Lecture 1

Hartree - Fock approximation

We begin to consider electron interactions. The simplest approximation to solve interacting Hamiltonians is the Hartree - Fock approx, which is also often called the mean-field theory. The Hartree part is classic, and the Fock part takes into account the effect of Pauli's exclusion principle, i.e. the many-body wavefunctions of fermions need to be anti-symmetrized.

§1. A quick review of 2nd quantization — quantization of wavefunction.

$\boxed{\text{Single-body operator}}$ (no interaction). In the 1st quantization, the total kinetic and external potential energy is $\boxed{H_1 = \sum_{i=1}^{N} h_1(i), \text{ and } h_1(i) = -\frac{\hbar^2}{2m}\nabla_i^2 + U(r_i)}$

we need to fix the particle number N, and the many-body wavefunction is also complicated. If we neglect electron spin for the moment, a N-body wavefunction typically can be written as a Slater derterminaint type as:

$$\psi(x_1, \cdots x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \cdots & \phi_2(x_N) \\ \vdots & \vdots & & \vdots \\ \phi_N(x_1) & \phi_N(x_2) & \cdots & \phi_N(x_N) \end{vmatrix},$$

where ϕ_i $(i=1, \cdots N)$ is a set of orth-normal single-particle state. $\psi(x_1, \cdots x_N)$ describes a N-particle state in which each single-particle state is filled with one electron. The Slater determinaint wavefunction satisfies the anti-symmetric property,

$$\boxed{\psi(r_1, \cdots r_i, \cdots r_j \cdots r_N) = -\psi(r_1, \cdots r_j \cdots r_i \cdots r_N)}.$$

We introduce field operator $\psi_\alpha^\dagger(\vec{r})$ and $\psi_\alpha(\vec{r})$, They anti-commute ~~wi~~ satisfying

$$\boxed{\begin{aligned}&\{\psi_\alpha(\vec{r}), \psi_\beta^\dagger(\vec{r}')\} \\ &= \delta_{\alpha\beta}\, \delta(\vec{r}-\vec{r}')\end{aligned}} = \psi_\alpha(\vec{r})\psi_\beta^\dagger(\vec{r}') + \psi_\beta^\dagger(\vec{r}')\psi_\alpha(\vec{r}) =$$

α, β are spin indices.

Apply $\psi_\alpha^\dagger(\vec{r})$ on the vaccum, we obtain a single-particle state with spin α, and it's a coordinate eigenstate located at $\vec{r}$, i.e

$$\langle \vec{r}', \alpha' | \psi_\alpha^\dagger(\vec{r}) | vac \rangle = \delta(\vec{r}-\vec{r}')\, \delta_{\alpha\alpha'}.$$

We define the density operator $\rho(r) = \sum_\alpha \psi_\alpha^\dagger(r)\psi_\alpha(r)$, For a many-body state $|\Psi\rangle$, $\langle \Psi | \rho(\vec{r}) | \Psi \rangle$ gives to electron density at $\vec{r}$.

So, 2nd quantization can be viewed as quantization of wavefunctions $\longrightarrow$ field operators.

using field operator, the single-body operator H_1 can be represented as

$$\boxed{H_1 = \sum_\sigma \int \psi_\sigma^\dagger(r)\, h_1(\vec r)\, \psi_\sigma(r)\, d\vec r = \sum_\sigma \int d\vec r\, \psi_\sigma^\dagger(\vec r)\left(\frac{-\hbar^2}{2m}\nabla_r^2 + U(r)\right)\psi_\sigma(\vec r)}$$

In many situation, we need to work with different single-particle basis, say, the momentum representation. We expand the field operator in a general basis as

$$\begin{cases} \psi_\sigma(r) = \sum_{i,\sigma} \varphi_{i,\sigma}(r)\, a_{i,\sigma} \\ \psi_\sigma^\dagger(r) = \sum_{i,\sigma} \varphi_{i,\sigma}^*(r)\, a_{i,\sigma}^\dagger \end{cases}$$

where $\{a_{i,\sigma}, a_{j\sigma'}^\dagger\} = \delta_{ij}\delta_{\sigma\sigma'}$, and $a_{i,\sigma}^\dagger, a_{i,\sigma}$ are creation/annihilation operators for the mode of $\varphi_{i,\sigma}$. $N_{i,\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$ represent the occupation number of the state $\varphi_{i,\sigma}$. Under the basis of $\varphi_{i,\sigma}(r)$, we have

