

§2. Electron gas

*) Interacting electron gas (Jellium model)

$$H = H_0 + H_I$$

$$H_0 = \sum_{\vec{k}} \epsilon_{\vec{k}} C_{\vec{k},\sigma}^{\dagger} C_{\vec{k},\sigma}$$

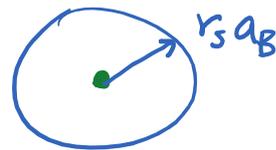
$$H_I = \frac{1}{2} \sum_{\vec{p}, \vec{q}, \vec{k}} \frac{e^2}{\epsilon_0 V |\vec{k}|^2} C_{\vec{p}+\vec{k},\sigma}^{\dagger} C_{\vec{q}-\vec{k},\sigma'}^{\dagger} C_{\vec{q},\sigma'} C_{\vec{p},\sigma}$$

Develop a perturbative expansion when H_0 is dominant over H_I .

$$|F_S\rangle = \prod_{|\vec{k}| < k_F} \prod_{\sigma=\uparrow,\downarrow} C_{\vec{k},\sigma}^{\dagger} |0\rangle$$

$$E_0 = \langle F_S | H_0 | F_S \rangle$$

$$= \frac{3}{5} \epsilon_F \cdot N_e$$



$$\left\{ \begin{aligned} \frac{1}{n} &= \frac{V}{N_e} = \frac{4}{3} \pi (r_s a_B)^3 \\ k_F &= (3\pi^2 n)^{1/3} \end{aligned} \right.$$

$$\Rightarrow \frac{E_0}{N_e} = \frac{3}{5} \epsilon_F \approx \frac{2.21}{r_s^2} \text{ Ry}$$

Rydberg energy unit: $1 \text{ Ry} \approx 13.6 \text{ eV}$

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(2)

Before calculating the interaction energy, we need to "fix" a divergence issue:

$$H_I = \frac{1}{2} \sum_{\vec{p}, \vec{q}, \vec{k}} \frac{e^2}{\epsilon_0 V |\vec{k}|^2} C_{\vec{p}+\vec{k}, \sigma}^+ C_{\vec{q}-\vec{k}, \sigma'}^+ C_{\vec{q}, \sigma'} C_{\vec{p}, \sigma}$$

$\underbrace{\hspace{10em}}_{= V_{\vec{k}}}$

$\vec{k}=0$ term causes a divergence since $V_{\vec{k}=0} \rightarrow \infty$

$\vec{k}=0$ term in H_I

$$= \frac{1}{2} \sum_{\vec{p}, \vec{q}} V_{\vec{k}=0} C_{\vec{p}, \sigma}^+ C_{\vec{q}, \sigma'}^+ C_{\vec{q}, \sigma'} C_{\vec{p}, \sigma}$$

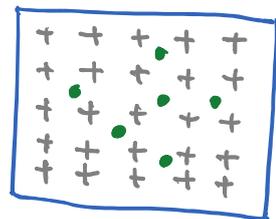
$$\approx \frac{1}{2} V_{\vec{k}=0} \underbrace{\sum_{\vec{p}, \sigma} C_{\vec{p}, \sigma}^+ C_{\vec{p}, \sigma}}_{= N_e} \cdot \underbrace{\sum_{\vec{q}, \sigma'} C_{\vec{q}, \sigma'}^+ C_{\vec{q}, \sigma'}}_{= N_e}$$

$$= \frac{1}{2} N_e^2 V_{\vec{k}=0}$$

To compensate this divergence, we consider **uniformly** distributed **positive** charges (ions):

$$n(\vec{r}) = \frac{N_e}{V}$$

↓
Actually, no \vec{r} dependence (uniform)



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③

Electrostatic potential from the "background charge":

$$\phi(\vec{r}) = \int d\vec{r}' \frac{+en(\vec{r}')}{4\pi\epsilon_0|\vec{r}-\vec{r}'|} = \int d\vec{r}' \frac{e \cdot \frac{N_e}{V}}{4\pi\epsilon_0|\vec{r}-\vec{r}'|}$$

$$\Rightarrow E_{\text{ion-el}} = \int d\vec{r} [-en(\vec{r})] \phi(\vec{r})$$

$$= - \left(\frac{N_e}{V} \right)^2 \int d\vec{r} d\vec{r}' \frac{e^2}{4\pi\epsilon_0|\vec{r}-\vec{r}'|}$$

$$= -N_e^2 V_{\vec{k}=0}$$

↑
 $\vec{k}=0$ Fourier component
of the Coulomb potential;
(see ⑤, ⑥ in electron-3.pdf)

Similarly,

$$E_{\text{ion-ion}} = \frac{1}{2} \int d\vec{r} [+en(\vec{r})] \phi(\vec{r})$$

↖ avoid double counting

$$= \frac{1}{2} N_e^2 V_{\vec{k}=0}$$

⇒ $E_{\text{ion-el}} + E_{\text{ion-ion}}$ exactly compensate
the divergent $\vec{k}=0$ term in H_z !

