Lecture FYS4480/9480, October 11, 2024

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HF-eqs

$$\langle pq | H | \Phi_0 \rangle = 0 = \langle i | f | a \rangle$$

$$\langle \Phi_i^a |$$

$$(*) \left[\begin{array}{l} \langle a | f | a \rangle = \varepsilon_a^{HF} \\ \langle i | f | i \rangle = \varepsilon_i^{HF} \end{array} \right. \qquad \langle i | f | a \rangle = 0$$

$$(**) \left[\begin{array}{l} \langle a | f | a \rangle = 0 \\ \langle i | f | i \rangle = \varepsilon_i^{HF} \end{array} \right. \qquad \Big| \ \varepsilon_a = \frac{\hbar^2 k_a^2}{2m}$$

Ground state energy

$$H = \underbrace{T_e + V_{ee}}_{} + \underbrace{V_{eB} + V_{BB}}_{}$$

(lim $\mu \to 0$)

$$\sum_{i=1}^{N} \frac{\hbar^2 k_i^2}{2m} + \frac{1}{2} e^2 \sum_{i,j}^{N} \frac{e^{-\mu|\vec{r}_i - \vec{r}_j|}}{|\vec{r}_i - \vec{r}_j|}$$

$N \to \infty$, $V \to \infty$, $n = \frac{N}{V} = \text{const}$

$V = L^3$ L - side of box

$\mu L \ll 1$

$$\sum_{i=1}^{N} \frac{\hbar^2 k_i^2}{2m} \longrightarrow \sum_{\substack{k_1 k_2 \\ \sigma_1 \sigma_2}} \langle k_1 \sigma_1 | \hat{t} | k_2 \sigma_2 \rangle \, a^\dagger_{k_1 \sigma_1} a_{k_2 \sigma_2}$$

$$\langle k_1 \sigma_1 | \hat{t} | k_2 \sigma_2 \rangle = \delta_{\sigma_1 \sigma_2} \delta_{k_1 k_2} \frac{\hbar^2 k_1^2}{2m}$$

$$\begin{pmatrix} 1 & 0 \end{pmatrix} \qquad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

can rewrite

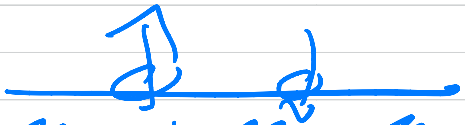
$$\sum_{k\sigma} \frac{\hbar^2 k^2}{2m} a^\dagger_{k\sigma} a_{k\sigma}$$

$$= 2 \sum_{k} \frac{\hbar^2 k^2}{2m} a^\dagger_{k} a_{k}$$

3-d

2

12

$n_1^2+n_2^2+n_3^2 = 1$ ( $n_1=-1$ $n_2=n_3=0$ + 5 more) 14

$n_1^2+n_2^2+n_3^2 = 0$  $n_1=n_2=n_3=0$ 2

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle \qquad \frac{1}{V}\sum_{k \le k_F} \rightarrow \frac{1}{(2\pi)^3}\int d^3k$$

$$\overset{N}{\underset{1}{\overline{}}}$$

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

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle =$$

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

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

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

$$\langle \Phi_0 | H_0 | \Phi_0 \rangle = \frac{\hbar^2 \cdot V}{10\pi^2 m} \left(\frac{3\pi^2 N}{V} \right)^{5/3}$$

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

$$a_0 = \hbar^2 / me^2 \qquad 1\,Ry = \frac{me^4}{2\hbar^2} = 13,6\,eV$$

$$\frac{\langle \Phi_0 | H | \Phi_0 \rangle}{N} = 2,21 \left(\frac{a_0}{r_s} \right)^2 \cdot 1\,Ry$$

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

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

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

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

$$\times \int dx_1 \, dx_2 \; \varphi^{*}_{k_1}(x_1)\, \varphi^{*}_{k_2}(x_2) \frac{e^2}{|x_1 - x_2|} \varphi_{k_3}(x_1)$$