$$\boxed{\begin{aligned} H_1 &= \sum_{\substack{ij\\ \sigma\sigma'}} \langle i\sigma | h_1 | j\sigma' \rangle\, a_{i\sigma}^\dagger a_{j\sigma'} = \sum_{ij,\sigma} \langle i | h_1 | j \rangle\, a_{i\sigma}^\dagger a_{j\sigma} \\ \text{where} \quad &\langle i\sigma | h_1 | j\sigma' \rangle = \delta_{\sigma\sigma'} \langle i_\sigma | h_1 | j_\sigma \rangle = \int \varphi_{i\sigma}^*(r)\left(-\frac{\hbar^2}{2m}\nabla^2 + U(r)\right)\varphi_{j\sigma}(r)\, dr \end{aligned}}$$

if $U(r) = 0$, we can use the momentum representation, or, the plane-wave basis: $\quad \varphi_k(r) = \frac{1}{\sqrt{V}} e^{i\vec k\cdot\vec r}$

$$\Rightarrow \boxed{H_1 = \sum_{k,\sigma} a_{k\sigma}^\dagger a_{k\sigma} \frac{\hbar^2 k^2}{2m}}$$

$\boxed{\text{two-body operators (interaction).}}$ $\boxed{h_2 = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}}$

1st quantization: $H_2 = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} = \frac{1}{2} \sum_{i \neq j} h_2(\vec{r}_i, \vec{r}_j)$

→ 2nd quantization (using $\psi^\dagger_\sigma, \psi_\sigma$)

$$\boxed{H_2 = \frac{e^2}{2} \sum_{\sigma\sigma'} \int dr\, dr' \, \frac{\psi^\dagger_\sigma(r)\, \psi^\dagger_{\sigma'}(r')\, \psi_{\sigma'}(r')\, \psi_\sigma(r)}{|\vec{r} - \vec{r}'|}}$$

Please note the sequence of field operators.

→ change to a general basis

$$H_2 = \frac{1}{2} \sum_{\substack{ijlk \\ \sigma_i \sigma_j \sigma_l \sigma_k}} \langle i\sigma_i\, j\sigma_j | h_2 | l\sigma_l, k\sigma_k \rangle\, a^\dagger_{i\sigma_i} a^\dagger_{j\sigma_j} a_{l\sigma_l} a_{k\sigma_k}$$

$$\boxed{H_2 = \frac{1}{2} \sum_{\substack{ijlk \\ \sigma,\sigma'}} \langle \underset{\sigma}{i} \underset{\sigma'}{j} | h_2 | \underset{\sigma'}{l} \underset{\sigma}{k} \rangle\, a^\dagger_{i\sigma} a^\dagger_{j\sigma'} a_{l\sigma'} a_{k\sigma}}$$

$$\langle i\sigma_i\, j\sigma_j | h_2 | l\sigma_l\, k\sigma_k \rangle = \delta_{\sigma_i \sigma_k} \delta_{\sigma_j \sigma_l} \langle i_{\sigma_i}\, j_{\sigma_j} | h_2 | l_{\sigma_j}\, k_{\sigma_i} \rangle$$

$$\langle i\sigma\, j\sigma' | h_2 | l_{\sigma'}\, k_\sigma \rangle = e^2 \int dr\, dr' \, \varphi^*_{i\sigma}(r)\, \varphi^*_{j\sigma'}(r') \frac{e^2}{|r - r'|} \varphi_{l\sigma'}(r')\, \varphi_{k\sigma}(r)$$

→ $H = H_1 + H_2$

$$\boxed{H = \sum_{ij\sigma} \langle \underset{\sigma}{i} | h_1 | j\sigma \rangle\, a^\dagger_{i\sigma} a_{j\sigma} + \frac{1}{2} \sum_{\substack{ijlk \\ \sigma\sigma'}} \langle \underset{\sigma}{i} \underset{\sigma'}{j} | h_2 | \underset{\sigma'}{l} \underset{\sigma}{k} \rangle\, a^\dagger_{i\sigma} a^\dagger_{j\sigma'} a_{l\sigma'} a_{k\sigma}.}$$

Hamiltonian interacting electrons (2nd quantized form!)

