Solution to HW 3

1. a) $\psi_\sigma(r) = \sum_{i\sigma} \phi_{i\sigma}(r)\, a_{i\sigma}$

$$H_1 = \int dr\, \psi^\dagger_\sigma(r)\left(-\frac{\hbar^2}{2m}\nabla_i^2 + u(r)\right)\psi_\sigma(r) = \sum_{i\sigma j\sigma'} \int \phi^*_{i\sigma}(r)\, \underbrace{\phi_{j\sigma'}(r)}_{(-\frac{\hbar^2}{2m}\nabla + u(r))}\, dr\; a^\dagger_{i\sigma} a_{j\sigma}$$

$$= \sum_{ij,\sigma} \int dr\, \phi^*_{i\sigma}(r)\left[-\frac{\hbar^2}{2m}\nabla^2 + u(r)\right]\phi_{j\sigma}(r)\quad a^\dagger_{i\sigma} a_{j\sigma}$$

$$H_2 = \frac{1}{2}\int dr_1 dr_2\; \psi^\dagger_\sigma(r_1)\psi^\dagger_{\sigma'}(r_2)\, V(r_1-r_2)\, \psi_{\sigma'}(r_2)\, \psi_\sigma(r_1)$$

$$= \frac{1}{2}\int dr_1 dr_2 \sum_{\substack{ijlk\\ \sigma\sigma'}} \phi^*_{i\sigma}(r_1)\, a^\dagger_{i\sigma}\, \underbrace{\phi^*_{j\sigma'}(r_2)}_{V(r_1-r_2)}\, a^\dagger_{j\sigma'}\; \phi_{l\sigma'}(r_2)\, a_{l\sigma'}\; \phi_{k\sigma'}(r_1)\, a_{k\sigma}$$

for Coulumb interaction:

$$H_2 = \frac{e^2}{2}\sum_{\substack{ijlk\\ \sigma\sigma'}} \int dr_1 dr_2\, \frac{\phi^*_i(r)\,\phi^*_j(r')\,\phi_l(r')\,\phi_k(r)}{|r-r'|}\; a^\dagger_{i\sigma} a^\dagger_{j\sigma'} a_{l\sigma'} a_{k\sigma}$$

1. b) in the plane-wave basis.

$$\phi_{k\sigma}(r) = \frac{1}{\sqrt{V}} e^{i\vec{k}\vec{r}},\ \text{and if } u(r) \text{ is a constant}$$

$$H_1 = \sum_k \frac{\hbar^2 k^2}{2m}\, a^\dagger_{k\sigma} a_{k\sigma}$$

$$H_2 = \frac{e^2}{2}\sum_{k_1k_2k_3k_4} \int dr_1 dr_2\, \frac{e^{-ik_1\cdot r_1}\, e^{-ik_2 r_2}\cdot e^{ik_3 r_2}\, e^{ik_4 r_1}}{|r_1-r_2|}\, a^\dagger_{k_1\sigma} a^\dagger_{k_2\sigma'} a_{k_3\sigma'} a_{k_4\sigma}$$

introduce center of mass coordinate $R = \frac{r_1 + r_2}{2}$, $r = r_1 - r_2$

$\Rightarrow r_1 = R + \frac{r}{2}$, $r_2 = R - r/2$

$$\int dr_1 dr_2 \cdots = \int dR\, dr \; e^{-i(k_1+k_2-k_3-k_4)\cdot R} \; e^{-i(k_1-k_2+k_3-k_4)\cdot\frac{r}{2}} \times V(r)$$

$$= \delta_{k_1+k_2=k_3+k_4} \cdot V[(k_1-k_2+k_3-k_4)/2]$$

set $k_3 = k_2 - q$, $k_4 = k_1 + q \Rightarrow$

$$H_2 = \frac{1}{2} \sum_{k_1 k_2 q} V(q)\, a^+_{k_1\sigma} a^+_{k_2\sigma'} a_{k_2-q\,\sigma'} a_{k_1+q\,\sigma}, \quad \text{where } V(q) = \frac{4\pi e^2}{q^2}$$