Jellium model :

$$H_{\text{Jellium}} = H_0 + H_I + E_{\text{ion-el}} + E_{\text{ion-ion}}$$

$$= H_0 + H_I'$$

where

$$H_I' = \frac{1}{2} \sum_{\vec{p}, \vec{q}} \sum_{\vec{k} (\neq 0)} \frac{e^2}{\epsilon_0 V |\vec{k}|^2} C_{\vec{p}+\vec{k}, \sigma}^+ C_{\vec{q}-\vec{k}, \sigma'}^+ C_{\vec{q}, \sigma'} C_{\vec{p}, \sigma}$$

First-order perturbation :

$$E_I = \langle FS | H_I' | FS \rangle$$

$$= \frac{1}{2} \sum_{\vec{p}, \vec{q}} \sum_{\vec{k} (\neq 0)} \frac{e^2}{\epsilon_0 V |\vec{k}|^2} \langle FS | C_{\vec{p}+\vec{k}, \sigma}^+ C_{\vec{q}-\vec{k}, \sigma'}^+ C_{\vec{q}, \sigma'} C_{\vec{p}, \sigma} | FS \rangle$$

Case 1: $(\vec{p}+\vec{k}, \sigma) = (\vec{p}, \sigma)$
 $(\vec{q}-\vec{k}, \sigma') = (\vec{q}, \sigma')$

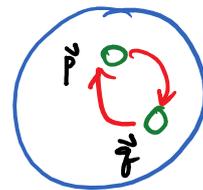
direct term (Hartree term)

Vannishing since $\vec{k}=0$ excluded.

dig two holes in the FS and refill them, otherwise no overlap with $\langle FS |$!

Case 2: $(\vec{p}+\vec{k}, \sigma) = (\vec{q}, \sigma')$
 $(\vec{q}-\vec{k}, \sigma') = (\vec{p}, \sigma)$

exchange term (Fock term) ✓

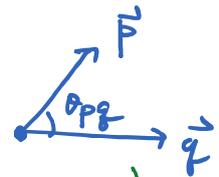


$$E_I = \frac{1}{2} \sum_{\vec{p}, \vec{q}} \sum_{\sigma} \frac{e^2}{\epsilon_0 V |\vec{q} - \vec{p}|^2} \langle F_S | \underbrace{C_{\vec{q}, \sigma}^+ C_{\vec{p}, \sigma}^+ C_{\vec{q}, \sigma} C_{\vec{p}, \sigma}}_{\equiv C_{\vec{p}, \sigma}^+ C_{\vec{q}, \sigma}^+} | F_S \rangle$$

within the FS
 $\vec{p} \neq \vec{q}$

$$= - \frac{1}{2} \sum_{\substack{|\vec{p}| < k_F, \\ |\vec{q}| < k_F, \\ \vec{p} \neq \vec{q}}} \sum_{\sigma} \frac{e^2}{\epsilon_0 V |\vec{q} - \vec{p}|^2}$$

$$= - \sum_{\substack{|\vec{p}| < k_F, \\ |\vec{q}| < k_F, \\ \vec{p} \neq \vec{q}}} \frac{e^2}{\epsilon_0 V |\vec{q} - \vec{p}|^2}$$



$$\stackrel{V \rightarrow \infty}{=} - \frac{e^2}{\epsilon_0 V} \cdot \frac{V^2}{(2\pi)^6} \int_{\substack{|\vec{p}| < k_F, \\ |\vec{q}| < k_F}} d\vec{p} d\vec{q} \frac{1}{p^2 + q^2 - 2pq \cos \theta}$$

$\equiv 4\pi^2 k_F^4$ (see page 8 - 9)

$$= - \frac{e^2 V}{16\pi^4 \epsilon_0} k_F^4 \leftarrow k_F = (3\pi^2 n)^{1/3}$$

$$= - \frac{3e^2 N_e}{16\pi^2 \epsilon_0} k_F \leftarrow \begin{cases} k_F = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_s a_B} \\ a_B = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \end{cases}$$