§ Hartree-Fock state

We seek a trial wavefunction of the Slater determinant type

$$\Psi = a^{+}_{i\sigma_i} a^{+}_{j\sigma_j} \cdots a^{+}_{l\sigma_l} |0\rangle , \quad N = \text{total particle number}$$

we minimize $\langle \Psi | H | \Psi \rangle$ under the constraint that each basis is orth-normal, i.e $\int \varphi^*_{i\sigma}(r)\, \varphi_{i\sigma}(r)\, dr = 1$. This constraint can be imposed by introducing Langragian multiplier $\lambda_{i\sigma}$, $\Rightarrow$

we need to minimize the functional

$$E[\varphi^*_{i\sigma}, \varphi_{i\sigma}] = \langle \Psi | H | \Psi \rangle - \sum_{i\sigma} \lambda_{i\sigma} \left[\int dr \left(\phi^*_{i\sigma} \phi_{i\sigma} \right) - 1 \right].$$

① $$\langle \Psi | H_1 | \Psi \rangle = \sum_{ij\sigma} \langle i\sigma | h_1 | j\sigma \rangle \langle \Psi | a^{+}_{i\sigma} a_{j\sigma} | \Psi \rangle$$

we need $i=j$, otherwise $\langle \Psi | a^{+}_{i\sigma} a_{j\sigma} | \Psi \rangle = 0 \Rightarrow$

$$\langle \Psi | H_1 | \Psi \rangle = \sum_{i,\sigma} \langle i\sigma | h_1 | i\sigma \rangle \langle \Psi | a^{+}_{i\sigma} a_{i\sigma} | \Psi \rangle$$

$n_{i\sigma}$

$$= \sum_{i,\sigma} n_{i\sigma} \int dr\, \varphi^*_{i\sigma} \left[-\frac{\hbar^2}{2m} \nabla^2 + u(r) \right] \varphi_{i\sigma}(r)$$

② $$\langle \Psi | H_2 | \Psi \rangle = \frac{1}{2} \sum_{\substack{ijlk \\ \sigma\sigma'}} \langle i\sigma\, j\sigma' | h_2 | l\sigma'\, k\sigma \rangle \langle \Psi | a^{+}_{i\sigma} a^{+}_{j\sigma'} a_{l\sigma'} a_{k\sigma} | \Psi \rangle$$

Hartree contribution $j=l$, $i=k$, but we need to exclude $i=j=l=k$ and $\sigma=\sigma'$

$$\langle \Psi | a^{+}_{i\sigma} a^{+}_{j\sigma'} a_{j\sigma'} a_{i\sigma} | \Psi \rangle = \left(n_{i\sigma} n_{j\sigma'} - n_{i\sigma} \delta_{ij} \delta_{\sigma\sigma'} \right)$$

Hartree

Fock contribution $\sigma=\sigma'$, $i=l$, $j=k$, but exclude $i=l=j=k$ & $\sigma=\sigma'$

$$\langle\Psi|\, a^{+}_{i\sigma}\, a^{+}_{j\sigma}\, a_{i\sigma}\, a_{j\sigma}\, |\Psi\rangle = -\,(n_{i\sigma}n_{j\sigma} - n_{i\sigma}\delta_{ij}\delta_{\sigma\sigma'})$$

minus sign comes from Fermi statistics

$$\Rightarrow \langle\Psi|H_2|\Psi\rangle = \frac{1}{2}\sum_{ij,\sigma\sigma'}\Big\{\langle i\sigma\, j\sigma'|h_2|j\sigma'\, i\sigma\rangle\,(n_{i\sigma}n_{j\sigma'} - n_{i\sigma}\delta_{ij}\delta_{\sigma\sigma'})$$

$$-\,\langle i\sigma\, j\sigma'|h_2|i\sigma'\, j\sigma\rangle\,\delta_{\sigma\sigma'}\,(n_{i\sigma}n_{j\sigma} - n_{i\sigma}\delta_{ij})\Big\}$$

$$= \frac{1}{2}\sum_{\substack{ij\\ \sigma\sigma'}}\Big\{\underbrace{\langle i\sigma\, j\sigma'\,|\,h_2\,|\,j\sigma'\, i\sigma\rangle}_{\text{Hartree}} - \underbrace{\delta_{\sigma\sigma'}\langle i\sigma\, j\sigma'|\,h_2\,|\,i\sigma' j\sigma\rangle}_{\text{Fock}}\Big\}\, n_{i\sigma}n_{j\sigma'}$$

