

Lecture 3 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.

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

operator (no interaction)
Single-body

In the 1st quantization, the total kinetic and external potential energy is $H_1 = \sum_{i=1}^N h_i(i)$, and $h_i(i) = -\frac{\hbar^2}{2m} \nabla_i^2 + U(r_i)$

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 determinant type as:

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

where ϕ_i ($i=1, \dots, N$) is a set of orth-normal single-particle state. (2)

$\psi(x_1, \dots, x_N)$ describes a N -particle state in which each single-particle state is filled with one electron. The Slater determinant wavefunction satisfies the anti-symmetric property,

$$\psi(r_1, \dots, r_i, \dots, r_j, \dots, r_N) = -\psi(r_1, \dots, r_j, \dots, r_i, \dots, r_N)$$

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

satisfying

$$\{\psi_\alpha(\vec{r}), \psi_\beta^\dagger(\vec{r}')\} = \psi_\alpha(\vec{r})\psi_\beta^\dagger(\vec{r}') + \psi_\beta^\dagger(\vec{r}')\psi_\alpha(\vec{r}) = \delta_{\alpha\beta} \delta(\vec{r}-\vec{r}') \leftarrow \alpha, \beta \text{ are spin indices.}$$

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

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

We define the density operator $\rho(\vec{r}) = \sum_\alpha \psi_\alpha^\dagger(\vec{r})\psi_\alpha(\vec{r})$, 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 (3)

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

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

$$\psi_{\sigma}(\vec{r}) = \sum_{i,\sigma} \varphi_{i,\sigma}(\vec{r}) a_{i,\sigma}$$

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

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 $\varphi_{i,\sigma}(\vec{r})$, we have

$$H_1 = \sum_{\substack{i,j \\ \sigma,\sigma'}} \langle i\sigma | h_1 | j\sigma' \rangle a_{i\sigma}^{\dagger} a_{j\sigma'} = \sum_{i,j,\sigma} \langle i | h_1 | j \rangle a_{i\sigma}^{\dagger} a_{j\sigma}$$

where $\langle i\sigma | h_1 | j\sigma' \rangle = \delta_{\sigma\sigma'} \langle i | h_1 | j \rangle = \int \varphi_{i\sigma}^*(\vec{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right) \varphi_{j\sigma}(\vec{r}) d\vec{r}$

if $U(\vec{r}) = 0$, we can use the momentum representation, or, the plane-

wave basis:

$$\varphi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

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

$$h_2 = \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

two-body operators (interaction).

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 $\psi_\sigma^\dagger, \psi_\sigma$)

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

Please note the sequence of field operators.

→ change to a general basis

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

$$H_2 = \frac{1}{2} \sum_{\substack{ijkl \\ \sigma_i \sigma'}} \langle ij | h_2 | lk \rangle_{\sigma_i \sigma'} a_{i\sigma_i}^\dagger a_{j\sigma'}^\dagger a_{l\sigma_l} a_{k\sigma}$$

$$\langle i\sigma_i j\sigma_j | h_2 | l\sigma_l k\sigma_k \rangle = \delta_{\sigma_i \sigma_k} \delta_{\sigma_j \sigma_l} \langle i\sigma_i j\sigma_j | h_2 | l\sigma_j k\sigma_i \rangle$$

$$\langle i\sigma_j \sigma' | h_2 | l\sigma_l k\sigma \rangle = e^2 \int dr dr' \frac{\phi_{i\sigma}^*(r) \phi_{j\sigma'}^*(r')}{|\vec{r} - \vec{r}'|} \phi_{l\sigma_l}(r') \phi_{k\sigma}(r)$$

$$H = H_1 + H_2$$

$$H = \sum_{ij\sigma} \langle i | h_1 | j \sigma \rangle a_{i\sigma}^\dagger a_{j\sigma} + \frac{1}{2} \sum_{ijkl \sigma\sigma'} \langle ij | h_2 | lk \rangle_{\sigma\sigma'} a_{i\sigma}^\dagger a_{j\sigma'}^\dagger a_{l\sigma_l} a_{k\sigma}$$

Hamiltonian interacting electrons (2nd quantized form!)