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⑥

$$\Rightarrow \frac{E_I}{N_e} = - \frac{3}{16\pi^2} \left(\frac{9\pi}{4}\right)^{1/3} \cdot \frac{1}{r_s} \underbrace{\frac{me^4}{4\pi\epsilon_0^2\hbar^2}}_{8\pi R_y}$$

$$= - \frac{3}{2\pi} \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_s} R_y$$

$$R_y = \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}$$

$$\approx - \frac{0.916}{r_s} R_y \quad (\text{Minus sign means total energy is lowered after turning on } H'_I.)$$

Compare: $\frac{E_0}{N_e} \approx \frac{2.21}{r_s^2} R_y$

$$\frac{E_I}{N_e} \approx - \frac{0.916}{r_s} R_y$$

$E_I \ll E_0$ if $r_s \rightarrow 0$ high density limit!

Higher-order expansion:

$$\frac{E}{N_e} \approx R_y \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \underbrace{0.622 \ln r_s - 0.096}_{\text{"RPA"}} + O(r_s) \right]$$

In neutron stars, $r_s \rightarrow 0$ is a good starting point.

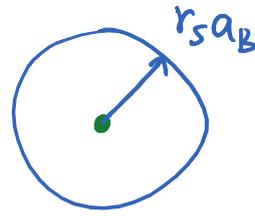
However, for metals, $r_s = 2 \sim 6$!

(perturbative treatment is problematic.)

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Simple argument why H_0 is dominant for $r_s \rightarrow 0$:

$$\begin{aligned}\frac{E_0}{N_e} &\sim \frac{\hbar^2 k_F^2}{2m} \\ &\sim \frac{\hbar^2}{2ma_B^2} \cdot \frac{1}{r_s^2} \\ &\quad \underbrace{\hspace{1cm}}_{1 Ry} \\ &\sim \frac{1}{r_s^2} Ry\end{aligned}$$



Heisenberg's uncertainty principle:

$$k_F \sim \frac{1}{r_s a_B}$$

$$\frac{E_I}{N_e} \sim \frac{e^2}{4\pi\epsilon_0 \cdot r_s a_B} \sim \frac{1}{r_s} Ry$$

The minus sign in E_I cannot be obtained,
but the scalings with r_s are correct!

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⑧

Appendix: Evaluating an integral in Page ⑤

$$I = \int_{\substack{|\vec{p}| < k_F, \\ |\vec{q}| < k_F}} d\vec{p} d\vec{q} \frac{1}{p^2 + q^2 - 2pq \cos \theta_{pq}}$$

We first evaluate the integration over \vec{p} in spherical coordinate (with \vec{q} as \hat{z} direction $\Rightarrow \theta_{pq} = \theta$):

$$\begin{aligned} & \int_{|\vec{p}| < k_F} d\vec{p} \frac{1}{p^2 + q^2 - 2pq \cos \theta_{pq}} \\ &= \int_0^{k_F} dp \cdot p^2 \underbrace{\int_0^{2\pi} d\phi}_{= 2\pi} \underbrace{\int_0^\pi \sin \theta d\theta}_{=} \frac{1}{p^2 + q^2 - 2pq \cos \theta} \\ &= -2\pi \int_0^{k_F} dp \frac{p}{q} \ln \left| \frac{p-q}{p+q} \right| \int_{-1}^1 dx \frac{1}{p^2 + q^2 - 2pqx} \\ & \quad - \frac{1}{2pq} \ln(p^2 + q^2 - 2pqx) \Big|_{-1}^1 \\ & \quad = -\frac{1}{pq} \ln \left| \frac{p-q}{p+q} \right| \end{aligned}$$

The integration over \vec{q} is also done in spherical coordinate.

The integration over angles is $\int_0^\pi \sin \theta_q d\theta_q \int_0^{2\pi} d\phi_q = 4\pi$

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$$I = -2\pi \int_0^{k_F} dq \, 4\pi q^2 \int_0^{k_F} dp \, \frac{p}{q} \ln \left| \frac{p-q}{p+q} \right|$$

$$= -8\pi^2 \int_0^{k_F} dp \int_0^{k_F} dq \, pq \ln \left| \frac{p-q}{p+q} \right|$$

$$p = k_F x$$

$$q = k_F y$$

$$= -8\pi^2 k_F^4 \int_0^1 dx \int_0^1 dy \, xy \ln \left| \frac{x-y}{x+y} \right|$$

$$\parallel$$

$$-\frac{1}{2}$$

$$= 4\pi^2 k_F^4$$