FYS4480/9480, lecture October 10, 2025

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Exchange in HF-energy

$$\frac{e^2}{\Omega(2\pi)^3}\int d\vec{r}\int d\vec{r}\,'\int d\vec{k}\,'$$

$$\times\ e^{i(\vec{k}\,'-\vec{k})(\vec{r}-\vec{r}\,')}\ \frac{e^{-\mu|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}$$

$$\frac{1}{\Omega}\sum_{\vec{k}\leq|k_F|}$$

$$\vec{k}=\frac{2\pi}{L}\vec{n}$$

$$\vec{n}=n_1\vec{e}_1+n_2\vec{e}_2+n_3\vec{e}_3$$

$n_i = 0, \pm 1, \pm 2, \ldots$

neighboring points are separated by $\Delta k_i = \dfrac{2\pi}{L}$ in each cartesian coordinate

$$\frac{1}{\Omega} \sum_{\vec{k}} \rightarrow \frac{1}{(2\pi)^3} \int d^3k$$

$$\sum_{\vec{k}} = \sum_{\vec{n}},$$ which, taking into account the components

$$\sum_{n_i} \qquad \Delta k_i \rightarrow dk_i$$
$$\Delta n_i \rightarrow dn_i$$

$$\sum_{n_i} \rightarrow \int dn_i$$

$$dn_i = \frac{L}{2\pi} dk_i$$

$$\sum_{\vec{k}} \rightarrow \int \underset{(1)}{dn_x}\, \underset{(2)}{dn_y}\, \underset{(3)}{dn_z} =$$

$$= \left(\frac{L}{2\pi}\right)^3 \int dk_x\, dk_y\, dk_z$$

$$= \frac{\Omega}{(2\pi)^3} \int d^3k$$

$$\frac{1}{\Omega} \sum_{\vec{k} \leq k_F} \longrightarrow \frac{1}{(2\pi)^3} \int_0^{k_F} d^3k$$

Density operator

$$n(\vec{r}) = \sum_{\vec{k} \leq k_F} |\varphi_{\vec{k}}(\vec{r})|^2$$

$$\varphi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\vec{r}}$$

$$= \frac{N}{\Omega}$$

$$n(\vec{r}) = \frac{1}{\Omega} \sum_{\vec{k} \leq k_F} \cdot 1 \longrightarrow$$

$$\Rightarrow \frac{1}{(2\pi)^3} \int_0^{k_F} d^3k = \frac{4\pi}{(2\pi)^3} \int_0^{k_F} k^2 dk$$

Take into account spin degrees of freedom, get a factor of 2

$$n(\vec{r}) = 2 \, \frac{1}{3} \, \frac{4\pi}{8\pi^3} k_F^3$$

$$= \frac{k_F^3}{3\pi^2} = \frac{N}{\Omega}$$

charge density

$$\rho(\vec{r}) = n(\vec{r}) \cdot e$$

$$\frac{e^2}{\Omega(2\pi)^3}\int d\vec{r}\int d\vec{r}\,'\int d\vec{k}\,'\, e^{i(\vec{k}\,'-\vec{k})(\vec{r}-\vec{r}\,')}$$

$$\times\, e^{-\mu|\vec{r}-\vec{r}\,'|}\,\frac{e}{|\vec{r}-\vec{r}\,'|}$$

$$\vec{x} = |\vec{r}-\vec{r}\,'| \qquad \vec{y} = \vec{r}\,'$$

$$\lim_{\mu\to 0}\frac{e^2}{\Omega(2\pi)^3}\int d\vec{k}\,'\int d\vec{y}\int d\vec{x}\; e^{i(\vec{k}\,'-\vec{k})\vec{x}}\, e^{-\mu|\vec{x}|}\,\frac{e}{|\vec{x}|}$$

$(x = |\vec{x}|)$

intermediate step

$$\int d\vec{x}\, e^{i(\vec{k}'-\vec{k})\vec{x}} \frac{e^{-\mu x}}{x}$$

$$= \int_0^\infty dx\, x^2 \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi$$

$$\times e^{i|\vec{k}'-\vec{k}||\vec{x}|\cos\theta} \frac{e^{-\mu x}}{x}$$

$$= 2\pi \int_0^\infty x^2 dx \frac{e^{-\mu x}}{x} \int_0^\pi d\theta \sin\theta\, e^{i|\vec{k}'-\vec{k}|x\cos\theta}$$

$$= \frac{4\pi}{\mu^2 + |\vec{k}' - \vec{k}|^2}$$

$$\times$$

$$\lim_{\mu \to 0} \frac{e^2}{\Omega (2\pi)^3} \int_0^{k_F} d\vec{k}'$$

$$\times \int d\vec{q} \; \frac{4\pi}{\mu^2 + |\vec{k}' - \vec{k}|^2} = \frac{e^2}{2\pi^2} \times$$

