LECTURE # 28

Note Title 3/30/2009

HARTREE - FOCK MEAN FIELD

CORRELATION (BEYOND MEAN FIELD)

SCREENING

VACUUM:

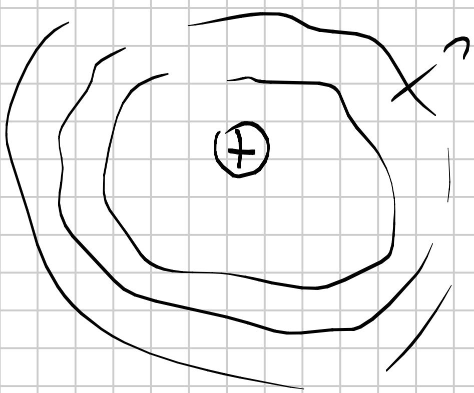
$\oplus$

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

COULOMB SEEN BY A "TEST" e

IN THE PRESENCE OF ELECTRON GAS:

e "CLOUD"

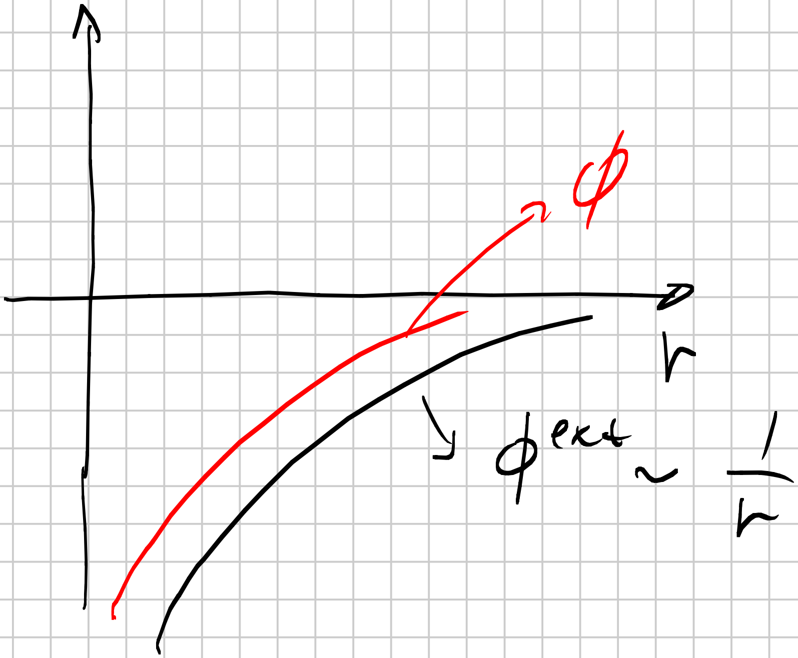


TEST CHARGE

MEASURE $\phi \neq \phi^{ext}$

TOTAL CHARGE

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



D

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

$$\vec{D} = \vec{\varepsilon} \cdot \vec{E}$$

$$\int f(x)\, g(y-x)\, dx \xrightarrow{FT} \tilde{f}(q)\, \tilde{g}(q)$$

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

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

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

TRIVIAL CASE $\quad \varepsilon(q) \sim \varepsilon_0$

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

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

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

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

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

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

FIND LINK BETWEEN $\varepsilon(q)$ AND $\chi(q)$

POISSON EQUATION

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

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

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

$$q^2 \phi^{ext}(q) = 4\pi\rho^{ext}(q) \qquad \phi^{ext}(q) = \varepsilon(q)\,\phi(q)$$

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

$$q^2\left(1 - \varepsilon(q)\right)\cancel{\phi(q)} = 4\pi\chi(q)\,\cancel{\phi(q)}$$

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

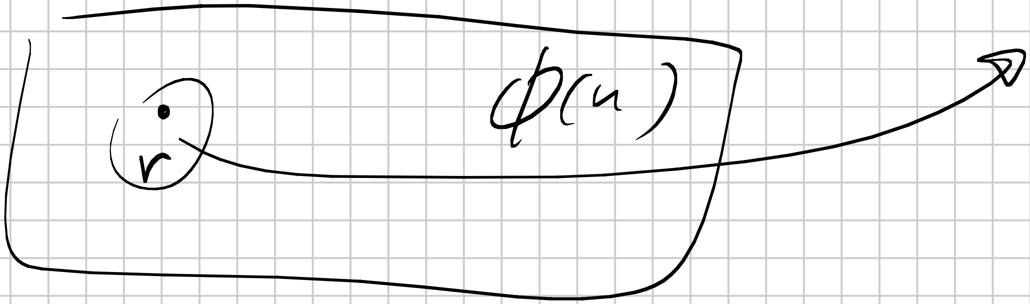
$$\boxed{\varepsilon(q) = 1 - \frac{4\pi}{q^2}\frac{\rho^{IND}(q)}{\phi(q)}}$$

THOMAS - FERMI APPROXIMATION

ASSUMPTION $\phi(r)$ WEAK DEPENDENCE ON r

SOMMERFELD MODEL

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



ELECTRON AT r
WITH AVERAGE $\langle k \rangle$
AND ENERGY $\varepsilon^0(k) = \frac{\hbar^2 k^2}{2m}$
(WITH NO ϕ)