Hartree → classic electrostatics

Fock: Quantum statistics

$$\langle i\sigma\, j\sigma'|h_2|j\sigma'\, i\sigma\rangle = \int dr\,dr'\;\frac{\varphi^{*}_{i\sigma}(r)\,\varphi^{*}_{j\sigma'}(r')\,\varphi_{j\sigma'}(r')\,\varphi_{i\sigma}(r)}{|\vec{r}-\vec{r}'|}$$

$$\langle i\sigma\, j\sigma'|\,h_2\,|i\sigma'\, j\sigma\rangle = \int dr\,dr'\;\frac{\varphi^{*}_{i\sigma}(r)\,\varphi^{*}_{j\sigma'}(r')\,\varphi_{i\sigma'}(r')\,\varphi_{j\sigma}(r)}{|\vec{r}-\vec{r}'|}$$

$$\rightarrow\ \boxed{\begin{aligned} E[\varphi^{*}_{i\sigma}\varphi_{i\sigma}] = {} & \sum_{i\sigma} n_{i\sigma}\int dr\;\varphi^{*}_{i\sigma}(r)\left(-\frac{\hbar^2\nabla^2}{2m} + u(r)\right)\varphi_{i\sigma}(r) - \sum_{i\sigma}\lambda_{i\sigma}\int dr\left(\varphi^{*}_{i}\varphi_{i} - 1\right) \\ & + \sum_{ij,\sigma\sigma'} n_{i\sigma}n_{j\sigma'}\Big(\int dr\,dr'\;\frac{\varphi^{*}_{i\sigma}(r)\,\varphi^{*}_{j\sigma'}(r')\,\varphi_{j\sigma'}(r')\,\varphi_{i\sigma}(r) - \delta_{\sigma\sigma'}\,\varphi^{*}_{i\sigma}(r)\,\varphi^{*}_{j\sigma'}(r')\,\varphi_{i\sigma'}(r')\,\varphi_{j\sigma}(r)}{|\vec{r}-\vec{r}'|}\end{aligned}}$$

Do variation with respect to $\varphi^*_{i\sigma}$, and set $n_{i\sigma}=1$ for occupied state $\Rightarrow$

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

$$-\sum_j n_{j\sigma}\int dr' \frac{\varphi^*_{j\sigma}(r')\,\varphi_{j\sigma}(r)}{|\vec{r}-\vec{r}\,'|}\quad \varphi_{i\sigma}(r') = \lambda_{i,\sigma}\,\varphi_{i\sigma}(r)$$

The Hartree-potential is local, but Fock-one is not.

H-F equation need to be solved self-consistently, and it's often complicated!

(*) If $u(r) =$ constant, we can use plane-wave $\varphi_{i\sigma}(r) = \frac{1}{\sqrt{V}}e^{i\vec{k}_i\cdot\vec{r}}$

$\Rightarrow$ Hartree part $\frac{1}{V}\sum_{k\sigma'} n_{k\sigma}\int dr \frac{1}{|\vec{r}-\vec{r}\,'|} = n\cdot V(q\to 0)$

$$V(q) = \frac{4\pi e^2}{q^2}.\quad \left(\text{Fourier transform of } \frac{e^2}{r}\right).$$

Hartree term diverge reflecting long range nature of Coulomb force. We set $u(r) =$ Hartree to cancel, which is the contribution from positive charge background.

$\Rightarrow$ Fock $-\frac{1}{V}\sum_{K_j} n_{K_j}\int dr' \frac{e^{i(\vec{k}_i-\vec{k}_j)\cdot\vec{r}\,'}}{|\vec{r}-\vec{r}\,'|}\left(\frac{1}{\sqrt{V}}e^{i(\vec{k}_j\cdot\vec{r})}\right)$

$$= \underbrace{-\left[\int\frac{d^3k}{(2\pi)^3} n_k\, V(k-k_i)\right]}_{\text{Fock - self energy}}\frac{1}{\sqrt{V}}e^{i\vec{k}_i\cdot\vec{r}}$$

Koopman's theorem: let us try to understand the physical meaning of $\lambda_{i\sigma}$, which equals

$$\lambda_{i\sigma} = \int dr\, \varphi^*_{i\sigma} \left(-\frac{\hbar^2}{2m}\nabla^2 + u(r)\right) \varphi_{i\sigma} + \sum_{j\sigma'} n_{j\sigma'} \int dr dr' \frac{|\varphi_i(r)|^2 |\varphi_j(r')|^2}{|r-r'|}$$

$$- \sum_j n_{j\sigma} \int dr dr' \frac{\varphi^*_i(r)\, \varphi^*_j(r')\, \varphi_j(r)\, \varphi_i(r')}{|r-r'|} .$$

This expression can be obtained by $\boxed{\lambda_{i,\sigma} = \delta E / \delta n_{i,\sigma}}$. Thus $\lambda_{i,\sigma}$ can be considered as the "energy" of the electron in the state (i, σ).