$$\int d\vec{q} = \Omega \Bigg| \int_0^{k_F} \frac{d\vec{k}'}{|\vec{k}' - \vec{k}|^2}$$

$$= \frac{e^2}{2\pi^2} \int_0^{k_F} k'^2 \, dk' \int_0^{\pi} 2\pi \, d\theta \sin\theta$$

$$k = |\vec{k}|$$

$$\times \left(\frac{1}{\sqrt{k'^2 + k^2 - 2|\vec{k}'||\vec{k}|\cos\theta}} \right)^2$$

$$u = \cos\theta$$

$$= \frac{e^2}{2\pi^2} \int_0^{k_F} k'^2 \, dk' \int_{-1}^{1} 2\pi \, du$$

$$\times \frac{1}{k'^2 + k^2 - 2k'k\,u}$$

$$= \frac{e^2}{\pi k} \int_0^{k_F} k' dk' \ln \left| \frac{k+k'}{k'-k} \right|$$

$$= \frac{e^2}{\pi k} \left\{ \frac{k_F^2 - k^2}{2} \ln \left| \frac{k_F + k}{k_F - k} \right| + k k_F \right\}$$

$$\Rightarrow$$

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2 k_F}{\pi} \left\{ 2 + \frac{k_F^2 - k^2}{k k_F} \ln \left| \frac{k_F + k}{k_F - k} \right| \right\}$$

$$x = k/k_F$$

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

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

non-interacting energy at the Fermi level

$$\varepsilon_0^F = \hbar^2 k_F^2/2m$$

$$E_k^{HF}/E_0^F = x^2 - \frac{4e^2 m}{\hbar^2 k_F \pi} F(x)$$

Bohr Radius $= a_0 = \frac{\hbar^2}{e^2 m}$

$$n = \frac{N}{\Omega} = 2\int_0^{k_F} k^2 dk \int d\theta \sin\theta \, d\phi \times \frac{1}{(2\pi)^3} = \frac{k_F^3}{3\pi^2}$$

Total volume : $N.\Omega_e$

volume each electron occupy

$$\Omega_e = \frac{4\pi r_s^3}{3}$$ $r_s \rightarrow$ radius of a sphere whose volume is the volume per electron

$$\frac{N}{N\Omega_e} = \frac{N}{\Omega} = \frac{3}{4\pi r_s^3} = \frac{k_F^3}{3\pi^2}$$

$$\mathcal{E}_K^{HF} / \mathcal{E}_0^F = x^2 - \left(\frac{r_s}{a_0}\right) 0.663\, F(x)$$

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

HF ground state energy

$$\hat{\mathcal{H}} = \hat{T} + \hat{V}$$

(i) $$\hat{T} = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} a^{+}_{k\sigma} a_{k\sigma}$$

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

$$\langle \Phi_0^{HF} | \hat{T} | \Phi_0^{HF} \rangle$$

$$\overset{\parallel}{\hat{H}_0}$$

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

$$\langle \Phi_0^{HF} | \hat{T} | \Phi_0^{HF} \rangle =$$

$$2 \frac{1}{(2\pi)^3} \int_0^{k_F} k^2 dk \int_0^{\pi} d\theta \sin\theta$$

$$\times \int_0^{2\pi} d\varphi \, \frac{\hbar^2 k^2}{2m}$$

$$= \frac{2 \cdot \Omega \, 4\pi}{(2\pi)^3} \int_0^{k_F} \frac{k^2 dk \, \hbar^2 k^2}{2m} = \frac{\Omega \hbar^2}{\pi^2 10 m} k_F^5$$

$$\frac{N}{\Omega} = \frac{k_F^3}{3\pi^2} = \frac{3}{4\pi r_s^3}$$

$$\langle \Phi_0^{HF} | \hat{T} | \Phi_0^{HF} \rangle = \frac{\hbar^2 \Omega}{10\pi^2 m} \left(\frac{3\pi^2 N}{\Omega} \right)^{5/3}$$

$$= \frac{3\hbar^2}{10m} \left(\frac{9\pi}{4} \right)^{2/3} \frac{N}{r_s^3}$$

$$a_0 = \frac{\hbar^2}{me^2} \qquad 1\,Ry = \frac{me^4}{2\hbar^2}$$

$$= 13.6\ eV$$

$$\frac{\langle \Phi_0^{HF} | \hat{T} | \Phi_0^{HF} \rangle}{N} =$$

$$2{,}21 \left(\frac{a_0}{r_s} \right) \cdot 1\,Ry$$

$$\hat{V}_{ee} = \frac{1}{2} \sum_{\substack{k_1 k_2 k_3 k_4 \\ \sigma_1 \sigma_2 \sigma_3 \sigma_4}} \langle k_1\sigma_1\, k_2\sigma_2 | v | k_3\sigma_3\, k_4\sigma_4 \rangle$$

