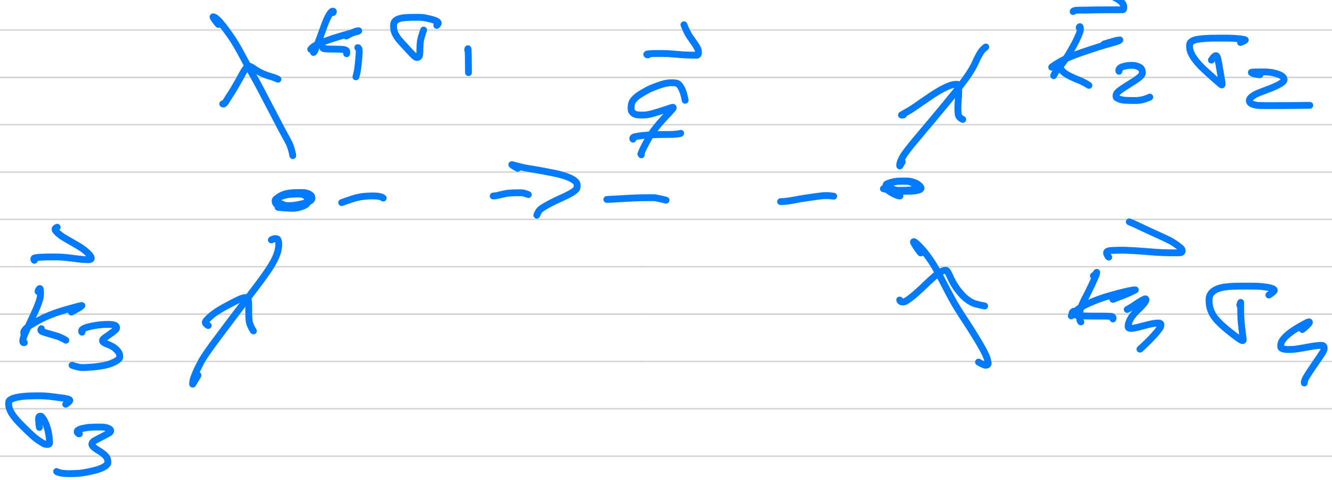
FYS4480/9480 October 16

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

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

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



$$\boxed{\begin{aligned} \vec{q} &= \vec{k}_2 - \vec{k}_4 \\ \vec{k}_1 &= \vec{k}_3 - \vec{q} \\ \vec{k}_3 &= \vec{p} \\ \vec{k}_4 &= \vec{k} \end{aligned}}$$

$$\vec{k}_1 = \vec{p} + \vec{q} \quad \wedge \quad \vec{k}_2 = \vec{k} - \vec{q}$$

$$\frac{1}{2} \sum_{\substack{\sigma_1 \sigma_2 \\ \sigma_3 \sigma_4 \\ \vec{k}_1 \vec{k}_2 \\ \vec{k}_3 \vec{k}_4}} \langle \vec{k}_1 \sigma_1 \, \vec{k}_2 \sigma_2 | v | \vec{k}_3 \sigma_3 \, \vec{k}_4 \sigma_4 \rangle \times a^{+}_{\vec{k}_1 \sigma_1} a^{+}_{\vec{k}_2 \sigma_2} a_{\vec{k}_4 \sigma_4} a_{\vec{k}_3 \sigma_3}$$

rewrite $\displaystyle \sum_{\substack{\vec{p}\,\vec{q} \\ \vec{k}}} = \sum_{\substack{\vec{p}\,\vec{k} \\ q = 0}} + \sum_{\substack{\vec{p}\,\vec{k} \\ \vec{q} \neq 0}}$

(i) $$\frac{e^2 4\pi}{2\Omega \mu^2} \sum_{\substack{\vec{p}\,\vec{k} \\ \sigma_1 \sigma_2}} a^\dagger_{\sigma_1 \vec{p}+\underset{=0}{\vec{q}}}\, a^\dagger_{\sigma_2 \vec{k}-\underset{=0}{\vec{q}}}$$

$$\times\, a_{\sigma_2 \vec{k}}\, a_{\sigma_1 \vec{p}}$$

$$\sum_{\substack{\vec{p}\,\vec{k} \\ \sigma_1 \sigma_2}} \langle \Phi_0^{HF} | a^\dagger_{\sigma_1 \vec{p}}\, a^\dagger_{\sigma_2 \vec{k}}\, a_{\sigma_2 \vec{k}}\, a_{\sigma_1 \vec{p}} | \Phi_0^{HF} \rangle$$

$$a^\dagger_{\sigma_1 \vec{p}}\, a^\dagger_{\sigma_2 \vec{k}}\, a_{\sigma_2 \vec{k}}\, a_{\sigma_1 \vec{p}}$$

$$\delta_{\sigma_1 \sigma_2}\, \delta_{\vec{p}\vec{k}}$$

$$\sum_{(p\sigma)\le F} = N$$

$\vec{p}_N \sigma_N$

$\vdots$

$\vec{p}_2 \sigma_2$

$\vec{p}_1 \sigma_1$

$$q = 0 : \quad \frac{e^2 4\pi}{2\Omega \mu^2}\left(N^2 - N\right)$$

(ii)

$$+ \sum_{\sigma_1 \sigma_2} \sum_{\substack{\vec{p}\,\vec{k} \\ \vec{q} \neq 0}} \frac{e^2}{\Omega\, 2} \frac{4\pi}{\mu^2 + q^2}$$

$$\times\, a_{\sigma_1, \vec{p}+\vec{q}}\; a_{\sigma_2\, \vec{k}-\vec{q}}\; a_{\sigma_2 \vec{k}}\; a_{\sigma_1 \vec{p}}$$

$$q \neq 0$$

$$\langle \Phi_0^{HF} | a^{+}_{\sigma_1 \vec{p}+\vec{q}} \, a^{+}_{\sigma_2 \vec{k}-\vec{q}} \, a_{\sigma_2 \vec{k}} \, a_{\sigma_1 \vec{p}} | \Phi_0^{HF} \rangle$$