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Hartree - Fock state

We seek a trial wavefunction of the Slater determinant type

$$\Psi = a_{i\sigma}^+ a_{j\sigma'}^+ \dots a_{\ell\sigma\ell}^+ |0\rangle, \quad N = \text{total particle number}$$

We minimize $\langle \Psi | H | \Psi \rangle$ under the constraint that each basis is orth-normal, i.e $\int \phi_{i\sigma}^*(r) \phi_{i\sigma}(r) dr = 1$. This constraint

can be imposed by introducing Lagrangian multiplier $\lambda_{i\sigma}$, \Rightarrow

we need to minimize the functional

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

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

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

$$\begin{aligned} \langle \Psi | H_1 | \Psi \rangle &= \sum_{i\sigma} \langle i\sigma | h_1 | i\sigma \rangle \langle \Psi | a_{i\sigma}^+ a_{i\sigma} | \Psi \rangle \\ &= \sum_{i\sigma} n_{i\sigma} \int dr \phi_{i\sigma}^* \left[-\frac{\hbar^2}{2m} \nabla^2 + U(r) \right] \phi_{i\sigma} \end{aligned}$$

$$\textcircled{2} \langle \Psi | H_2 | \Psi \rangle = \frac{1}{2} \sum_{\substack{ijkl \\ \sigma\sigma'}} \langle ij | h_2 | lk \rangle \langle \Psi | a_{i\sigma}^+ a_{j\sigma'}^+ a_{\ell\sigma} a_{k\sigma'} | \Psi \rangle$$

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

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

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Fock contribution $\sigma = \sigma', i = l, j = k$, but exclude $i = l = j = k$ & $\sigma = \sigma'$ (6)

$$\langle \Psi | \underbrace{a_{i\sigma}^\dagger a_{j\sigma}^\dagger a_{i\sigma} a_{j\sigma}} | \Psi \rangle = - (n_{i\sigma} n_{j\sigma} - n_{i\sigma} \delta_{ij} \delta_{\sigma\sigma'})$$

↑
minus sign comes from Fermi statistics

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

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

↓
classic electrostatics
↓
Quantum statistics

$$\langle i\sigma j\sigma' | h_2 | j\sigma' i\sigma \rangle = \int d\mathbf{r} d\mathbf{r}' \frac{\varphi_{i\sigma}^*(\mathbf{r}) \varphi_{j\sigma'}^*(\mathbf{r}') \varphi_{j\sigma'}(\mathbf{r}') \varphi_{i\sigma}(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|}$$

$$\langle i\sigma j\sigma' | h_2 | i\sigma' j\sigma \rangle = \int d\mathbf{r} d\mathbf{r}' \frac{\varphi_{i\sigma}^*(\mathbf{r}) \varphi_{j\sigma'}^*(\mathbf{r}') \varphi_{i\sigma'}(\mathbf{r}') \varphi_{j\sigma}(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|}$$

$$\Rightarrow E[\varphi_i^* \varphi_i] = \sum_{i\sigma} n_{i\sigma} \int d\mathbf{r} \varphi_{i\sigma}^*(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} + u(\mathbf{r}) \right) \varphi_{i\sigma}(\mathbf{r}) - \sum_{i\sigma} n_{i\sigma} \int d\mathbf{r} (\varphi_i^* \varphi_i - 1) \\ + \sum_{ij, \sigma\sigma'} n_{i\sigma} n_{j\sigma'} \left[\int d\mathbf{r} d\mathbf{r}' \frac{\varphi_{i\sigma}^*(\mathbf{r}) \varphi_{j\sigma'}^*(\mathbf{r}') \varphi_{j\sigma'}(\mathbf{r}') \varphi_{i\sigma}(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} - \delta_{\sigma\sigma'} \int d\mathbf{r} d\mathbf{r}' \frac{\varphi_{i\sigma}^*(\mathbf{r}) \varphi_{j\sigma'}^*(\mathbf{r}') \varphi_{i\sigma'}(\mathbf{r}') \varphi_{j\sigma}(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} \right]$$

