Lecture FYS4480, October 26, 2023

Hartree-Fock sp-energy

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{2e^2}{\pi} k_F \, F(k/k_F)$$

$$F(k/k_F) = \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right|$$

$$x = k/k_F$$

$$\varepsilon_0^F = \frac{\hbar^2 k_F^2}{2m}$$ (kinetic energy at $k = k_F$)

$$\varepsilon_k^{HF}/\varepsilon_0^F = x^2 - \frac{4e^2 m}{\hbar^2 k_F \pi} F(x)$$

$$a_0 = \hbar^2/e^2 m$$

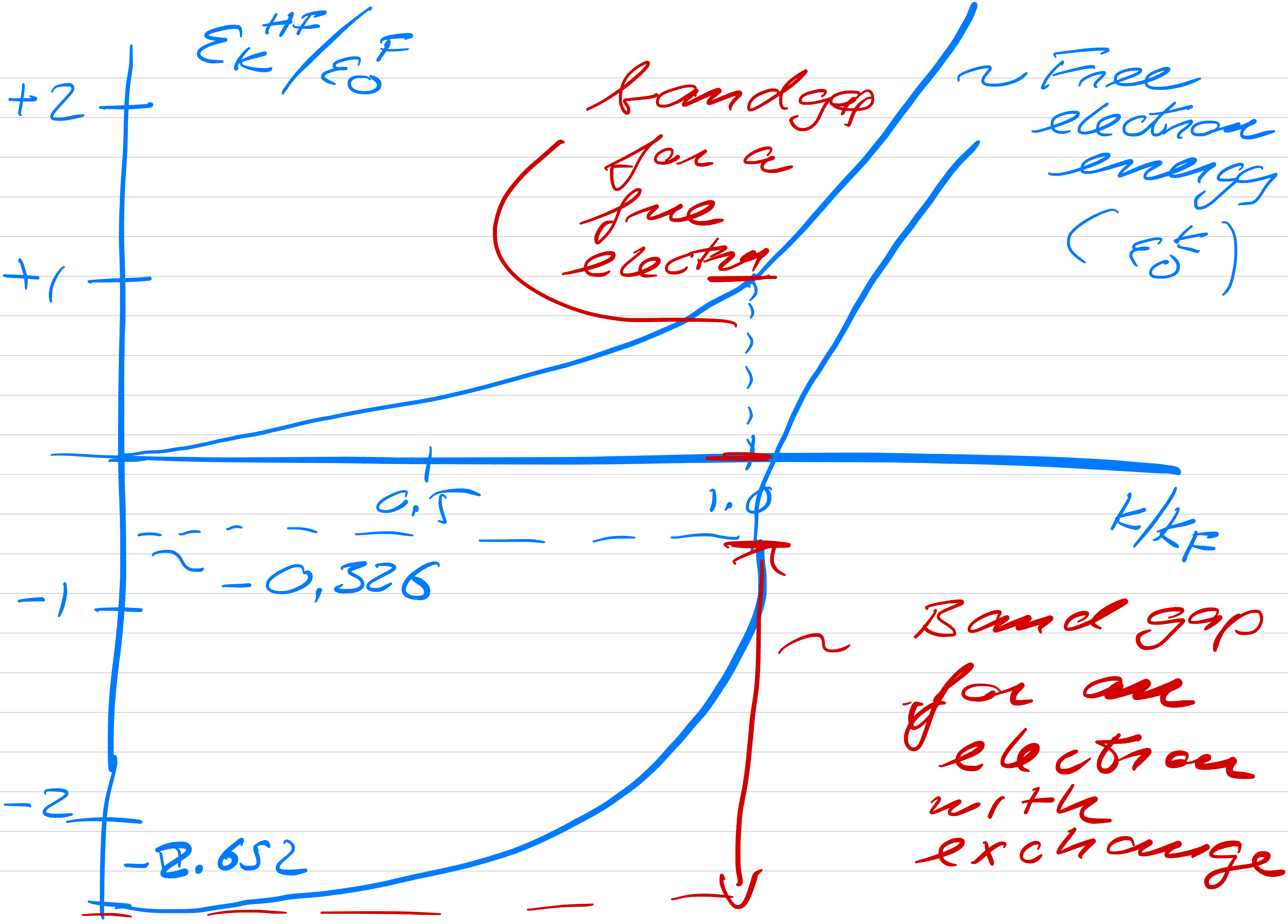
$$n = \frac{N}{V} = \text{density} = \frac{k_F^3}{3\pi^2} \quad (\text{at } T=0)$$

