$

$\downarrow$ ψ E_0

$\downarrow$ ψ', E_0'

THEN

$$E_0 = \langle \psi | T + v + H^{(2)} | \psi \rangle < \langle \psi' | T + v + H^{(2)} | \psi' \rangle = \quad +v' - v$$

$$\langle \psi' | T + v' + H^2 + v - v' | \psi' \rangle = E_0' + \langle \psi' | v - v' | \psi' \rangle$$

$$E_0 - E_0' < \int dr \; n(r) \, (v(r) - v'(r)) \qquad (a)$$

$$0$$

$$E_0' = \langle \psi' | T + v' + H^{(2)} | \psi' \rangle < \langle \psi | T + v' + H^{(2)} | \psi \rangle \quad +v - v$$

$$\Rightarrow E_0 - E_0' > \int dr \; n(r) \, (v(r) - v'(r)) \qquad (b)$$

(a) + (b) ARE TRUE ONLY IF $v(r) = v'(r)$

ABSURDUM

$$n(r) = \langle \psi' | \hat{\rho} | \psi' \rangle = \langle \psi | \rho | \psi \rangle$$

$E[v(r)] \rightarrow E[v[n]] \Rightarrow$

$E[n(r)] \Rightarrow$ GROUND STATE MANY BODY ENERGY

UNIQUECY DETERMINED BY $n(r)$

$$E[n(r)] = \int dr\, v(r)\, n(r) + F[n(r)]$$

F → KINETIC TERM + COULOMB

VARIATIONAL METHOD

$$\delta\left(E[n] - \mu \int dr\, n(r)\right) = 0$$

$$\frac{\delta E[n]}{\delta n} = \mu$$

DENSITY FUNCTIONAL EQUATION

$$\frac{\delta F[n]}{\delta n} + v(r) = \mu \qquad \leftarrow$$

HOW DO WE WRITE $F[n]$?

$F[n]$ FOR A NON-INTERACTING SYSTEM

$H^{(2)} = 0$ NO e-e COULOMB

$E_S[n] = \int dr\, v(r)\, n(r) + T_S[n(r)]$

$S \rightarrow$ NON-INTERACTING

$$\frac{\delta T_s[n]}{\delta n} + v(u) = \mu$$

(A) FROM DENSITY FUNCTIONAL THEORY

EQUIVALENT TO:

$$n(u) = \sum_j \vartheta(\mu - \varepsilon_j) |\phi_j(u)|^2$$

$$\left[\frac{-\hbar^2 \nabla^2}{2m} + v(u)\right] \phi_j(u) = \varepsilon_j \phi_j(u)$$

(B) FROM SCHROED. EQ.

THIS LINK BETWEEN SE AND DFT IS USED IN THE

(C) KOHN - SHAM EQUATIONS

$$E[n(r)] = \underbrace{T_s[n]}_{(A)} + \int dr\, v(r)\, n(r) + \underbrace{\frac{1}{2}\int dr\, dr' \frac{n(r)\, n(r')}{|r - r'|}}_{(B)} + \underbrace{E_{xc}[n]}_{(C)}$$

(A) $T_s[n]$ KINETIC ENERGY OF NON-INTERACTING SYSTEM WITH SAME DENSITY $n(r)$

(B) HARTREE

(C) EXCHANGE - CORRELATION

$$\frac{\delta E}{\delta n} = \mu$$

$$\frac{\delta T_s}{\delta n} + v(r) + \underbrace{\int dr' \frac{n(r')}{|r-r'|}}_{v^H(r)} + \underbrace{\frac{\delta E_{xc}[n]}{\delta n}}_{v^{xc}(r)} = \mu$$

EQUIVALENT TO

KOHN SHAM ORBITALS

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + v^{EFF}(r)\right] \phi_j(r) = \varepsilon_j \phi_j(r)$$

$$v^{EFF} = v(r) + v^H(r) + v^{xc}(r)$$

$$n(r) = \sum_j \theta(\mu - \varepsilon_j) |\phi_j(r)|^2$$

- SOLVED SELF-CONSISTENTLY
- BEYOND HF → DEPENDS ON WHAT IS IN $v^{xc}(r)$

$v^{xc}(r) \rightarrow E_{xc}[n]$

$E_{xc}[n]$ TAKEN OFTEN FROM

HOMOGENEOUS ELECTRON GAS

GOOD GUESS

GREEN'S FUNCTIONS

QUANTUM MONTECARLO

→ E_{xc}

LOCAL DENSITY APPROX LDA

DFT-LDA

$$E_{xc}[n] = \int d\vec{r}\; n(\vec{r})\, \varepsilon_{xc}(n(\vec{r}))$$

LOCALITY

YOU COULD USE HOMEGAS + HF FOR THE EXCHANGE

$$\frac{E^{HF}}{N} = \left(\frac{2.21}{(r_s/a_0)^2} - \frac{0.916}{(r_s/a_B)} \right)$$

KINETIC

EXCHANGE

$$\varepsilon_x(n)$$

$$\frac{4\pi}{3} r_s^3 = \frac{1}{n}$$

$$\varepsilon_x[n] = -\alpha n^{1/3}$$

$$E^{xc}[n] = -\alpha \int dr\, n(r)\, n^{1/3}(r)$$

$$v^x(r) \sim -\alpha \frac{4}{3} n^{1/3}(r)$$