2a): $|\psi\rangle = a^+_{i_1\sigma_1} a^+_{i_2\sigma_2} \cdots a^+_{i_n\sigma_n} |0\rangle$

$$\langle\psi| H_0 |\psi\rangle = \langle 0| a_{i_n\sigma_n} \cdots a_{i_1\sigma_1} \left[\sum_{ij\sigma} \langle i|\hat{h}|j\rangle a^+_{i\sigma} a_{j\sigma} \right] a^+_{i_1\sigma_1} \cdots a^+_{i_n\sigma_n} |0\rangle$$

we have to set $i=j$, which can be any one of $i_1, \cdots i_n$

$$\Rightarrow \langle\psi| H_0 |\psi\rangle = \sum_{i\sigma} \langle i|\hat{h}|i\rangle n_{i\sigma} = \sum_{i\sigma} n_{i\sigma} \int dr \left[\phi^*_i(r) \left(\frac{-\hbar^2}{2m}\nabla^2 + U(r)\right) \phi_i(r) \right]$$

$$\langle\psi| H_2 |\psi\rangle = \langle 0| a_{i_n\sigma_n} \cdots a_{i_1\sigma_1} \left(\frac{1}{2} \sum_{\substack{ijlk \\ \sigma\sigma'}} \langle ij|V|kl\rangle a^+_{i\sigma} a^+_{j\sigma'} a_{l\sigma'} a_{k\sigma} \right) a^+_{i\sigma_1} \cdots a^+_{i_n\sigma_n} |0\rangle$$

we have to pair the indices $i j l k$

① direct channel $\quad a^+_{i\sigma} a^+_{j\sigma'} a_{l\sigma'} a_{k\sigma}$

$i=k$, and $j=l$, each of them can take $i_1 \cdots i_n$

$$\Rightarrow \frac{e^2}{2} \sum_{ij\sigma\sigma'} n_{i\sigma} n_{j\sigma'} \int dr dr' \frac{|\phi_i(r)|^2 |\phi_j(r')|^2}{|r-r'|} \leftarrow \langle ij|V|ij\rangle$$

② exchange channel $\quad a^+_{i\sigma} a^+_{j\sigma'} a_{l\sigma'} a_{k\sigma}$

$i=l$, $j=k$ and $\sigma=\sigma'$, due to the cross. an extra minus sign

$$\Rightarrow \frac{e^2}{2}(-) \sum_{ij\sigma\sigma'} n_{i\sigma} n_{j\sigma'} \delta_{\sigma\sigma'} \langle ij|V|ji\rangle = -\frac{e^2}{2} \sum_{ij\sigma\sigma'} \underbrace{n_{i\sigma} n_{j\sigma'}}_{\delta_{\sigma\sigma'}} \int dr dr' \frac{[\phi^*_i(r) \phi^*_j(r') \times \phi_j(r) \phi_i(r')]}{|r-r'|}$$

add together $\Rightarrow$

$$\langle \psi | H | \psi \rangle = \sum_{i\sigma} n_{i\sigma} \int dr \left\{ \phi_i^*(r) \left(-\frac{\hbar^2}{2m}\nabla^2 + u(r)\right) \phi_i(r) \right\}$$

$$+ \frac{e^2}{2} \sum_{ij\sigma\sigma'} n_{i\sigma} n_{j\sigma'} \int dr dr' \left\{ \frac{|\phi_i(r)|^2 |\phi_j(r')|^2}{|r-r'|} - \delta_{\sigma\sigma'} \frac{\phi_i^*(r)\phi_j^*(r')\,\phi_j(r)\,\phi_i(r')}{|r-r'|} \right\}$$

b) introduce Lanrange multiplier λ_i for each $\int dr |\phi_i(r)|^2 = 1$.

