LECTURE #25

Note Title 3/22/2010

HARTREE-FOCK MEAN FIELD

CORRELATION EFFECTS = EFFECTS BEYOND MEAN FIELD

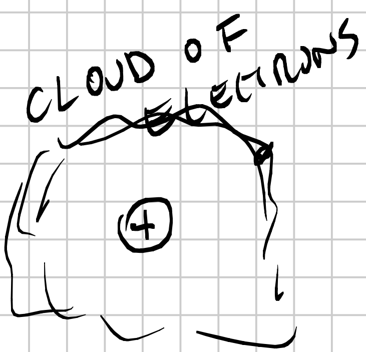
SCREENING

$\cdot\, e$ → TEST CHARGE

$$\phi^{ext} = -\frac{e^2}{r}$$

$\oplus$

IN THE PRESENCE OF ELECTRON GAS



$\cdot$ TEST CHARGE

$$\phi(r) \neq \underline{\underline{\phi^{ext}}}$$

$$\rho(\vec{r}) = \rho^{ext}(\vec{r}) + \rho^{INDUCED}(r)$$

D DISPLACEMENT VECTOR

$$\nabla \cdot D = 4\pi \rho^{ext}$$

$$\vec{D} = \overleftrightarrow{\varepsilon} \cdot \vec{E} \rightarrow \phi$$

$\rightarrow$ ASSUME ISOTROPIC SYSTEM

$$\varepsilon_{ij} = \varepsilon \delta_{ij}$$

$$\downarrow$$

$$\phi^{ext}$$

$$\phi^{ext}(\vec{r}) = \int dr' \, \varepsilon(r-r') \, \phi(r')$$

$\rightarrow$ NON LOCAL DEPENDENCE

$\varepsilon(r-r') \rightarrow$ TRANSLATIONAL INVARIANCE

$$\downarrow \text{FT}$$

$$\boxed{\phi^{ext}(q) = \varepsilon(q) \, \phi(q)}$$

$$\phi(q) = \frac{\phi^{ext}(q)}{\varepsilon(q)}$$

$$\int f(x) \, g(y-x) \, dx$$

$$\downarrow \text{FT}$$

$$\tilde{f}(q) \, \tilde{g}(q)$$

$\varepsilon(q) = \varepsilon_0$ CONSTANT IN q- SPACE

$\downarrow$

$\varepsilon(r - r') = \varepsilon_0 \, \delta(r - r')$

$$\phi^{ext} = -\frac{e^2}{r} \rightarrow \phi = -\frac{e^2}{\varepsilon_0 r}$$

$$\phi^{ext}(q) = \frac{4\pi e^2}{|q|^2} \rightarrow \frac{4\pi e^2}{\varepsilon_0 |q|^2}$$

$\vec{P} = \chi \vec{E}$

$$\boxed{\varepsilon(q) \overset{?}{\longleftrightarrow} \chi(q)}$$

$\downarrow$

$\rho^{INDUCED}(q) = \chi(q) \, \phi(q)$

$$-\nabla^2\phi(r) = 4\pi\rho(r) \qquad \rho(r) = \rho^{ext} + \rho^{IND}$$

$$-\nabla^2\phi^{ext}(r) = 4\pi\rho^{ext}(r)$$

$\downarrow$ FT

$$\rho^{IND}(q) \to \chi(q)\,\phi(q)$$

$$q^2\phi(q) = 4\pi\rho^{ext}(q) + 4\pi\rho^{IND}(q)$$

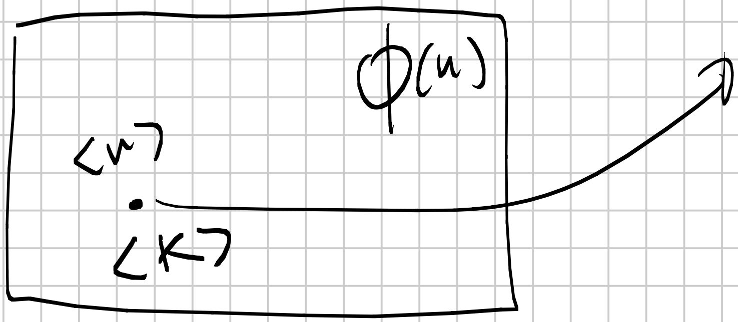
$$q^2\left(\phi(q) - \phi^{ext}(q)\right) = 4\pi\chi(q)\,\phi(q)$$

$$q^2\left(\cancel{\phi(q)} - \varepsilon(q)\,\cancel{\phi(q)}\right) = 4\pi\chi(q)\,\cancel{\phi(q)}$$

$$\varepsilon(q) = 1 - \frac{4\pi}{q^2}\chi(q) \to 1 - \frac{4\pi}{q^2}\frac{\rho^{IND}(q)}{\phi(q)}$$

