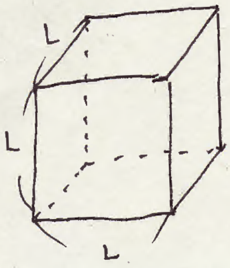
Notes on jellium model

Taisuke Ozaki (ISSP, Univ. of Tokyo)

Jellium model

Fig. 1



$V = L^3$

$n_b(x) = \frac{N}{V}$

$$\boxed{\text{Suppose that electrons occupy in a rectangular unit cell with a lattice constant, } L\text{, under the Born-von karman periodic boundary condition, and that the positive compensation changes also spread over the unit cell so that the total system can be neutral}}$$

The one-particle wave function is given by

$$\boxed{\psi_{k\lambda}(x) = V^{-\frac{1}{2}} e^{ik\cdot x}\,\eta_\lambda} \quad \cdots (1)$$

where λ is $\uparrow$ or $\downarrow$, and η_λ satisfies

$$\langle \eta_\lambda | \eta_{\lambda'} \rangle = \delta_{\lambda\lambda'} \quad \cdots (2)$$

We also assume the Born-von Karman periodic boundary conditions.

$$k_i = \frac{2\pi n_i}{L}, \quad i = x, y, z \qquad n_i = 0, \pm 1, \pm 2, \pm 3 \cdots$$
$$\cdots (3)$$

$$k_i \cdot x = k_x x + k_y y + k_z z$$
$$= \frac{2\pi n_x}{L} x + \frac{2\pi n_y}{L} + \frac{2\pi n_z}{L} \quad \cdots (4)$$

In this case, it is noted that

$$e^{i\frac{2\pi n_x}{L}(x+L)} = e^{i2\pi n_x} e^{i\frac{2\pi n_x}{L}x} = e^{i\frac{2\pi n_x}{L}x} \quad \cdots (5)$$

In fact, Eq. (5) is the Born-von Karman condition.

The Hamiltonian of the jellium model

is given by

$$\hat{H} = \hat{H}_{el} + \hat{H}_{b} + \hat{H}_{el-b} \quad \cdots \quad (6)$$

Electron part

$$H_{el} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} e^2 \sum_{i \neq j = 1}^{N} \frac{e^{-\mu |\mathbf{r}_i - \mathbf{r}_j|}}{|\mathbf{r}_i - \mathbf{r}_j|} \quad \cdots \quad (7)$$

positive back ground part

$$\hat{H}_b = \frac{1}{2} e^2 \iint dx\, dx' \frac{n(x) n(x') e^{-\mu |x - x'|}}{|x - x'|} \quad \cdots \quad (8)$$

Electron - positive back ground part

$$\hat{H}_{el-b} = - e^2 \sum_{i=1}^{N} \int dx \frac{n(x) e^{-\mu |x - \mathbf{r}_i|}}{|x - \mathbf{r}_i|} \quad \cdots \quad (9)$$

✱ In order to make each integration finite, $e^{-\mu \cdots}$ is introduced, and we will consider $\mu \to 0$ at last.

✱ In the thermodynamic limit that $N \to \infty$, $V \to \infty$ with a constant, $\rho = \frac{N}{V}$, each term in Eq. (6) diverges.

✱ However, the sum of three terms becomes finite.

✱ A procedure will be done :

First : $L \to \infty$ Assumption

Second : $\mu \to 0$ $\mu^{-1} \ll L$

Positive background part, $\hat{H}_b$

Let us evaluate H_b. Noting $n_b(x) = \frac{N}{V}$, --- (10)

one can evaluate H_b as

$$\hat{H}_b = \frac{1}{2} e^2 \iint dx\, dx' \frac{n(x)\, n(x')\, e^{-\mu|x-x'|}}{|x - x'|}$$

$$= \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \iint dx\, dx' \frac{e^{-\mu|x-x'|}}{|x-x'|}$$

$$= \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \int dx \int dz \frac{e^{-\mu z}}{z}$$

$$= \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \int dx \left[\int_{-\pi}^{\pi} d\phi \int_0^{\pi} d\theta \cdot \sin\theta \int_0^{\infty} dr \cdot r^2 \cdot \frac{e^{-\mu r}}{r} \right] \quad \text{--- (11)}$$

The integration in [ ] is

$$[\ \ ] = \int_0^{\pi} d\theta \sin\theta \int_{-\pi}^{\pi} d\phi \int_0^{\infty} dr\, r^2 \times \frac{e^{-\mu r}}{r}$$

$$= \left[-\cos\theta\right]_0^{\pi} \times \left[\phi\right]_{-\pi}^{\pi} \int r e^{-\mu r} dr$$

$$= (1+1) \times 2\pi \times \left[-\frac{e^{-\mu r}(\mu r + 1)}{\mu^2}\right]_0^{\infty}$$

$$= 4\pi \times \left(0 - \left(-\frac{e^{-\mu\cdot 0}(\mu\cdot 0 + 1)}{\mu^2}\right)\right) = \frac{4\pi}{\mu^2} \quad \text{--- (12)}$$

Putting Eq. (12) into Eq. (11), and performing $\int dx$, we have

$$\hat{H}_b = \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \times V \times \frac{4\pi}{\mu^2}$$

Thus

$$\boxed{\frac{\hat{H}_b}{N} = \frac{1}{2} e^2 \frac{N}{V} \frac{4\pi}{\mu^2}} \quad \text{---- (13)}$$

Electron - positive background part, $\hat{H}_{el-b}$

As well as H_b, one can evaluate H_{el-b} as

$$\hat{H}_{el-b} = -e^2 \sum_{i=1}^{N} \frac{N}{V} \int dx \, \frac{e^{-\mu|x - r_i|}}{|x - r_i|}$$

$$= -e^2 \sum_{i=1}^{N} \frac{N}{V} \int dz \, \frac{e^{-\mu z}}{z}$$

$$= -e^2 \sum_{i=1}^{N} \frac{N}{V} \left[\int_0^{\pi} d\theta \sin\theta \int_{-\pi}^{\pi} d\phi \int_0^{\infty} r^2 \times \frac{e^{-\mu r}}{r} \right]$$

$$= -e^2 \sum_{i=1}^{N} \frac{N}{V} \cdot \frac{4\pi}{\mu^2}$$

$$\boxed{\hat{H}_{el-b} = -e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}} \quad \cdots\cdots \quad (14)$$