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

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

$$\vec{k} - \vec{q} = \vec{p} \quad \wedge \quad \vec{p} + \vec{q} = \vec{k}$$

$$\langle \Phi_0^{HF} | \hat{v} | \Phi_0^{HF} \rangle = -(2)\, \frac{2\pi e^2}{\Omega} \sum_{\substack{\vec{p}\,\vec{k} \\ \vec{k} \neq \vec{p}}} \frac{1}{|\underbrace{\vec{p} - \vec{k}}_{q}|^2}$$

Spin

(we have taken limit $\mu \to 0$)

Only exchange term.

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

$$-\frac{4\pi e^2\Omega}{(2\pi)^6}\int_0^{k_F} d^3p\int_0^{k_F} d^3k \times \frac{1}{|\vec{p}-\vec{k}|^2}$$

$$\int_0^{k_F} d^3p\int_0^{k_F} d^3k \,\frac{1}{p^2+k^2-2kp\underbrace{\cos\theta}_{u}}$$

$$s = k/p$$

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

$p \neq k \qquad p > k \qquad s < 1$

$$\frac{1}{\sqrt{1+s^2-2su}} = \sum_l s^l P_l(u)$$

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

$$\int_{p\leq k_F} d^3p \int_{k<p} dk\, k^2\, 2\pi \int_{-1}^{1} du$$

$$\times \sum_{l\lambda} \left(\frac{k}{p}\right)^{l+\lambda} \frac{1}{p^2} P_l(u)\, P_\lambda(u)$$

$$+\left(\int_{p<k} \cdots \int_{k\leq k_F} \cdots \right)$$

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

First integral

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

$$\times \frac{1}{2l+1}$$

2 from the other int

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

$$= 8\pi^2 k_F^4 \sum_l \frac{1}{(2l+1)(2l+3)}$$

$$\sum_{i} \frac{1}{(2i+1)(2i+3)} =$$

$$\frac{1}{2} \sum_{i} \left(\frac{1}{2i+1} - \frac{1}{2i+3} \right)$$

$$= \frac{1}{2} + \frac{1}{2} \sum_{i=0}^{\infty} \underbrace{\left(\frac{1}{2i+3} - \frac{1}{2i+3} \right)}_{0}$$

$$= \frac{1}{2}$$

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

$$= \boxed{- e^2 \Omega\, k_F^4 / 4\pi^3}$$

Density $n = \dfrac{N}{\Omega}$

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

$$r_s = \left(\frac{3}{4\pi n}\right)^{1/3} \quad k_F^3 = 3\pi^2 n$$

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

$$= -\frac{e^2 \Omega}{4\pi^3} \left(\frac{3\pi^2 N}{\Omega} \right)^{4/3}$$

$$\langle \Phi_0^{HF} | \mathcal{H} | \Phi_0^{HF} \rangle / N$$

$$= \left(2.21 / (r_s/a_0)^2 - \frac{0.916}{r_s/a_0} \right) \times 1 Ry$$

$$1 Ry = 13.6 \, eV$$

$r_s/a_0 \sim 2-6$ metals

interaction term (V/N)

$$-\frac{e^2}{4\pi^3}\frac{\Omega}{N}\left(3\pi^2\frac{N}{\Omega}\right)^{4/3}$$

$$= -\frac{e^2\,3}{4\pi}(3\pi^2)^{1/3}\,n^{1/3}$$

$$= -\text{const}\; n^{1/3}$$

Forms the basis for the Local density approximation (LDA) in Density functional theory (DFT)

DFT

Reminder of HF theory
Energy is a functional of (an ansatz) a state function, in our case a slater det $|\Phi_0\rangle$

$$E_{HF}[\Phi_0]$$

$$|\Phi_0\rangle \to |\Phi_0\rangle + |\delta\Phi_0\rangle$$

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

$$|\delta\Phi_c\rangle = \sum_{ai} \delta c_i^a \, a_a^\dagger a_i \, |\Phi_0\rangle$$

$$\left(\varphi_i(\vec{r}) \rightarrow \varphi_i(\vec{r}) + \delta\varphi_a(\vec{r}) \right)$$

$$\langle |p|h| \, H \, | \Phi_0 \rangle = 0$$

$$\left(\frac{\delta E[\Phi_0]}{\delta \Phi_0} = 0 \right)$$

$$\rightarrow \langle i|\hat{f}|a\rangle = 0 = \langle i|\hat{h}_0|a\rangle$$

$$+ \sum_{j \leq F} \langle ij|v|aj\rangle_{AS}$$

$$\hat{f} = \hat{h}^{HF} \quad \hat{h}^{HF}|p\rangle = \varepsilon_p^{HF}|p\rangle$$

DFT : energy is a functional of density

$E[n]$

$$\frac{\delta E[n]}{\delta n} = 0$$

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number operator

$$\hat{N} = \sum_p a_p^+ a_p$$

$$\langle \Phi_0 | \hat{N} | \Phi_0 \rangle = N$$

$$\hat{n}(\vec{r}) = \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i)$$

$$n(\vec{r}) = \frac{\langle \Psi | \hat{n} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$\int d\vec{r}\, n(\vec{r}) = N$$

with a Slater det $|\Phi_0\rangle$

$$n(\vec{r}) = \sum_{i=1}^{N} |\varphi_i(\vec{r})|^2$$