Do variation with respect to $\varphi_{i\sigma}^*$, and set $n_{i\sigma} = 1$ for occupied state \Rightarrow ⑦

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

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

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

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

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

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

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

$$= \left[\frac{d^3k}{(2\pi)^3} n_{\vec{k}} V(\vec{k}-\vec{k}_i) \right] \frac{1}{\sqrt{V}} e^{i\vec{k}_i \cdot \vec{r}}$$

Fock-self energy

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 $\lambda_{i,\sigma} = \frac{\delta E}{\delta n_{i,\sigma}}$. 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!

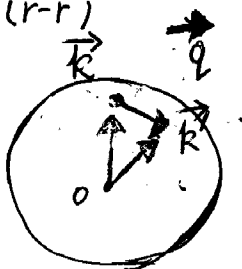
Jellium model Generally, speaking, the HF equation has to be solved numerically by iteration. If the external potential (ionic potential) is a constant, it is easy to show that the plane waves are still a solution to HF equation. This corresponds to the case that we average ionic charge as a uniform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

$$E_{HF}(k)_\sigma = \epsilon^0(k) - \frac{1}{V} \sum_{k'} n_{k',\sigma} \int dr' \frac{e^2}{|r-r'|} e^{i(k-k')(r-r')}$$

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


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

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

$$\Rightarrow \delta E_{HF}(k) = -\frac{4\pi e^2}{(2\pi)^3} \cdot 2\pi \int_0^\infty dq \int_{-1}^1 d \cos \theta \theta(k_F^2 - (k^2 + q^2 + 2kq \cos \theta))$$

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

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

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

* ex: the evaluation of $F(x)$

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

(6)

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

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

③ as $k \rightarrow k_F$, $\delta E_{HF}(k) \sim -e^2 (k - k_F) \ln[|k - k_F|/k_F]$

the velocity shift $v(k) = \hbar^{-1} \partial E / \partial k \Rightarrow v(k) \sim \ln(k_F/|k - k_F|)$
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 $\sim \frac{1}{q^2}$

$$\sum_{\mathbf{q}} n_{\mathbf{k}+\mathbf{q}} \frac{1}{q^2} \sim \int q^2 dq d\omega \frac{1}{q^2} \Theta_H(\epsilon_k + q v_F \cos \theta \leq \epsilon_F)$$

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

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

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

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

exchange hole

let us calculate the density correlation function

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

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

$$\begin{aligned} & - \frac{1}{V^2} \sum_{k k'} e^{i(k-k')(r-r')} n_k n_{k'} \\ & = - \frac{\rho}{(2\pi)^6} \int d\vec{k} d\vec{k}' e^{i(\vec{k}-\vec{k}') \cdot (\vec{r}-\vec{r}')} \Theta(k_F - k) \Theta(k_F - k') \\ & = - \left[\frac{1}{(2\pi)^3} \int d\vec{k} e^{i\vec{k} \cdot (\vec{r}-\vec{r}')} \Theta(k_F - k) \right]^2 \end{aligned}$$

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

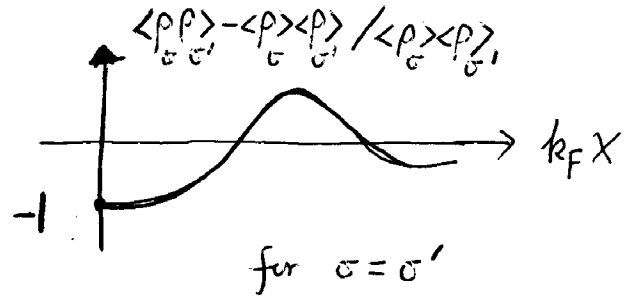
$$\left(n = \frac{k_F^3}{6\pi^2} \right)$$

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

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

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

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



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

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

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