Inserting Eqs. (13) and (14) into Eq. (6), we have

$$\boxed{\hat{H} = \hat{H}_{el} - \frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}} \quad \cdots\cdots \quad (15)$$

$\langle k_1 \lambda_1 | \hat{T} | k_2 \lambda_2 \rangle$

The expectation value of $\hat{T}$ is evaluated by

$$\langle k_1 \lambda_1 | \hat{T} | k_2 \lambda_2 \rangle$$

$$= \int \psi^*_{k_1\lambda_1}(x) \frac{(-\hbar^2)}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi_{k_2\lambda_2}(x)\, dx$$

$$= \frac{-\hbar^2}{2mV} \int d\sigma\, \eta^*_{\lambda_1}(\sigma)\, \eta_{\lambda_2}(\sigma) \int dr\, e^{-ik_1 \cdot r} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) e^{ik_2 \cdot r}$$

$$= \frac{-\hbar^2}{2mV} \delta_{\lambda_1\lambda_2} \int dr\, e^{-ik_1 \cdot r} (-|k_2|^2)\, e^{ik_2 \cdot r}$$

$$= \frac{\hbar^2 k_2^2}{2mV} \left[\int dr\, e^{i(k_2 - k_1)\cdot r} \right] \times \delta_{\lambda_1 \lambda_2} \quad \text{----} \quad (16)$$

The integration in [ ] is given by

<u>if $k_1 \neq k_2$</u>

$$[\ \ ] = \frac{1}{i(k_2^{(x)} - k_1^{(x)})} \left[e^{i(k_2^{(x)} - k_1^{(x)})x} \right]_0^L$$

$$\times \frac{1}{i(k_2^{(y)} - k_1^{(y)})} \left[e^{i(k_2^{(y)} - k_1^{(y)})y} \right]_0^L$$

$$\times \frac{1}{i(k_2^{(z)} - k_1^{(z)})} \left[e^{i(k_2^{(z)} - k_1^{(z)})z} \right]_0^L = 0 \quad \text{----} \quad (17)$$

<u>if $k_1 = k_2$</u>

$$[\ \ ] = \frac{\hbar^2 k_2^2}{2mV} \int dr = \frac{\hbar^2 k_2^2}{2m} \quad \text{----} \quad (18)$$

There fore, considering Eqs. (17) and (18),

$$\langle k_1 \lambda_1 | \hat{T} | k_2 \lambda_2 \rangle = \frac{\hbar^2 k_2^2}{2m} \delta_{\lambda_1 \lambda_2} \delta_{k_1 k_2} \quad \text{----} \quad (19)$$

So, the second quantized Hamiltonian for $\hat{T}$ is

$$\boxed{\hat{T} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} a^\dagger_{k\lambda} a_{k\lambda}} \quad \text{----} \quad (20)$$

$\langle k_1\lambda_1\, k_2\lambda_2 \mid V \mid k_3\lambda_3\, k_4\lambda_4 \rangle$

For the potential term of electron-electron interaction in Eq. (7), let us evaluate the expectation value.

$$\langle k_1\lambda_1\, k_2\lambda_2 \mid V \mid k_3\lambda_3\, k_4\lambda_4 \rangle$$

$$= e^2 \iint dx_1 dx_2 \left(\frac{e^{-ik_1\cdot x_1}}{\sqrt{V}} \eta^*_{\lambda_1}(\sigma_1)\right)\left(\frac{e^{-ik_2\cdot x_2}}{\sqrt{V}} \eta^*_{\lambda_2}(\sigma_2)\right)\left[\frac{e^{-\mu|x_1-x_2|}}{|x_1-x_2|}\right]$$

$$\times \left(\frac{e^{ik_3\cdot x_1}}{\sqrt{V}} \eta_{\lambda_3}(\sigma_1)\right)\left(\frac{e^{ik_4\cdot x_2}}{\sqrt{V}} \eta_{\lambda_4}(\sigma_2)\right)$$

$$= \frac{e^2}{V^2} \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4} \times \int e^{-ik_1\cdot x_1} e^{-ik_2\cdot x_2} \frac{e^{-\mu|x_1-x_2|}}{|x_1-x_2|} e^{ik_3\cdot x_1} e^{ik_4\cdot x_2} dx_1 dx_2 \quad \text{---- (21)}$$

Considering a variable change

$$x = x_2$$
$$y = x_1 - x_2 \longrightarrow x_1 = y + x \quad \text{---- (22)}$$

Eq. (21) can be written by

$$\text{Eq. (21)} = \frac{e^2}{V^2} \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4} \times$$

$$\iint dx\, dy\, e^{-ik_1\cdot(y+x)} e^{-ik_2\cdot x} \frac{e^{-\mu|y|}}{|y|} e^{ik_3\cdot(y+x)} e^{ik_4\cdot x}$$

$$= \frac{e^2}{V^2}\int dx\, e^{-i(k_1+k_2-k_3-k_4)\cdot x} \times \int dy\, e^{i(k_3-k_1)\cdot y} \frac{e^{-\mu|y|}}{|y|} \times \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4} \quad \text{--- (23)}$$

Noting $\displaystyle\int dx\, e^{-i(k_1+k_2-k_3-k_4)\cdot x} = \delta_{k_1+k_2,\, k_3+k_4} V$ ---- (24)

$$\text{Eq. (21)} = \frac{e^2}{V} \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4}\delta_{k_1+k_2,\, k_3+k_4} \int dy\, e^{i(k_3-k_1)\cdot y} \frac{e^{-\mu|y|}}{|y|} \quad \text{--- (25)}$$