r_s = radius of a sphere whose volume is given by volume per electron

$$\frac{k_F^3}{3\pi^2} = \frac{3}{4\pi r_s^3} \Rightarrow k_F = 1.92/r_s$$

$$\varepsilon_k^{HF}/\varepsilon_0^F = x^2 - (r_s/a_0)\, 0.663\, F(x)$$

$r_s/a_0 \sim 2-6$ for most metals



$\varepsilon_K^{HF}/\varepsilon_0^F$
+2
+1
-1
-2
0.5
1.0
k/k_F
~ -0,326
-2.652
band gap for a free electron
~ Free electron energy (ε_0^k)
~ Band gap for an electron with exchange

$x = 1$ $\quad \varepsilon_{k_F}^{HF} / \varepsilon_0^F = -0.326$

$r_s / a_0 = 4$

$x = 0$ $\quad \varepsilon_0^{HF} / \varepsilon_0^F = -2.652$

$$\Delta \varepsilon^{HF} = \varepsilon_{k_F}^{HF} - \varepsilon_{k=0}^{HF} = 2.326$$

Band gap due to exchange energy only, Band gap is the spread between max and min values in the band of k-values up to k_F

connection with exercise set.

$$\varepsilon_k^{HF} = \varepsilon_{k_F}^{HF} + \left(\frac{\partial \varepsilon_k^{HF}}{\partial k}\right)_{k_F} (k - k_F)$$

$$+ \ldots$$

$$\varepsilon_k^0 = \frac{\hbar^2 k_F^2}{2m} + \frac{\hbar^2 k_F}{m}(k - k_F) + \ldots,$$

introduce effective mass

m^*_{HF}

$$\varepsilon_k^{HF} = \varepsilon_{k_F}^{HF} + \frac{\hbar^2 k_F}{m^*_{HF}}(k - k_F) + \ldots,$$

$$m^*_{HF} = \hbar^2 k_F \Big/ \left(\frac{\partial \varepsilon_k^{HF}}{\partial k}\right)_{k_F}$$

$m^*_{HF} = 0$ for electron gas in 3-dim with HF only,

Density of states

$$n(\epsilon) = \frac{V k^2}{2\pi^2} \left(\frac{\partial \epsilon}{\partial k}\right)^{-1}$$

use $\frac{1}{V} \sum_{k} \to \frac{1}{(2\pi)^3} \int d\vec{k}$

$V \to \infty$

$$\sum_{\vec{k}} \Rightarrow \frac{V}{(2\pi)^3} \int_0^\infty d\vec{k}$$

$$= \int_{-\infty}^{\infty} g(\varepsilon)\, d\varepsilon$$

$$g(\varepsilon) = n(\varepsilon)$$

$$\frac{V}{(2\pi)^3} \int 4\pi k^2 dk = \int n(\varepsilon)\, d\varepsilon$$

$$dk = \frac{\partial k}{\partial \varepsilon}\, d\varepsilon$$

$$n(\varepsilon) = \frac{V}{2\pi^2} k^2 \left(\frac{\partial \varepsilon}{\partial k}\right)^{-1}$$

at $k = k_F$, $\varepsilon \to \varepsilon_k^{HF}$

$$\left(\frac{\partial (\varepsilon_k^{HF})}{\partial k} \right)_{k_F} = \infty$$