THOMAS - FERMI APPROXIMATION

$\phi(r)$ WEAK DEPENDENCE ON r



ELECTRON AT $\langle r\rangle$

WITH AVERAGE $\langle K\rangle$

AND ENERGY $\varepsilon(k) = \dfrac{\hbar^2\langle K\rangle^2}{2m}$

$\phi(r) = 0$

$$n(\mu) = 2\int \frac{d^3k}{(2\pi)^3}\,\frac{1}{e^{\beta(\varepsilon(k)-\mu)}+1}$$

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

ADD $\phi(r)$

$$\varepsilon(r,k) \longrightarrow \frac{\hbar^2 k^2}{2m} - e\phi(r) \rightarrow$$

MAKES SENSE BECAUSE OF SEMICLASSICAL APPROX

$$n'(r,\mu) = 2\int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta\left(\frac{\hbar^2k^2}{2m} - \underbrace{e\phi(r) - \mu}_{}\right)}}$$

$$\mu'(r) = \mu + e\phi(r)$$

$$n' = n(\mu + e\phi(r))$$

$$\rho^{\text{INDUCED}}(r) = -e\left[n(\mu + e\phi(r)) - n(\mu)\right]$$

$$e\phi(r) \ll \mu$$

$$\rho^{IND}(r) = -e \frac{dn}{d\mu} e\phi(r)$$

$$\varepsilon^{TF}(q) = 1 - \frac{4\pi}{q^2}\frac{\rho^{IND}(q)}{\phi(q)} = 1 - \frac{4\pi}{q^2}\left(-e^2 \frac{dn}{d\mu}\right) =$$

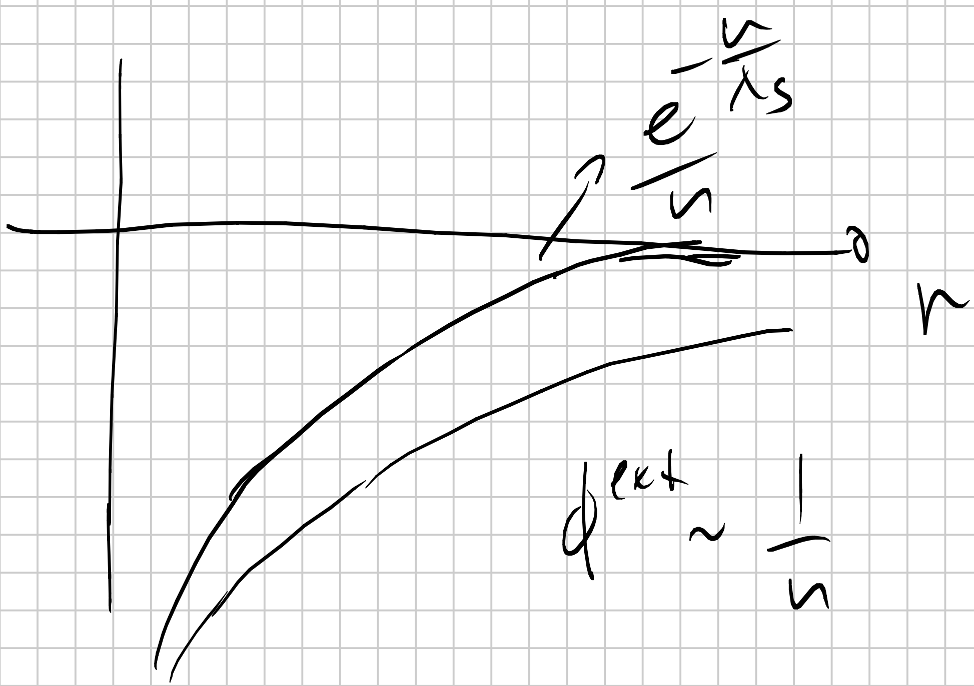
$$1 + \frac{\left(4\pi e^2 \frac{dn}{d\mu}\right)}{q^2} = 1 + \frac{q_s^2}{q^2}$$

q SCREENING

$$\phi^{ext}(q) = \frac{e^2 4\pi}{q^2} \rightarrow \phi(q) = \frac{\phi^{ext}(q)}{\varepsilon(q)} = \frac{4\pi e^2}{q^2 + q_s^2}$$

$$\phi^{ext}(r) = \frac{e^2}{r}$$

$$\phi^{TF}(r) = \frac{e^2}{r} e^{-q_s r} \rightarrow \text{YUKAWA POTENTIAL}$$



$$q_s = 4\pi e^2 \frac{dn}{d\mu}$$

$T = 0$

$$n = \int_0^\infty d\varepsilon \; g(\varepsilon) \, \theta(\mu - \varepsilon)$$

$$\frac{dn}{d\mu} = \int d\varepsilon \; g(\varepsilon) \frac{d}{d\mu} \theta(\mu - \varepsilon) = \int d\varepsilon \; g(\varepsilon) \, \delta(\varepsilon - \mu)$$

$$= g(\mu)$$

a_B = BOHR RADIUS

$$q_s \propto k_F \left(\frac{r_s}{a_B}\right)^{1/2} \sim \left(\frac{a_B}{r_s}\right)^{1/2}$$