We transform as

$$(k_3 - k_1)\cdot y = |k_3 - k_1||y| \cos\theta \qquad \cdots (26)$$

Using Eq. (26), the integral in Eq. (25) can be evaluated by

$$\int dy\, e^{i(k_3-k_1)\cdot y} \frac{e^{-\mu|y|}}{|y|}$$

$$= \int_0^{\pi} d\theta \sin\theta \int_{-\pi}^{\pi} d\phi \int_0^{\infty} dr \cdot r^2 e^{i|k_3-k_1| r \cos\theta} \frac{e^{-\mu r}}{r}$$

$$= \int_0^{\pi} d\theta \sin\theta \int_{-\pi}^{\pi} d\phi \int_0^{\infty} dr \cdot r\, e^{-\overbrace{[-i|k_3-k_1|\cos\theta + \mu]}^{\alpha} r}$$

$$= \int_0^{\pi} d\theta \sin\theta \int_{-\pi}^{\pi} d\phi \left[- \frac{e^{-\alpha r}(\alpha r + 1)}{\alpha^2} \right]_0^{\infty}$$

$$= 2\pi \int_0^{\pi} d\theta \cdot \sin\theta \times \frac{1}{\alpha^2}$$

$$= 2\pi \int_0^{\pi} \sin\theta \times \frac{1}{[\mu - i|k_3-k_1|\cos\theta]^2} \qquad \cdots (27)$$

Letting $t = \cos\theta$

$$\frac{dt}{d\theta} = -\sin\theta \qquad \theta = 0 \to t = -1$$
$$\theta = \pi \to t = 1 \qquad \cdots (28)$$
$$\to d\theta = -\frac{1}{\sin\theta} dt$$

Eq. (27) is given by

$$\text{Eq. (27)} = 2\pi \int_1^{-1} dt \times (-1) \frac{1}{(\mu - i|k_3-k_1| t)^2}$$

$$= 2\pi \left[\frac{1}{\mu \times i|k_3-k_1| + |k_3-k_1|^2 t} \right]_{-1}^{1}$$

$$= 2\pi \left(\frac{1}{i\mu|k_3-k_1| + |k_3-k_1|^2} - \frac{1}{i\mu|k_3-k_1| - |k_3-k_1|^2} \right)$$

$$= \frac{2\pi}{|k_3-k_1|} \left(\frac{1}{i\mu + |k_3-k_1|} - \frac{1}{i\mu - |k_3-k_1|} \right)$$

$$= \frac{2\pi}{|k_3-k_1|} \left(\frac{i\mu - |k_3-k_1| - i\mu - |k_3-k_1|}{(i\mu + |k_3-k_1|)(i\mu - |k_3-k_1|)} \right)$$

$$= \frac{4\pi}{\mu^2 + |k_3-k_1|^2}$$

Thus,

$$\int dy\, e^{i(k_3-k_1)\cdot y} \frac{e^{-\mu|y|}}{|y|} = \frac{4\pi}{\mu^2 + |k_3-k_1|^2} \quad \cdots\cdots (29)$$

putting Eq. (29) into Eq. (25), we obtain

$$\boxed{\langle k_1\lambda_1\, k_2\lambda_2 | V | k_3\lambda_3\, k_4\lambda_4 \rangle = \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4}\delta_{k_1+k_2,\,k_3+k_4} \frac{e^2}{V} \frac{4\pi}{\mu^2 + |k_3-k_1|^2}} \quad \cdots (30)$$

The second quantized expression

for $\frac{1}{2} e^2 \sum_{i\neq j=1}^{N} \frac{e^{-\mu|\mathbf{r}_i - \mathbf{r}_j|}}{|\mathbf{r}_i - \mathbf{r}_j|}$

becomes

$\longrightarrow$

$$\frac{e^2}{2V} \sum_{k_1\lambda_1} \sum_{k_2\lambda_2} \sum_{k_3\lambda_3} \sum_{k_4\lambda_4} \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4}\delta_{k_1+k_2,\,k_3+k_4} \times \frac{4\pi}{\mu^2 + |k_3-k_1|^2}$$

$$\times\, a^{\dagger}_{k_1\lambda_1} a^{\dagger}_{k_2\lambda_2} a_{k_4\lambda_4} a_{k_3\lambda_3} \quad \cdots\cdots (31)$$

Second quantized Hamiltonian for jellium model

Putting Eqs. (20) and (31) into Eq. (15),

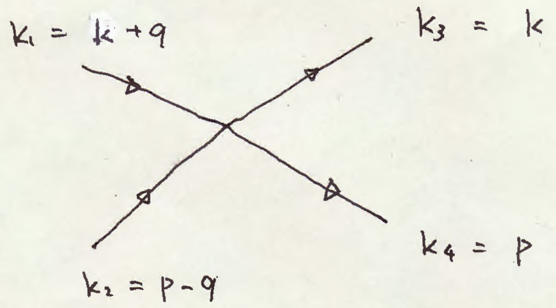
we obtain the second quantized Hamiltonian

for the jellium model as

$$\boxed{\begin{aligned}\hat{H} &= \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} a^{+}_{k\lambda} a_{k\lambda} \\ &+ \frac{e^2}{2V} \sum_{k_1\lambda_1} \sum_{k_2\lambda_2} \sum_{k_3\lambda_3} \sum_{k_4\lambda_4} \delta_{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_4} \delta_{k_1+k_2,\, k_3+k_4} \frac{4\pi}{(k_1-k_3)^2+\mu^2} \\ &\qquad \times a^{+}_{k_1\lambda_1} a^{+}_{k_2\lambda_2} a_{k_4\lambda_4} a_{k_3\lambda_3} \\ &- \frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}\end{aligned}} \quad \cdots\cdots (32)$$

Because of $\delta_{k_1+k_2,\, k_3+k_4}$ in the second term of Eq. (32),

the summations are limited.