$$\times \; \varphi_{k_4}(x_2)$$

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

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

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

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

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

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

$$\iint dx\, dy\, e^{+i(k_2-k_4)y} \frac{1}{y} e^{-i(k_1-k_3+k_2-k_4)x}$$

introduce $e^{-\mu y}$

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

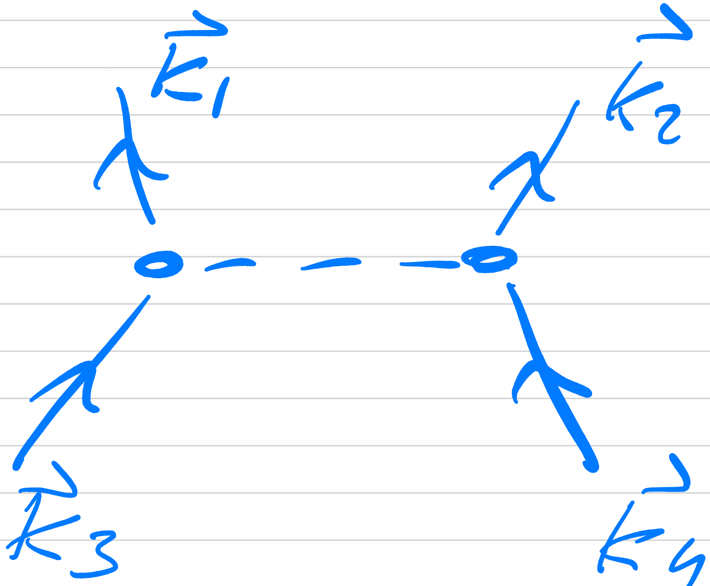
$$\times\, e^{-i(k_1-k_3+k_2-k_4)x}$$

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

$$(q = k_2-k_4)$$

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

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



$$\vec{k}_2 - \vec{k}_4 = \vec{q} \qquad \vec{k}_3 = \vec{p}$$

$$\vec{k}_1 = \vec{k}_3 - \vec{q} \qquad \vec{k}_4 = \vec{q}$$

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

$$\delta_{\sigma_1 \sigma_3} \quad \delta_{\sigma_2 \sigma_4}$$

$$V_{ee} = \frac{e^2}{V2} \sum_{\sigma_1 \sigma_2} \sum_{\vec{p}\vec{k}\vec{q}} \frac{4\pi}{M^2+q^2}$$

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

$$= \frac{e^2}{V2} \sum_{\sigma_1\sigma_2} \sum_{\vec{p}\vec{k}} \frac{4\pi}{M^2} \left\{ \underline{\qquad\qquad} \; \underset{q=0}{\iota} \; \underline{\qquad\qquad} \right\}$$

$$+ \frac{e^2}{V2} \sum_{\sigma_1\sigma_2} \sum_{\substack{\vec{p}\vec{k} \\ \vec{q}\neq 0}} \frac{4\pi}{M^2+q^2} \left\{ \underline{\qquad} \; \underset{q\neq 0}{\iota} \; \underline{\qquad} \right\}$$

The first term gives

$$\frac{e^2}{2V}\frac{4\pi}{\mu^2}\left(N^2 - N\right)$$

$$\sum_{\substack{pq\\ \sigma_1\sigma_2}} a^{+}_{\vec{p}\sigma_1} a^{+}_{\vec{q}\sigma_2} a_{q\sigma_2} a_{\vec{p}\sigma_1} = \Big(\underbrace{\sum_{\sigma k} a^{+}_{k\sigma} a_{k\sigma}}_{\hat{N}}\Big)^2 - \Big(\underbrace{\sum_{\sigma k} a^{+}_{k\sigma} a_{k\sigma}}_{\hat{N}}\Big)$$

This term cancels exactly $H_{eB} + H_{BB}$

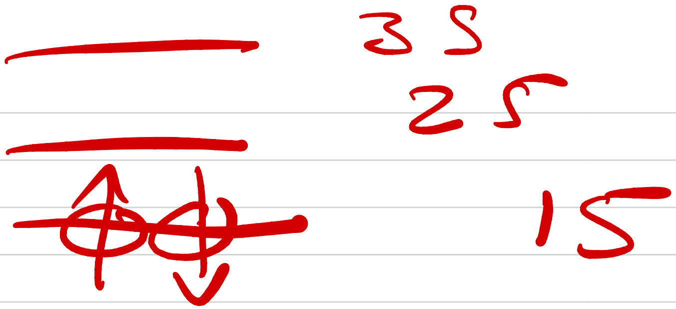
$$\langle \Phi_0 | V_{ee} | \Phi_0 \rangle$$

$$= \boxed{- \text{const}\ \rho^{1/3}}$$

local density used in DFT

$$\rho = \frac{N}{V}$$

$$\langle pq \| rs \rangle_{AS} = \langle pq | r | rs \rangle - \langle pq | r | sr \rangle$$



$$\underset{(1)\ \ (2)}{\langle 1S\ 1S} | v | \underset{(1)\ \ (2)}{1S\ 1S \rangle}$$

$$\sum_{\sigma_1 \sigma_2} \langle \underset{\substack{(1)\\(1\,0)\\(0\,1)}}{1S}\ \underset{\substack{(2)\\(0\,1)\\(1\,0)}}{1S} | v | \underset{\substack{(1)\\(1\,0)}}{1S}\ \underset{(2)}{1S} \rangle$$

$$- \langle \underset{\substack{(1)\\(1\,0)}}{1S}\ \underset{\substack{(2)\\(0\,1)}}{1S} | v | \underset{\substack{(2)\\ \binom{0}{1}}}{1S}\ \underset{\substack{(1)\\ \binom{1}{0}}}{1S} \rangle = 2 \langle 1S\,1S | v | 1S\,1S \rangle$$