$$\times\, a^{+}_{k_1\sigma_1}\, a^{+}_{k_2\sigma_2}\, a_{k_4\sigma_4}\, a_{k_3\sigma_3}$$

$$\langle \Phi_0^{HF} | \hat{V}_{ee} | \Phi_0^{HF} \rangle / N$$

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

$$= \chi^*_{\sigma_1}(1)\, \chi_{\sigma_3}(1)\, \chi^*_{\sigma_2}(2)\, \chi_{\sigma_4}(2)$$

$$\times \int dx_1\, dx_2\, \varphi^*_{k_1}(x_1)\, \varphi^*_{k_2}(x_2) \frac{e^2}{|x_1 - x_2|} =$$

$$\times\, \varphi_{k_3}(x_1)\, \varphi_{k_4}(x_2)$$

$$\left(\varphi_{\vec{k}}(\vec{x}) = \frac{1}{\sqrt{\Omega}} e^{i \vec{k} \vec{x}} \right)$$

$$\delta_{\sigma_1\sigma_3}\,\delta_{\sigma_2\sigma_4}\,\frac{e^2}{\Omega^2}\int dx_1\int dx_2$$

$$\times\; e^{-i(k_1-k_3)x_1}\, e^{-i(k_2-k_4)x_2}\,\frac{}{|x_1-x_2|}$$

$$\int dx_1\int dx_2\; e^{-i(k_2-k_4)(x_2-x_1)}\,\frac{1}{|x_1-x_2|}$$

$$\times\; e^{-i(k_1-k_3+k_2-k_4)x_1}$$

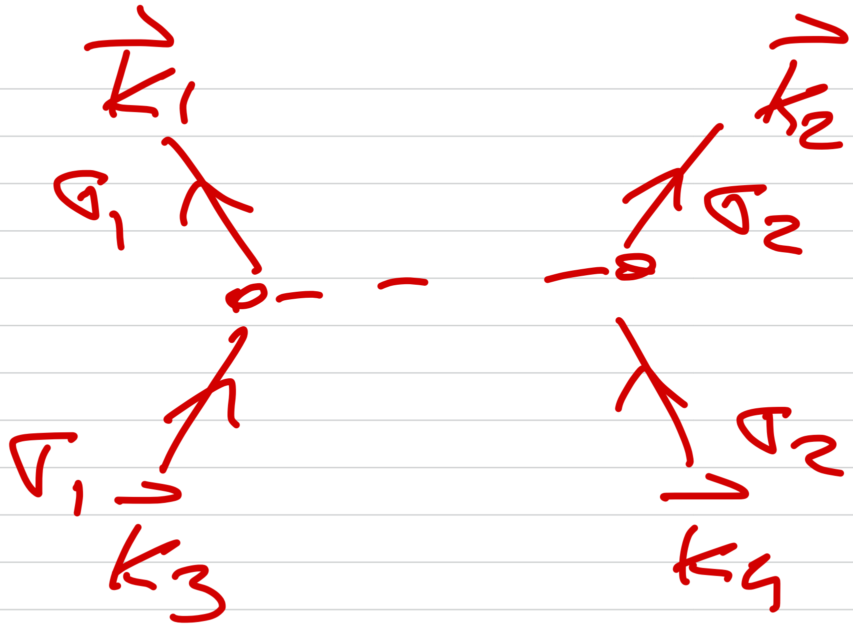
$$y = x_1 - x_2 \qquad\qquad x = x_1$$

introduce $e^{-\mu y}$ $\left(\lim_{\mu \to 0}\right)$

$$\lim_{\mu \to 0} \int dx \int dy \; e^{i(k_2 - k_4) y - \mu y} \; \frac{e}{y} \times e^{-i(k_1 - k_3 + k_2 - k_4) x} \times \frac{e^2}{\Omega^2}$$

$q = k_2 - k_4$

$$\lim_{\mu \to 0} \frac{e^2}{\Omega} \boxed{\delta_{k_1+k_2,\, k_3+k_4}} \cdot \int dy \; e^{i(k_2-k_4)y} \times e^{-\mu y}/y$$



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

conservation of momentum

$$= \lim_{\mu\to 0} \frac{e^2}{\Omega}\,\delta_{k_1+k_2,\,k_3+k_4} \times \frac{4\pi}{\mu^2+q^2}$$