Instead of four variables, k_1, k_2, k_3, and k_4, three new variables, k, p, and q, are introduced.

$$\left.\begin{aligned} k_1 + k_2 &= k+q+p-q = k+p \\ k_3 + k_4 &= k+p \end{aligned}\right) \longrightarrow \text{being consistent with } \delta_{k_1+k_2,\, k_3+k_4}$$

$$k_1 - k_3 = k+q-k = q \qquad \cdots\cdots (33)$$

Using the three variables, the second term in Eq. (32) (S.T.) becomes

$$S.T. = \frac{e^2}{2V} \sum_{kpq} \sum_{\lambda_1\lambda_2} \frac{4\pi}{q^2+\mu^2} a^+_{k+q,\lambda_1} a^+_{p-q,\lambda_2} a_{p,\lambda_2} a_{k,\lambda_1} \quad \text{---- (34)}$$

Eq. (34) is divided into terms with $q \neq 0$ and and terms with $q = 0$.

$$\boxed{\begin{aligned} S.T. &= \frac{e^2}{2V} \sum_{kpq}{}' \sum_{\lambda_1\lambda_2} \frac{4\pi}{q^2+\mu^2} a^+_{k+q,\lambda_1} a^+_{p-q,\lambda_2} a_{p,\lambda_2} a_{k,\lambda_1} \\ &+ \frac{e^2}{2V} \sum_{kp} \sum_{\lambda_1\lambda_2} \frac{4\pi}{\mu^2} a^+_{k,\lambda_1} a^+_{p\lambda_2} a_{p,\lambda_2} a_{k,\lambda_1} \end{aligned}} \quad \text{--- (35)}$$

where

$\sum'$ means that terms with $q = 0$ are omitted in the summation.

Noting
$$a_{p\lambda_2} a_{k\lambda_1} = - a_{k\lambda_1} a_{p\lambda_2}, \qquad \text{we see}$$
$$a^+_{p\lambda_2} a_{k\lambda_1} = - a_{k\lambda_1} a^+_{p\lambda_2} + \delta_{kp}\delta_{\lambda_1\lambda_2}$$

$$\begin{aligned} a^+_{k\lambda_1} a^+_{p\lambda_2} a_{p\lambda_2} a_{k\lambda_1} &= - a^+_{k\lambda_1} a^+_{p\lambda_2} a_{k\lambda_1} a_{p\lambda_2} \\ &= a^+_{k\lambda_1} \left(a_{k\lambda_1} a^+_{p\lambda_2} - \delta_{kp}\delta_{\lambda_1\lambda_2} \right) a_{p\lambda_2} \\ &= a^+_{k\lambda_1} a_{k\lambda_1} a^+_{p\lambda_2} a_{p\lambda_2} - \delta_{kp}\delta_{\lambda_1\lambda_2} a^+_{k\lambda_1} a_{p\lambda_2} \\ &= a^+_{k\lambda_1} a_{k\lambda_1} \left(a^+_{p\lambda_2} a_{p\lambda_2} - \delta_{kp}\delta_{\lambda_1,\lambda_2} \right) \end{aligned}$$

---- (36)

By making use of Eq. (36), the second term in Eq. (35) can be expressed by

$$\frac{e^2}{2V}\sum_{kp}\sum_{\lambda_1\lambda_2}\frac{4\pi}{\mu^2}a^+_{k\lambda_1}a^+_{p\lambda_2}a_{p\lambda_2}a_{k\lambda_1}$$

$$=\frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{k\lambda_1}\sum_{p\lambda_2}a^+_{k\lambda_1}a_{k\lambda_1}\left(a^+_{p\lambda_2}a_{p\lambda_2}-\delta_{kp}\delta_{\lambda_1\lambda_2}\right)$$

$$=\frac{e^2}{2V}\frac{4\pi}{\mu^2}\left[\left(\sum_{k\lambda_1}a^+_{k\lambda_1}a_{k\lambda_1}\right)\left(\sum_{p\lambda_2}a^+_{p\lambda_2}a_{p\lambda_2}\right)-\left(\sum_{k\lambda_1}a^+_{k\lambda_1}a_{k\lambda_1}\right)\right] \quad ----(37)$$

Since "$a^+_{k\lambda_1}a_{k\lambda_1}$" is the number operator, we now define the sum of the number operator, $\hat{N}$ by

$$\hat{N}=\sum_{k\lambda_1}a^+_{k\lambda_1}a_{k\lambda_1} \quad ----(38)$$

Using Eq. (38), Eq. (37) can be written by

$$\text{Eq. (37)}=\frac{e^2}{2V}\frac{4\pi}{\mu^2}\left[\hat{N}^2-\hat{N}\right] \quad ----(39)$$

If the number of total electrons does not change, the eigenvalue of $\hat{N}$ is N, i.e., $\hat{N}|\psi\rangle=N|\psi\rangle$

the eigenvalue of $\hat{N}^2$ is N^2, i.e., $\hat{N}^2|\psi\rangle=N^2|\psi\rangle$

---(40)

So, Eq. (37) can be simplified as

$$\boxed{\begin{aligned}\frac{e^2}{2V}\sum_{kp}\sum_{\lambda_1\lambda_2}\frac{4\pi}{\mu^2}a^+_{k\lambda_1}a^+_{p\lambda_2}a_{p\lambda_2}a_{k\lambda_1}&=\frac{e^2}{2V}\frac{4\pi}{\mu^2}(N^2-N)\\&=\frac{e^2}{2}\frac{N^2}{V}\frac{4\pi}{\mu^2}-\frac{e^2}{2}\frac{N}{V}\frac{4\pi}{\mu^2}\end{aligned}}$$

---(41)

It should be noted that the first term in Eq. (41) exactly cancels out with the third term in Eq. (32).