This result reflects the long-range character of the Coulomb interaction, if we change $\frac{1}{|r|}$ (Fourier transfo[rm] $\sim \frac{1}{q^2}$)

to $\frac{e^{-\mu|r|}}{|r|}$ $\left(\sim \frac{1}{q^2+\mu^2} \right)$

$$\langle \Phi_0^{HF} | H | \Phi_0^{HF} \rangle$$

$$H = H_0 + H_I$$

$$H_0 = \sum_{\substack{k_1 k_2 \\ \sigma_1 \sigma_2}} \langle k_1 \sigma_1 | h_0 | k_2 \sigma_2 \rangle a^+_{k_1 \sigma_1} a_{k_2 \sigma_2}$$

$$H_1 = \frac{1}{2} \sum_{\substack{k_1 k_2 k_3 k_4 \\ \sigma_1 \sigma_2 \sigma_3 \sigma_4}} \langle k_1 \sigma_1 k_2 \sigma_2 | v | k_3 \sigma_3 k_4 \sigma_4 \rangle \times a^+_{k_1 \sigma_1} a^+_{k_2 \sigma_2} a_{k_4 \sigma_4} a_{k_3 \sigma_3}$$

$$\langle k_1 \sigma_1 | h_0 | k_2 \sigma_2 \rangle = \frac{1}{V} \sum_{\substack{\sigma_1 = \pm 1 \\ \sigma_2}} \chi^*_{\sigma_1} \chi_{\sigma_2} \int e^{-i \vec{k}_1 \vec{r}} \left(\frac{-\hbar^2 \nabla^2}{2m} \right) e^{i \vec{k}_2 \vec{r}} d\vec{r}$$

$$= \frac{\hbar^2 k^2}{2m} \delta_{\sigma_1 \sigma_2} \delta_{k_1 k_2} \Rightarrow$$

$$H_0 = \sum_{k_1 \sigma_1} \frac{\hbar^2 k^2}{2m} a^{+}_{k_1 \sigma_1} a_{k_1 \sigma_1}$$

$$= \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} a^{+}_{k\sigma} a_{k\sigma}$$

$$\langle \Phi_0^{HF} | H_0 | \Phi_0^{HF} \rangle$$

$$a^{+}_{k_i \sigma_i} = a_i^{+}$$

$$\Phi_0^{HF} = \prod_{i=1}^{N} a_i^{+} |0\rangle$$

$$\langle \Phi_0^{HF} | \sum_{p(k_p \sigma_p)} \frac{\hbar^2 k_p^2}{2m} a_p^+ a_p | \Phi_0^{HF} \rangle$$

factor of 2

$$\sum_p = \sum_{k_p \sigma}$$

$$= 2 \sum_{k_p} \to \frac{2V}{(2\pi)^3} \int_0^{k_F} d\vec{k}$$

$$= \frac{2 \cdot 4\pi V}{(2\pi)^3} \int_0^{k_F} k^2 dk \, \frac{\hbar^2 k^2}{2m}$$

$$= \frac{V \hbar^2}{\pi^2 10 m} k_F^5$$

$$\langle k_1\sigma_1 k_2\sigma_2 | v | k_3\sigma_3 k_4\sigma_4 \rangle$$

$$= \sum_{\xi_1 \xi_2} \chi^*_{\sigma_1}(\xi_1)\, \chi^*_{\sigma_2}(\xi_2)\, \chi_{\sigma_3}(\xi_1)\, \chi_{\sigma_4}(\xi_2)$$

$$\times \int \psi^*_{k_1}(x_1)\, \psi^*_{k_2}(x_2)\, \frac{e^2}{x_1 - x_2}\, \psi_{k_3}(x_1)\, \psi_{k_4}(x_2)$$

$$\times\, dx_1\, dx_2$$

$$= \delta_{\sigma_1\sigma_3}\, \delta_{\sigma_2\sigma_4}\, \frac{e^2}{V^2}$$

$$\times \int dx_1 \int dx_2\, \frac{e^{-i(k_1-k_3)x_1}\, e^{-i(k_2-k_4)x_2}}{x_1 - x_2}$$

$$\int dx_1\, dx_2\, \frac{e^{-i(k_2-k_4)x_2}\, e^{-i(k_1-k_3)x_1}}{x_1-x_2}$$

$$\int dx_1\, dx_2\, \frac{e^{-i(k_2-k_4)(x_2-x_1)} \times e^{-i(k_1-k_3+k_2-k_4)x_1}}{x_1-x_2}$$

