Lecture FYS4480/9480, October 17, 2024

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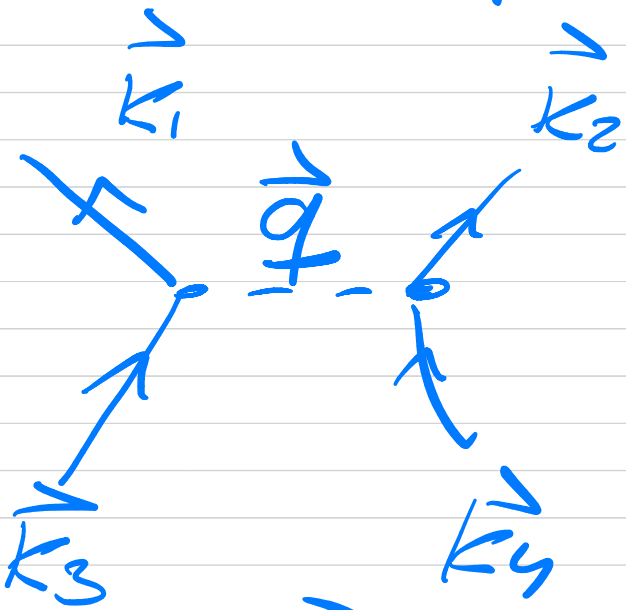
$$V_{int} = \sum_{\sigma_1 \sigma_2} \frac{e^2}{V^2} \sum_{\substack{pk\\q}} \frac{4\pi}{\mu^2+q^2} a^+_{\sigma_1, \vec{k}+\vec{p}}$$

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

$$\vec{q} = \vec{k}_1 - \vec{k}_3$$
$$= \vec{k}_2 - \vec{k}_4$$



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

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

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

$$+ \underbrace{\sum_{\vec p \vec k} \sum_{\sigma_1 \sigma_2} \frac{4\pi}{\mu^2} \;\text{———}\; 1 \;\text{———}}$$

$$\langle \Phi_0 | \sum_{\substack{\vec p \vec k \\ \sigma_1 \sigma_2}} -1 \;\text{———}\; | \Phi_0 \rangle = \frac{e^2 4\pi}{2 V \mu^2} (N^2 - N)$$

$$\langle \Phi_0 | V | \Phi_0 \rangle =$$

$$\frac{1}{2} \sum_{ij \leq F} \left(\langle ij | v | ij \rangle - \langle ij | v | ji \rangle \right)$$

$$\langle ij | v | ij \rangle = 0$$

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

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

i : Braside : $\vec{p}+\vec{q}$ σ_1 Ketside $\vec{p}$ σ_1

Direct

$$-\langle i' j' | v | j\, i \rangle$$

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

σ_1

$\vec{p} + \vec{q}$ $\qquad$ $\vec{k}$

σ_1 $\qquad$ σ_2

$\delta_{\sigma_1 \sigma_2}$

$\vec{p} + \vec{q} = \vec{k}$

$\vec{p} = \vec{k} + \vec{q}$; $\vec{q} = \vec{p} - \vec{k}$

$$\langle \Phi_0 | H_{int} | \Phi_c \rangle$$

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

spin deg.

$\left(\lim_{\mu \to 0} \right)$

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

$$\langle \Phi_0 | V_{int} | \Phi_0 \rangle =$$

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

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

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

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

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

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

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

$\Rightarrow$

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

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

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

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

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

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

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

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

$$\int dp\, p^3$$

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

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

$$\int d^3p \int d^3k \, \frac{1}{|p-k|^2} = 4\pi^2 k_F^4$$

$$\langle \Phi_0 | V_{int} | \Phi_0 \rangle = -\frac{e^2 V k_F^4}{4\pi^3}$$

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

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

$$\langle \Phi_0 | V_{int} | \Phi_0 \rangle = -\frac{e^2 V}{4\pi^3} \left(\frac{3\pi^2 N}{V} \right)^{4/3}$$

$$= -0.916 \, Ry \, a_0 / r_s \cdot N$$

$$\frac{\langle H \rangle}{N} = \left(\frac{2.21}{(r_s/a_0)^2} - \frac{0.916}{r_s/a_0} \right) Ry$$

$$1 \, Ry = 13.6 \, eV$$

Density functional theory vs Hartree-Fock

Energy is a functional of

$|\Phi_0\rangle$

$E_{HF}[\Phi_0]$ $\quad |\Phi_0\rangle \rightarrow |\Phi_0\rangle + |\delta\Phi_0\rangle$

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

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

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

$$\langle 1p1h | H | \Phi_0 \rangle = 0$$

$$\frac{\delta E[\Phi_0]}{\delta \Phi_0} = 0$$

$$\langle i | f | a \rangle = \langle i | h_0 | a \rangle$$

$$+ \sum_{j \in F} \langle ij | v | aj \rangle_{AS} = 0$$

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

DFT

$$E[\rho] = E[n]$$

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

$$\hat{H} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i=1}^{N} V_{ext}(\vec{r}_i)$$

$$+ \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} v(r_{ij})$$

$$r_{ij} = |\vec{r}_i - \vec{r}_j|$$

one body density

$$\rho(\vec{r}, \sigma; \vec{r}', \sigma') = \delta_{\sigma\sigma'} \sum_i \psi_i^*(\vec{r}) \psi_i(\vec{r}')$$

Diagonal part

$$\rho(\vec{r}) = \sum_i |\psi_i(\vec{r})|^2 = n(\vec{r})$$

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

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

$$n(\vec{r})\Big|_{\vec{r}=\vec{r}_1} \propto \frac{\int d\vec{r}_2\, d\vec{r}_3 \ldots d\vec{r}_N \times |\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots \vec{r}_N)|^2}{\langle \psi | \psi \rangle}$$

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

Thomas-Fermi-Dirac functional

$$E_{TFD}[n] = \underbrace{C_1 \int d\vec{r}\, n(\vec{r})^{5/3}}_{\text{kinetic energy term}}$$

$$+ \int d\vec{r}\; V_{ext}(\vec{r})\; n(\vec{r})$$

$$\varphi^*(\vec{r}) \qquad \varphi(\vec{r})$$

$$+ \frac{1}{2} \underbrace{\int d\vec{r} \int d\vec{r}\,' \frac{n(\vec{r})\, n(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}}_{\text{Hartree}}$$

$$\left(\frac{1}{2} \sum_{i,j} \left(\langle i,j | v | i,j \rangle \right) \right)^2$$

$$n(\vec{r}) = \sum_i |\varphi_i(\vec{r})|^2$$

$$+ \boxed{\underbrace{C_2 \int d\vec{r}\, n(\vec{r})^{4/3}}_{\text{exchange from elgas}}}$$