The second term in Eq. (41) vanishes when $L \to \infty$, $\mu \to 0$, and $\mu^{-1} \ll L$ as shown below

$L = \gamma \mu^{-1}$, then, we can evaluate the second term in Eq. (41)
(γ : constant)

$$\frac{-\frac{e^2}{2}\frac{N}{V}\frac{4\pi}{\mu^2}}{N} = -\frac{e^2}{2}\frac{4\pi}{\gamma^3\mu^{-3}\mu^2} = -2\pi e^2 \frac{\mu}{\gamma^3} \xrightarrow{\mu \to 0} 0$$

Thus, we conclude

$$\lim_{\mu \to 0} \lim_{L \to \infty} \left(-\frac{1}{N}\frac{e^2}{2}\frac{N}{V}\frac{4\pi}{\mu^2} \right) = 0 \qquad \text{---- (42)}$$

It is also noticed that letting μ be zero in the first term of Eq. (35) is allowed. Thus, the second quantized Hamiltonian given by Eq. (32) is simplified as

$$\boxed{\hat{H} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} a^{+}_{k\lambda} a_{k\lambda} + \frac{e^2}{2V} \sum_{kpq}{}' \sum_{\lambda_1\lambda_2} \frac{4\pi}{q^2} a^{+}_{k+q,\lambda_1} a^{+}_{p-q\,\lambda_2} a_{p\lambda_2} a_{k\lambda_1}}$$

---- (43)

High density limit of the jellium model

We now consider the high density limit of the jellium model. Let us introduce r_0 which corresponds to essentially interparticle spacing.

$$V \equiv \frac{4}{3}\pi r_0^3 N \quad \text{-----} \quad (44)$$

Bohr radius, a_0

$$a_0 = \frac{\hbar^2}{me^2} \quad \text{----} \quad (45)$$

Moreover, a dimensionless parameter, r_s, is defined by

$$r_s \equiv \frac{r_0}{a_0} \quad \text{----} \quad (46)$$

Using r_0, four dimensionless parameters are introduced by

$$\bar{V} \equiv r_0^{-3} V, \quad \bar{k} \equiv r_0 k, \quad \bar{p} \equiv r_0 p, \quad \bar{q} \equiv r_0 q \quad \text{----} \quad (47)$$

$$\downarrow \qquad \downarrow \qquad \downarrow \qquad \downarrow$$

$$\bar{V} = (a_0 r_s)^{-3} V \qquad \bar{k} = a_0 r_s k \qquad \bar{p} = a_0 r_s p \qquad \bar{q} = a_0 r_s q$$

Then, we see

$$\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\bar{k}}{a_0 r_s}\right)^2 = \frac{\hbar^2 \bar{k}^2}{2m a_0^2 r_s^2} = \frac{\hbar^2 \bar{k}^2}{2m a_0 r_s^2}\left(\frac{me^2}{\hbar^2}\right)$$

$$= \frac{e^2}{a_0 r_s^2}\frac{1}{2}\bar{k}^2 \quad \text{----} \quad (48)$$

$$\frac{e^2}{2V}\frac{4\pi}{q^2} = \frac{e^2}{2(a_0 r_s)^3 \bar{V}} \frac{4\pi}{\left(\frac{\bar{q}}{a_0 r_s}\right)^2}$$

$$= \frac{e^2}{2a_0 r_s \bar{V}}\frac{4\pi}{\bar{q}^2} \quad \text{-----} \quad (49)$$

Putting Eqs. (48) and (49) into Eq. (43),

we obtain

$$\boxed{\hat{H} = \frac{e^2}{a_0 r_s^2}\left(\sum_{\bar{k}\lambda} \frac{1}{2}\bar{k}^2 a^{+}_{\bar{k}\lambda} a_{\bar{k}\lambda} + \frac{r_s}{2V} \sum_{\bar{k}\bar{p}\bar{q}}{}' \sum_{\lambda_1\lambda_2} \frac{4\pi}{q^2} a^{+}_{\bar{k}+\bar{q}\,\lambda_1} a^{+}_{\bar{p}-\bar{q}\,\lambda_2} a_{\bar{p}\lambda_2} a_{\bar{k}\lambda_1} \right)}$$

----- (50)

Firstly, it is noted that

$r_s \to 0$ corresponds to high density limit.

In this case, the second term can be regarded as "a small perturbation".

So, for the high density limit. we evaluate the zero-th order term and the first order term by employing the perturbation theoy

$$E = E_0 + E_1 \quad \text{----- (51)}$$

$$E_0 = \langle F | \hat{H}_0 | F \rangle \quad \text{----- (52)}$$

$$E_1 = \langle F | \hat{H}_1 | F \rangle \quad \text{----- (53)}$$

$|F\rangle$ is the eigen state of $\hat{H}_0$, corresponding to "Free" electrons.

$$\hat{H}_0 = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} a^{+}_{k\lambda} a_{k\lambda} \quad \text{---- (54)}$$

$$\hat{H}_1 = \frac{e^2}{2V} \sum_{kpq}{}' \sum_{\lambda_1\lambda_2} \frac{4\pi}{q^2} a^{+}_{k+q,\lambda_1} a^{+}_{p-q,\lambda_2} a_{p\lambda_2} a_{k\lambda_1} \quad \text{--- (55)}$$

Total number of electrons, $N = \langle F | \hat{N} | F \rangle$

The conversion from the summation to the integration can be done by the following consideration.