$$E = \langle \psi | H | \psi \rangle - \sum_{i\sigma} \lambda_{i\sigma} \int |\phi_{i\sigma}(r)|^2 dr \,,$$

where $\phi_{i\sigma}(r) = \phi_i(r)\,\chi_\sigma$

χ_σ is the spin WF

$$\frac{\delta E}{\delta \phi_{i\sigma}^*} = \left(-\frac{\hbar^2}{2m}\nabla^2 + u(r)\right) \phi_i(r)\,\chi_\sigma$$

$$- \frac{e^2}{2} \sum_{j\sigma'} \delta_{\sigma\sigma'} \, n_{j\sigma'} \int dr' \frac{\phi_j^*(r')\,\phi_j(r)}{|r-r'|} \, \phi_i(r')\,\chi_\sigma$$

$$+ \frac{e^2}{2} \sum_{j\sigma'} n_{j\sigma'} \int dr' \frac{|\phi_j(r')|^2}{|r-r'|} \, \phi_i(r)\,\chi_\sigma - \lambda_{i\sigma}\,\phi_i(r)\,\chi_\sigma = 0$$

(set $n_{i\sigma} = 1$ (occupied)).

i.e

$$\left\{ -\frac{\hbar^2}{2m}\nabla^2 + u(r) + \sum_{j\sigma'} n_{j\sigma'} \int dr' \frac{|\phi_j(r')|^2}{|r-r'|} \right\} \phi_i(r)\,\chi_\sigma$$

$$- \sum_{j} \delta_{\sigma\sigma'} n_{j\sigma'} \int dr' \frac{\phi_j^*(r')\,\phi_j(r)}{|r-r'|} \, \phi_i(r')\,\chi_\sigma = \lambda_{i\sigma}\,\phi_i(r)$$

3c) $\phi_{i\sigma}(r) = e^{ik_i \cdot r} \chi_\sigma$, plug in to the HF equation

and set $U(r) = 0$.

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + \sum_{j\sigma'} \int dr' \frac{n_{j\sigma'}}{|r-r'|} \right\} \begin{matrix} e^{ik_i r} \\ \chi_\sigma \end{matrix}$$

$$- \sum_j \delta_{\sigma\sigma'} n_{j\sigma'} \int dr' \frac{e^{ik_j(r-r')}}{|r-r'|} \cdot e^{ik_i r'} \chi_\sigma$$

$$= \left\{ -\frac{\hbar^2}{2m} \nabla^2 + \sum_{j\sigma'} \int dr' \frac{n_{j\sigma'}}{|r-r'|} \right\} e^{ik_i r} \chi_\sigma$$

$$- \left\{ \sum_j \delta_{\sigma\sigma'} n_{j\sigma'} \int dr' \frac{e^{i(k_j - k_i)(r-r')}}{|r-r'|} \right\} e^{ik_i r} \chi_\sigma = \lambda_{i\sigma} e^{ik_i r} \chi_\sigma$$

Thus $\lambda_{i\sigma} = \frac{\hbar^2 k^2}{2m} + \sum_{j\sigma'} \int dr' \frac{n_{j\sigma'}}{|r-r'|}$

$$- \sum_j \delta_{\sigma\sigma'} n_{j\sigma'} \int d(r'-r) \frac{e^{i(k_j - k_i)(r-r')}}{|r-r'|}$$

thus $\lambda_{i\sigma}$ has the meaning of particle energy

= Kinetic + Hartree (direct) + Fock (exchange)

③ $\rho_\sigma(r) = \psi^+_\sigma(r)\,\psi_\sigma(r) = \sum_{ij} \phi_i^*(r)\,\phi_j(r)\, a^+_{i\sigma}\, a_{j\sigma}$

$$\langle\psi|\,\rho_\sigma(r)\,\rho_{\sigma'}(r')\,|\psi\rangle = \langle\psi|\sum_{\substack{ij\sigma \\ i'j'\sigma'}} \phi_i^*(r)\,\phi_j(r)\,\phi^*_{j'}(r')\,\phi_{i'}(r')\, a^+_{i\sigma}a_{j\sigma}\,a^+_{j'\sigma'}a_{i'\sigma'}\,|\psi\rangle$$