$$\left(y = x_1 - x_2 \qquad x = x_1 \right)$$

$$= \int dx \int dy\, \frac{e^{i(k_2-k_4)y}}{y}\, e^{-i(k_1-k_3+k_2-k_4)x}$$

convergence factor μ

add $\dfrac{e^2}{V^2}$

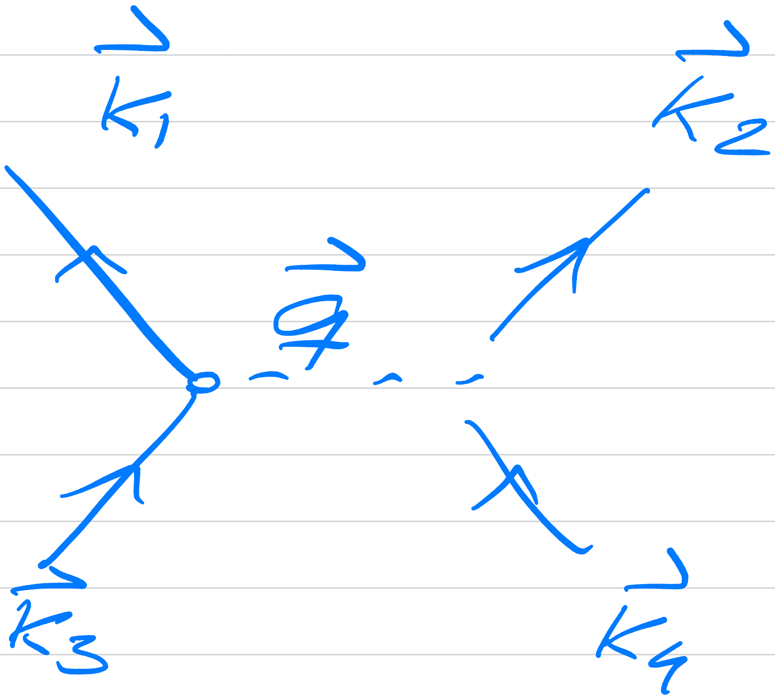
$$\frac{e^2}{V^2}\int dx \int dy \, e^{i(k_2-k_4)y} \, \frac{e^{-\mu y}}{y}$$

$$\times\, e^{-i(k_1-k_3+k_2-k_4)x}$$

$$= \frac{e^2}{V}\,\delta_{k_1+k_2,\,k_3+k_4}\int dy \; e^{i(k_2-k_4)y} \times e^{-\mu y}/y$$

$$q = k_2 - k_4$$

$$= \frac{e^2}{V} \delta_{k_1+k_2,\, k_3+k_4} \frac{4\pi}{M^2+q^2}$$



$$\vec{k}_1 - \vec{k}_3 = \vec{q}$$

$$= \vec{k}_2 - \vec{k}_4$$

$$\vec{k}_1 = \vec{k}_3 - \vec{q}$$

$$\vec{k}_1 = \vec{p} - \vec{q}$$

$$\vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{k}_4$$

$$\boxed{\vec{k}_4 = \vec{k}} \qquad \boxed{\vec{k}_3 = \vec{p}}$$

$$\frac{1}{2}\sum_{\substack{k_1k_2k_3k_4\\ \sigma_1\sigma_2\sigma_3\sigma_4}} \langle \cdots |v| \quad \rangle\, a^{+}_{k_1\sigma_1} a^{+}_{k_2\sigma_2} a_{k_4\sigma_4} a_{k_3\sigma_3}$$

$$= \sum_{\sigma_1\sigma_2} \frac{e^2}{2V} \sum_{\substack{\vec p\,\vec q\\ \vec k}} \frac{4\pi}{\mu^2+q^2}$$

$$a^{+}_{\vec p+\vec q\,\sigma_1}\, a^{+}_{\vec k-\vec q\,\sigma_2}\, a_{\vec k\sigma_2}\, a_{\vec p\sigma_1}$$

$$= \left(\sum_{\vec q\neq 0} \frac{4\pi}{\mu^2+q^2} - \cdot\ \cdot\right) + \left(\sum_{\substack{\sigma_1\sigma_p\\ p\,q}} \frac{4\pi}{\mu^2}\cdots\right)$$

$$\mu \neq 0$$

The last term $\dfrac{e^2}{2V}\dfrac{4\pi}{\mu^2}(N^2-N)$

this cancels a corresponding term from the positive ion background in the limit $N \to \infty$ and $\mu \to 0$