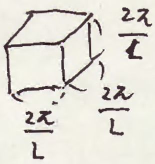
$$\sum_{k\lambda} f_\lambda(k) = \sum_{n_x}\sum_{n_y}\sum_{n_z}\sum_{\lambda} f_\lambda\left(\frac{2\pi n}{L}\right)$$

$$= \sum_{n_x}\sum_{n_y}\sum_{n_z} \frac{1}{\Delta V} \times \Delta V \times f_\lambda(k)$$

$$= \frac{1}{\Delta V} \sum_{\lambda} \sum_{n_x}\sum_{n_y}\sum_{n_z} \Delta V\, f_\lambda(k)$$

$$\simeq \frac{1}{\Delta V} \sum_{\lambda} \int dk\ f_\lambda(k) \qquad \cdots\ (56)$$

where



$$\longrightarrow \quad \Delta V = \left(\frac{2\pi}{L}\right)^3 \qquad \cdots\ (57)$$

Thus,

$$\boxed{\sum_{k\lambda} f_\lambda(k) \longrightarrow \frac{V}{(2\pi)^3} \sum_{\lambda} \int dk\ f_\lambda(k)} \qquad \cdots\ (58)$$

We now evaluate the total number of electrons as the expectation value of the number operator $\hat{N}$.

$$N = \langle F | \hat{N} | F \rangle = \sum_{k\lambda} \langle F | \hat{n}_{k\lambda} | F \rangle \qquad \text{------}\ (59)$$

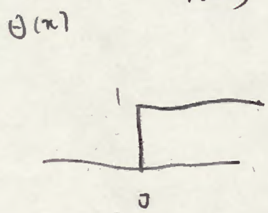
Noting

$$|F\rangle = |\,1\,1\,1\,1\,1\,1\,1\,0\,0\,0\,\cdots\cdots\rangle \qquad \cdots\ (60)$$

$\uparrow$
k_F

N is given by

$$N = \sum_{k\lambda} \theta(k_F - k) \qquad \cdots\ (61)$$



where $\theta(x)$ is a step function.

One can convert the summation of Eq. (61) using Eq. (58) as

$$N = \sum_{k\lambda} \theta(k_F - k)$$

$$= \frac{V}{(2\pi)^3} \sum_{\lambda} \int dk\, \theta(k_F - k)$$

$$= \frac{V}{(2\pi)^3} \times 2 \times \frac{4}{3}\pi k_F^3$$

$$= \frac{V k_F^3}{3\pi^2} \quad \text{----} \quad (62)$$

$$\longrightarrow \quad k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}} \quad \text{---} \quad (63)$$

From Eq. (44),

$$\frac{N}{V} = \frac{3}{4\pi} r_0^{-3} \quad \text{---} \quad (64)$$

putting Eq. (64) into Eq. (63), we have

$$\boxed{\begin{aligned} k_F &= \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} r_0^{-1} \\ &= \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} (a_0 r_s)^{-1} \end{aligned}} \quad \text{---} \quad (65)$$

Zero-th order energy, E_0

As the expectation value of $\hat{H}_0$ with respect to $|F\rangle$, we evaluate E_0 as follows:

$$E_0 = \langle F | \hat{H}_0 | F \rangle \quad \leftarrow \text{ note that } n_{k\lambda} = a^{+}_{k\lambda} a_{k\lambda}$$

$$= \frac{\hbar^2}{2m} \sum_{k\lambda} k^2 \langle F | n_{k\lambda} | F \rangle$$

$$= \frac{\hbar^2}{2m} \sum_{k\lambda} k^2 \, \theta(k_F - k)$$

$$= \frac{\hbar^2}{2m} \sum_{\lambda} \frac{V}{(2\pi)^3} \int dk \cdot k^2 \, \theta(k_F - k)$$

$$= \frac{\hbar^2}{2m} \times 2 \times \frac{V}{(2\pi)^3} \times 4\pi \int_0^\infty d|k| \cdot |k|^4 \, \theta(|k_F| - |k|)$$

$$= \frac{\hbar^2}{\cancel{2}m} \cancel{\times 2} \times \frac{V}{(2\pi)^3} \times 4\pi \times \frac{1}{5} k_F^5 \leftarrow \text{Eq. (65)}$$

$$= \underbrace{\frac{\hbar^2}{m}}_{e^2 a_0} \times \frac{4}{3} \cancel{\pi} \cancel{(a_0 r_s)^3} N \times \frac{1}{\cancel{8}_{2} \pi^{\cancel{3}}} \times \cancel{4\pi} \times \frac{1}{5} \times \left(\frac{9\pi}{4}\right)^{\frac{5}{3}} \times (a_0 r_s)^{\cancel{-5}\,2}$$

$$= e^2 a_0 \times \frac{2}{3} N \times \frac{1}{\pi} \times \frac{1}{5} \times \left(\frac{9}{4}\pi\right)^{\frac{5}{3}} \times (a_0 r_s)^{-2}$$

$$= e^2 \cancel{a_0} \times \cancel{\frac{2}{3}} N \times \frac{1}{\cancel{\pi}} \times \frac{1}{5} \times \cancel{\frac{9}{4}}\cancel{\pi} \times \left(\frac{9}{4}\pi\right)^{\frac{2}{3}} \times \frac{1}{a_0^{\cancel{2}} r_s^2}$$

$$\boxed{E_0 = \frac{e^2}{2a_0} \frac{N}{r_s^2} \frac{3}{5} \left(\frac{9}{4}\pi\right)^{\frac{2}{3}}} \quad \text{----- (66)}$$

Comparison of E_0 with $\varepsilon_F^0 = \frac{\hbar^2 k_F^2}{2m}$

The kinetic energy at k_F is given by

← Eq. (65)

$$\varepsilon_F^0 = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{9\pi}{4}\right)^{\frac{2}{3}} \frac{1}{a_0^2 r_s^2}$$

← $\frac{\hbar^2}{m} = a_0 e^2$

$$= \frac{1}{2} a_0 e^2 \left(\frac{9\pi}{4}\right)^{\frac{2}{3}} \times \frac{1}{a_0^2 r_s^2}$$

$$= \frac{e^2}{2a_0} \frac{1}{r_s^2} \left(\frac{9\pi}{4}\right)^{\frac{2}{3}} \quad \text{---- (67)}$$

Comparing Eq. (67) with Eq. (66),

we get a well-known result:

$$\boxed{\frac{E_0}{N} = \frac{3}{5}\varepsilon_F^0} \quad \text{--- (68)}$$

First order energy correction E_1

As the expectation value of $\hat{H}_1$ with respect to $|F\rangle$,

we evaluate E_1 as follows:

$$E_1 = \langle F | \hat{H}_1 | F \rangle$$

$$= \frac{e^2}{2V} \sum_{kpq}{}' \sum_{\lambda_1 \lambda_2} \frac{4\pi}{q^2} \langle F | a^{\dagger}_{k+q\,\lambda_1} a^{\dagger}_{p-q\,\lambda_2} a_{p\lambda_2} a_{k\lambda_1} | F \rangle \quad \text{---- (69)}$$