But the ground state energy should not be written as

$$E = \sum_{i\sigma} n_{i\sigma} \lambda_{i,\sigma}, \quad (\text{wrong}).$$

The interaction energy is double counted!

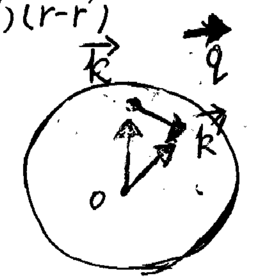
Jellium model Generally, speaking, the HF equation has to solved numerically by iteration. If the external potential (ionic potential) is a constant, it is easy to show that the plane waves are still a solution to HF equation. This correspondes to the case that we averge ionic charge as a uniform positive background to maintain the charge neutrality.

☆ ex: check plane waves are indeed a solution to the HF equation.

let us evaluate the HF energy. for the filled Fermi surface:

The Hartree part cancels with background charge, but the Fock part

$$\mathcal{E}_{HF}(k)_\sigma = \overset{0}{\mathcal{E}}(k) - \frac{1}{V}\sum_{k'} n_{k'\sigma} \cdot \int dr' \frac{e^2}{|r-r'|} e^{i(k-k')(r-r')}$$



$$= \overset{0}{\mathcal{E}}(k) - \frac{1}{V}\sum_{k'} n_{k',\sigma} \frac{4\pi e^2}{|k-k'|^2} \qquad \theta(k'<k_F)$$

$$\delta\mathcal{E}_{HF}(k) = -\frac{1}{V}\sum_{k'} n_{k'\sigma}\frac{4\pi e^2}{|k-k'|^2} = -\frac{1}{(2\pi)^3}\int_0 d\vec{k}' \cdot \frac{4\pi e^2}{|\vec{k}-\vec{k}'|^2}$$

define $\vec{q} = \vec{k}' - \vec{k} \Rightarrow \vec{k}' = \vec{k} + \vec{q} \Rightarrow k'^2 = k^2 + q^2 + 2k\cdot q\cos\theta$

$$\Rightarrow \delta\mathcal{E}_{HF}(k) = -\frac{4\pi e^2}{(2\pi)^3} \cdot 2\pi \int_0^\infty dq \int_{-1}^{1} d\cos\theta \;\; \theta_1\left(k_F^2 - (k^2+q^2+2k\cdot q\cos\theta)\right)$$

$$= -\frac{2e^2}{\pi}k_F \;\frac{1}{2}\int_0^\infty dz \int_{-1}^{1} d(\cos\theta)\;\theta\left(1 - (x^2+z^2+2xz\cos\theta)\right)$$

$$= -\frac{2e^2}{\pi}k_F\; F(x), \qquad (z = q/k_F,\; x = k/k_F)$$

$$F(x) = \frac{1}{2}\int_0^\infty f(z)\,dz, \qquad \begin{cases} f(z) = 2 & |x+z|<1 \\ f(z) = \dfrac{1-(x-z)^2}{2x^2} & \text{otherwise} \\ f(z) = 0 & |x-z|>1 \end{cases}$$

☆ ex: <u>the evaluation of $F(x)$</u>

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

comments: ① exchange interaction is negative, which only exists between electrons with the same spin.

② $\delta \mathcal{E}_{HF} \sim k_F$, while the $\mathcal{E}_F \sim k_F^2$. thus in the low density region, $\delta \mathcal{E}_{HF}$ could dominate over $\mathcal{E}_{kinetic}$. The naive analysis would give a Ferromagnetic state at low density. But this is a unreliable result.

③ as $k \to k_F$, $\delta \mathcal{E}_{HF}(k) \sim -e^2 (k-k_F) \ln[|k-k_F|/k_F]$

the velocity shift $v(k) = \hbar^{-1} \partial \mathcal{E}/\partial k \Rightarrow v(k) \sim \underbrace{\ln(k_F/|k-k_F|)}_{\text{divergence}}$

This would give a specific heat suppression as $\sim T/\ln(T_F/T)$

This is not correct!