ADD $\phi(r)$

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

$$n'(r) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta(\varepsilon^0(k) - e\phi(r) - \mu)}+1} =$$

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

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

$e\phi(r) \ll \mu \Rightarrow$ EXPAND $\rho^{\text{IND}}(r)$

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

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

$$1 + \frac{4\pi e^2 \frac{dn}{d\mu} \to q_s^2}{q^2} = 1 + \frac{q_s^2}{q^2}$$

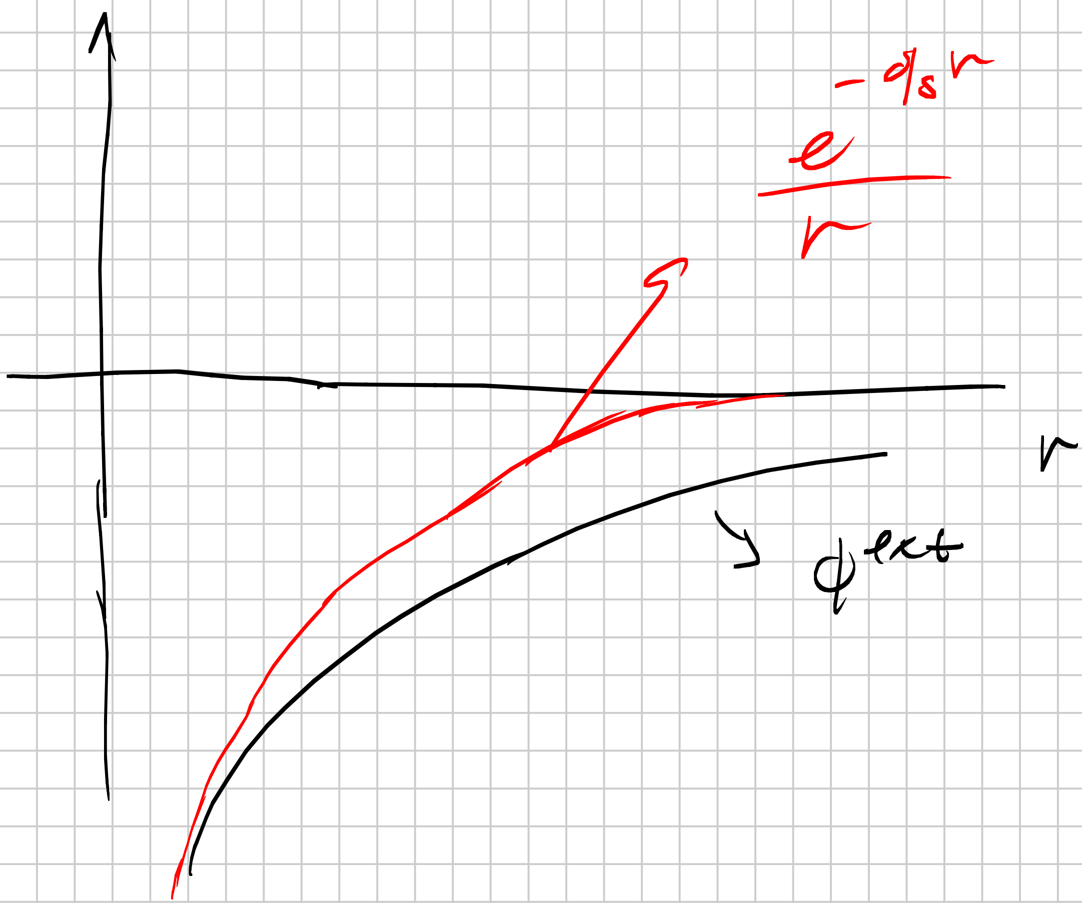
$$\phi^{\text{ext}}(q) = \frac{e^2 4\pi}{q^2} \Rightarrow \phi(q) = \frac{e^2 4\pi}{q^2 \varepsilon(q)} = \frac{e^2 4\pi}{q^2 + q_s^2}$$

FOURIER TRANSFORM

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

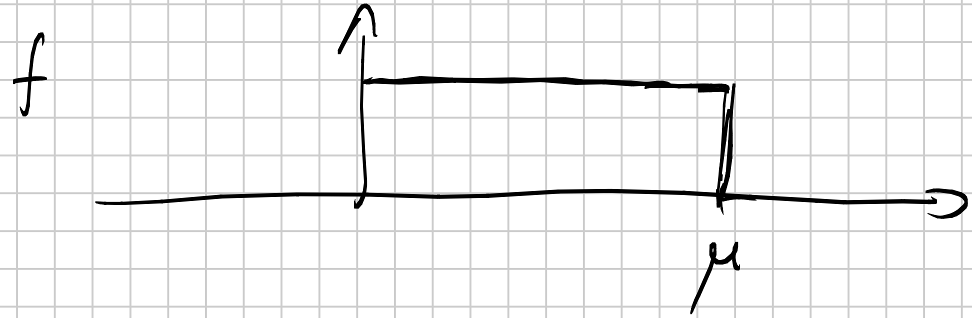
$$\phi(r) \to \frac{e^2}{r} e^{-q_s r}$$

YUKAWA POTENTIAL



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

$\boxed{T=0}$



$$n = \int d\varepsilon \; g(\varepsilon)\, \vartheta(\mu-\varepsilon)$$

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

$$= g(\mu)$$

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

<u>BOHR RADIUS</u>