The expectation value

$\langle F | a^{\dagger}_{k+q\,\lambda_1} a^{\dagger}_{p-q\,\lambda_2} a_{p\lambda_2} a_{k\lambda_1} | F \rangle$

survives only if

$$a^{\dagger}_{k+q\,\lambda_1} a^{\dagger}_{p-q\,\lambda_2} a_{p\lambda_2} a_{k\lambda_1} | F \rangle = | F \rangle \quad \text{---- (70)}$$

To satisfy Eq. (70), there are just two posibilities:

(A)

$$\boxed{\begin{aligned} k+q,\ \lambda_1 &= k,\ \lambda_1 \\ p-q,\ \lambda_2 &= p\ \lambda_2 \end{aligned}}$$

(B)

$$\boxed{\begin{aligned} k+q,\ \lambda_1 &= p\ \lambda_2 \\ p-q\ \lambda_2 &= k\ \lambda_1 \end{aligned}}$$

---- (71)

The case (A) is forbidden because of the exclusion of terms with $q = 0$. Thus, we only have to consider the case (B)

Let us consider the case (B).

$$\langle F | a^\dagger_{k+q\lambda_1} a^\dagger_{p-q} \cancel{a}_{\lambda_2} a_{p\lambda_2} a_{k\lambda_1} | F \rangle$$

$$\longrightarrow \delta_{k+q,p}\, \delta_{\lambda_1\lambda_2} \langle F | a^\dagger_{k+q\lambda_1} \underbrace{a^\dagger_{k\lambda_1} a_{k+q\lambda_1}}_{-a_{k+q\lambda_1} a^\dagger_{k\lambda_1}} a_{k\lambda_1} | F \rangle$$

$$= -\delta_{k+qp}\, \delta_{\lambda_1\lambda_2} \langle F | a^\dagger_{k+q\lambda_1} a_{k+q\lambda_1} a^\dagger_{k\lambda_1} a_{k\lambda_1} | F \rangle$$

$$= -\delta_{k+qp}\, \delta_{\lambda_1\lambda_2} \langle F | \hat{n}_{k+q\lambda_1} \hat{n}_{k\lambda_1} | F \rangle \qquad \cdots (72)$$

Noting

$$|F\rangle = |1\,1\,1\,1\,1\,1 \cdots 1\,1\,1 \underset{\substack{\uparrow \\ k_F}}{} \; 0\, 0\, 0\, 0 \rangle \qquad \cdots (73)$$

we see

$$n_{k\lambda_1} |F\rangle = \theta(k_F - k)|F\rangle \qquad \cdots (74)$$

$$\langle F | n_{k+q,\lambda_1} = \langle F | \theta(k_F - |k+q|) \qquad \cdots (75)$$

Putting Eqs. (74) and (75) into Eq. (72), we get

$$\delta_{k+q,p}\, \delta_{\lambda_1\lambda_2} \langle F | a^\dagger_{k+q\lambda_1} a^\dagger_{k\lambda_1} a_{k+q\lambda_1} a_{k\lambda_1} | F \rangle$$

$$= -\delta_{k+qp}\, \delta_{\lambda_1\lambda_2}\, \theta(k_F - |k+q|)\, \theta(k_F - k) \qquad \cdots (76)$$

Using Eq. (76), one can write E_1 given by Eq. (69),

$$E_1 = -\frac{e^2}{2V} \sum_{\lambda_1} \sum_{kq}{}' \frac{4\pi}{q^2}\, \theta(k_F - |k+q|)\, \theta(k_F - k)$$

$$= -\frac{e^2}{\cancel{2}\,\cancel{V}} \frac{V^{\cancel{2}}}{(2\pi)^6} \times \cancel{2} \times 4\pi \iint dk\, dq \cdot q^{-2}\, \theta(k_F - |k+q|)\, \theta(k_F - k)$$

$$\boxed{E_1 = -\frac{4\pi e^2 V}{(2\pi)^6} \iint dk\, dq \cdot q^{-2}\, \theta(k_F - |k+q|)\, \theta(k_F - k)} \qquad \cdots (77)$$

In order to make the expression of Eq. (77) symmetric, we introduce a variable, p defined by

$$p = k + \frac{1}{2}q \longrightarrow k = p - \frac{1}{2}q \quad \text{---} \quad (78)$$

Then, we see

$$k+q = k + \frac{1}{2}q \quad \text{---} \quad (79)$$

By putting Eqs. (78) and (79) into Eq. (77), we have

$$E_1 = -\frac{4\pi e^2 V}{(2\pi)^6}\int dq \cdot q^{-2}\int dp \; \theta\left(k_F - \left|p + \frac{1}{2}q\right|\right)\theta\left(k_F - \left|p - \frac{1}{2}q\right|\right) \quad \text{---} \quad (80)$$

The range for the integration is found from the shaded region in the following figure.