direct channel $i=j$ and $j'=i'$, $\Rightarrow$ $\underbrace{a^+_{i\sigma}a_{j\sigma}}\ \underbrace{a^+_{j'\sigma'}a_{i'\sigma'}}$

$$\sum_{ij\sigma\sigma'} |\phi_i(r)|^2\,|\phi_j(r')|^2\, n_{i\sigma}\, n_{j\sigma'} \quad (\text{for } i\neq j \text{ or } \sigma\neq\sigma')$$

which is just $\langle\rho_\sigma(r)\rangle\langle\rho_{\sigma'}(r')\rangle$

exchange channel $i=i'$ & $j=j'$ & $\sigma=\sigma'$ $\quad a^+_{i\sigma}\ a_{j\sigma}\ a^+_{j'\sigma'}\ a_{i'\sigma'}$

$$\rightarrow -\sum_{ij\sigma'} \delta_{\sigma\sigma'}\,\varphi_i^*(r)\,\varphi_j^*(r')\,\varphi_j(r)\,\varphi_i(r')\; n_{i\sigma}(n_{j\sigma}-1)$$

$$= -\sum_{ij\sigma'} \delta_{\sigma\sigma'}\,\varphi_i^*(r)\,\varphi_j^*(r')\,\varphi_j(r)\,\varphi_i(r')\, n_{i\sigma} n_{j\sigma} + \sum_{ij\sigma'} \delta_{\sigma\sigma'}\,\varphi_i^*(r)\,\varphi_i(r')\, n_{i\sigma} \cdot \sum_j \varphi_j(r)\,\varphi_j^*(r')$$

$$= -\sum_{ij\sigma'} \delta_{\sigma\sigma'}\,\varphi_i^*(r)\,\varphi_j^*(r')\,\varphi_j(r)\,\varphi_i(r')\, n_{i\sigma} n_{j\sigma} + \sum_{i\sigma'} \delta_{\sigma\sigma'}\,|\varphi_i(r)|^2\, n_{i\sigma}\,\delta(r-r')$$

↳ this an articfact due to normalization

$$\Rightarrow\quad G_{\sigma\sigma'}(r\,r') = \langle\psi|\,\rho_\sigma(r)\,\rho_{\sigma'}(r')\,|\psi\rangle - \langle\psi|\,\rho_\sigma(r)\,|\psi\rangle\langle\psi|\,\rho_{\sigma'}(r')\,|\psi\rangle$$

at $r \neq r'$ $\Rightarrow$

$$G_{\sigma\sigma'}(r, r') = 0 \quad \text{if} \quad \sigma \neq \sigma'$$

$$= - \sum_{ij} \varphi_i^*(r) \varphi_j^*(r') \varphi_j(r) \varphi_i(r') n_{i\sigma} n_{j\sigma} \quad \text{if} \quad \sigma = \sigma'$$

For plane wave $\Rightarrow$

$$G_{\sigma\sigma'}(rr') = -\frac{1}{V^2} \sum_{k_i k_j'} e^{i k_i (r-r')} e^{i k_j (r'-r)} n_{k_i \sigma} n_{k_j \sigma}$$

$$= - \Big[\sum_{k_i} \underbrace{e^{i k_i (r-r')} n_{k_i \sigma}}_{\left(\frac{1}{V}\right)} \Big]^2$$

$$= - \left| \frac{1}{(2\pi)^3} \int d^3\vec{k} \, e^{i \vec{k} \cdot (\vec{r} - \vec{r}')} \, \Theta(|k| < |k_F) \right|^2 . \; (\text{for } \sigma = \sigma')$$

The detail of how to do the integral is in the lecture notes

and I won't repeat.

$$G_{\sigma\sigma}(r\, r') / \langle \rho_\sigma \rangle \langle \rho_{\sigma'} \rangle = -9 \left(\frac{x \cos x - \sin x}{x^3} \right)^2$$