$$H = H_0 + \sum_{\substack{q\neq 0\\ p,q\\ \sigma_1\sigma_2}} \frac{4\pi}{\mu^2+q^2}\, a^{\dagger}_{\vec{k}+\vec{q}\,\sigma_1}\, a^{\dagger}_{\vec{p}-\vec{q}\,\sigma_2}\, a_{p\sigma_2}\, a_{k\sigma_1}$$

$$\langle \Phi_0^{HF} | H_1 | \Phi_0^{HF} \rangle$$

$$= \frac{2\pi e^2}{V} \sum_{\substack{p q \neq 0 \\ k \\ \sigma_1 \sigma_2}} \langle \Phi_0^{HF} | a^{+}_{k+q\,\sigma_1} a^{+}_{p-q\,\sigma_2} a_{p\sigma_2} a_{k\sigma} | \Phi_0^{HF} \rangle$$

$$\times \frac{1}{\mu^2 + q^2}$$

when performing contraction

$$- \delta_{\vec{k}+\vec{q},\,p}\ \delta_{\vec{p}-\vec{q},\,\vec{k}}\ \delta_{\sigma_1 \sigma_2}$$

$$\langle \Phi_0^{HF} | H_1 | \Phi_0^{HF} \rangle =$$

$$- 2 \, \frac{2\pi e^2}{V} \sum_{p,\, k \neq p} \frac{1}{|\vec{p} - \vec{k}|^2}$$

$$\frac{1}{V} \sum_{p(k)} \longrightarrow \frac{1}{(2\pi)^3} \int d\vec{p} \; (d\vec{k})$$

$$= - \frac{4\pi e^2 V}{(2\pi)^6} \int_0^{k_F} d\vec{p} \int_0^{k_F} d\vec{k} \, \frac{1}{|\vec{p} - \vec{k}|^2}$$

$$\int_0^{k_F} d\vec{p} \int_0^{k_F} d\vec{k} \frac{1}{|\vec{p}-\vec{k}|^2}$$

$$= \int d\vec{p} \int d\vec{k} \frac{1}{p^2+k^2-2|\vec{k}||\vec{p}|\cos\theta}$$

$$(\mu = \cos\theta \qquad s = k/p)$$

$$= \int d^3p \int d^3k \frac{1}{p^2} \frac{1}{1+s^2-2s\mu}$$

Legendre expansion

$$\frac{1}{\sqrt{1+s^2-2\mu s}} = \sum_{l} s^{l} P_l(\mu)$$

$$\frac{1}{1+s^2-2\mu s} = \sum_{l\lambda} s^{l+\lambda} P_l(\mu) P_\lambda(\mu)$$

$$\int d^3p \int d^3k \frac{1}{|\vec{p}-\vec{k}|^2} =$$

$$\int_{p \le k_F} d^3p \int_{k<p} dk\, k^2\, 2\pi \int_{-1}^{1} d\mu \sum_{l\lambda} \left(\frac{k}{p}\right)^{l+\lambda}$$

$$\frac{1}{p^2} P_l(\mu) P_\lambda(\mu) + \left(\int_{p<k} \int_{k \le k_F} - - \ldots \right)$$

$$\int_{-1}^{1} P_l(\mu) P_\lambda(\mu) \, d\mu = \frac{2}{2l+1} \delta_{l\lambda}$$

$$= 4\pi \int_{p \le k_F} d^3p \int_{k<p} dk \sum_l \left(\frac{k}{p} \right)^{2l+2} \frac{1}{2l+1}$$

$$\frac{\times 2}{k > p}$$

$$= 8\pi \int_{p \le k_F} d^3p \int_0^p dk \sum_l \left(\frac{k}{p}\right)^{2l+2} \frac{1}{2l+1}$$

$$= 8\pi \int_0^{k_F} d^3p \; p \underbrace{\sum_l \frac{1}{(2l+1)(2l+3)}}$$

$$\left(\frac{1}{2} \sum_l \left(\frac{1}{2l+1} - \frac{1}{2l+3} \right) = \frac{1}{2} \right)$$

$$= -\frac{e^2 V k_F^4}{4\pi^3}$$