This difficulty lies in the long wavelength part of Coulomb potential $\sim 1/q^2$

$$\sum_q n_{k+q} \frac{1}{q^2} \sim \int q^2 dq \, d\cos\theta \, \frac{1}{q^2} \, \theta_H(\mathcal{E}_k + q v_F \cos\theta < \mathcal{E}_F)$$

$$= \int q^2 dq \, d\cos\theta \, \frac{1}{q^2} \, \theta_H[v_F (k_F - k) - q v_F \cos\theta]$$

$$\frac{\partial}{\partial k}\left(\sum_q n_{k+q} \frac{1}{q^2}\right) \sim \int q^2 dq \, d\cos\theta \, \frac{1}{q^2} \, \delta[(k_F - k) - q \cos\theta]$$

$$= \int dq \, \frac{1}{q} \, \theta(|k_F - k| < q) \sim \ln \frac{k_F}{|k-k_F|}.$$

we will see the this difficulty can be removed by taking into account of screening. — the Coulomb potential becomes short ranged!

$\boxed{\text{exchange hole}}$ let us calculate the density correlation function

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

the first term is just $\langle \rho_\sigma(r) \rangle \langle \rho_{\sigma'}(r') \rangle$, thus

$$\langle \rho_\sigma(r)\, \rho_{\sigma'}(r') \rangle - \langle \rho_\sigma(r) \rangle \langle \rho_{\sigma'}(r') \rangle = -\sum_{ij} \delta_{\sigma\sigma'} \varphi_i^*(r) \varphi_j^*(r') \varphi_j(r) \varphi_i(r'),$$

where means nearby an electron it is unlikely to find another electron with the same spin, i.e. the appearance of a hole.

For uniform system, the above express reduces to

$$-\frac{1}{V^2} \sum_{kk'} e^{i(k-k')(r-r')} n_k n_{k'}$$

$$= -\frac{1}{(2\pi)^6} \int d\vec{k}\, d\vec{k}'\, e^{i(\vec{k}-\vec{k}')\cdot(\vec{r}-\vec{r}')}\, \Theta(k_F - k)\, \Theta(k_F - k')$$

$$= -\left[\frac{1}{(2\pi)^3} \int d\vec{k}\, e^{i(\vec{k})\cdot(\vec{r}-\vec{r}')}\, \Theta(k_F - k) \right]^2$$

$$\int_0^{k_F} \frac{d\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} = \frac{n}{2} \cdot \int_0^{k_F} dk \cdot k^2 \int_{-1}^{1} dx\, e^{ik|r-r'|x} \Big/ 2\int_0^{k_F} k^2\, dk$$

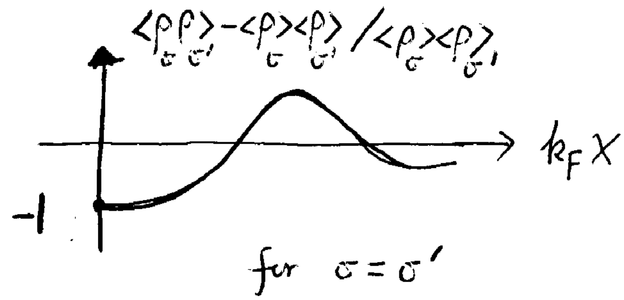
$$\left(\frac{n}{2} = \frac{k_F^3}{6\pi^2} \right)$$

$$= \frac{1}{2\pi^2 |r-r'|} \int_0^{k_F} dk.\, k \sin k|r-r'| = \frac{1}{2\pi^2 |r-r'|} \frac{d}{d(|r-r'|)} \int_0^{k_F} \cos k(|r-r'|)\, dk$$

$$= \frac{1}{2\pi^2 |r-r'|} \frac{d}{d(|r-r'|)} \left(\frac{\sin k_F(|r-r'|)}{|r-r'|} \right)$$

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

with $x \equiv k_F |r-r'|$



For electrons with opposite spin, there are no correlation at HF level

However, this is not ture. Interactions can also bring correlations $\langle\rho_\uparrow(r)\rho_\downarrow(r')\rangle$.

~~In other words which can exhibit correlation hole.~~