Fig. 2

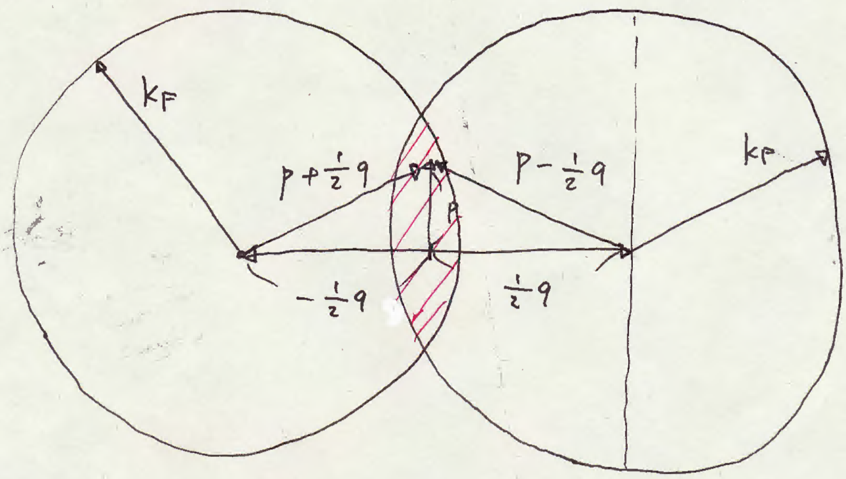
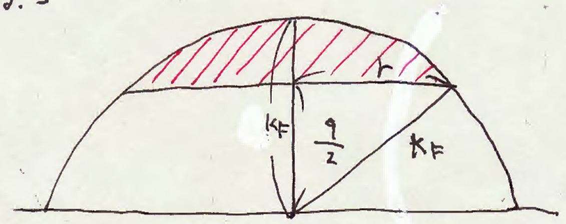


Fig. 3



$$y = \frac{q}{2}$$

$$\longrightarrow r^2 + \left(\frac{q}{2}\right)^2 = k_F^2$$

$$r^2 + y^2 = k_F^2$$

$$r = \sqrt{k_F^2 - y^2} \quad \text{----} \quad (81)$$

Condition:

$$k_F \geq \frac{q}{2} \longrightarrow 2k_F \geq q$$

$$\longrightarrow 1 \geq \frac{q}{2k_F} \quad \text{----} \quad (82)$$

The two integrations in Eq. (80) can be evaluated by the following way:

(i) Evaluate the volume of the shaded region with a fixed q.

(ii) Evaluate the integral over q

(i) Evaluate the volume of shaded region

The volume can be calculated by integrating the area of circle with a radius of r.

Thus, considering Fig. 3, we can calculate as

$$\text{Volume of the shaded region} = 2\int_{\frac{q}{2}}^{k_F} \pi r^2\, dy$$

$$= 2\pi \int_{\frac{q}{2}}^{k_F} (k_F^2 - y^2)\, dy$$

$$= 2\pi \left[k_F^2 y - \frac{1}{3} y^3 \right]_{\frac{q}{2}}^{k_F}$$

$$= 2\pi \left(k_F^3 - \frac{1}{3} k_F^3 - k_F^2 \frac{q}{2} + \frac{1}{3}\left(\frac{q}{2}\right)^3 \right)$$

$$= \frac{4\pi}{3} k_F^3 \left(1 - \frac{3}{2}\frac{q}{2k_F} + \frac{1}{2}\left(\frac{q}{2k_F}\right)^3 \right) \quad \text{---- (83)}$$

Letting $\frac{q}{2k_F}$ be x, Eq. (83) is rewritten by

$$\text{Eq. (83)} = \frac{4\pi}{3} k_F^3 \left(1 - \frac{3}{2} x + \frac{1}{2} x^3 \right) \quad \text{--- (84)}$$

Thus

$$\boxed{\int d\mathbf{p}\, \theta\left(k_F - |\mathbf{p} + \tfrac{1}{2}\mathbf{q}|\right) \theta\left(k_F - |\mathbf{p} - \tfrac{1}{2}\mathbf{q}|\right) = \frac{4}{3}\pi k_F^3 \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) \theta(1-x)} \quad \text{---- (85)}$$

where $\theta(1-x)$ comes from Eq. (82)

(ii) Evaluate the integral over q

Noting $x = \frac{q}{2k_F} \rightarrow \frac{dx}{dq} = \frac{1}{2k_F} \rightarrow dq = 2k_F\, dx$,

and putting Eq. (85) into Eq. (80), one can evaluate Eq. (80) as

$$E_1 = -\frac{4\pi e^2 V}{(2\pi)^6} \times \frac{4\pi}{3} k_F^3 \times 2k_F \int_0^1 dx \cdot 4\pi \cdot (2k_F x)^2 \cdot (2k_F x)^{-2} \times \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right)$$

$$= -\frac{4\pi e^2 V}{(2\pi)^6} \times \frac{4\pi}{3} k_F^3 \times 2k_F \times 4\pi \left[x - \frac{3}{4}x^2 + \frac{1}{8}x^4\right]_0^1$$

$$= -\frac{4\pi e^2 V}{(2\pi)^6} \times \frac{4\pi}{3} k_F^3 \times 2k_F \times 4\pi \times \frac{3}{8} \qquad \text{---- (86)}$$

From Eqs. (44) and (46),

$$V = \frac{4}{3}\pi r_0^3 N = \frac{4}{3}\pi (a_0 r_s)^3 N \qquad \text{--- (87)}$$

Inserting Eqs. (65) and (87) into Eq. (86), we have

$$E_1 = -\frac{4\pi e^2}{(2\pi)^6} \times \frac{4\pi}{\cancel{3}} \cancel{(a_0 r_s)^3} N \times \frac{4\pi}{\cancel{3}} \times \frac{9\pi}{\cancel{4}} \times \cancel{\frac{1}{(a_0 r_s)^3}} \times \cancel{2} \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} (a_0 r_s)^{-1} \times \frac{3\pi}{\cancel{2}}$$

$$= -\frac{\cancel{4\pi} e^2}{\cancel{2\pi} \cdot \cancel{2\pi} \cdot \cancel{2\pi} \cdot \cancel{2\pi} \cdot \cancel{2\pi} \cdot 2\pi} \times \cancel{4\pi} N \cdot \cancel{\pi} \cdot \cancel{\pi} \cdot \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} (a_0 r_s)^{-1} \cdot 3\cancel{\pi}$$

$$= -\frac{3e^2}{4\pi} N \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{1}{a_0 r_s} = -\frac{e^2}{2a_0} \frac{N}{r_s} \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{3}{2\pi}$$

Thus,

$$\boxed{E_1 = -\frac{e^2}{2a_0} \frac{N}{r_s} \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{3}{2\pi}} \qquad \text{---- (88)}$$

Comparison of the approximated energy with an experiment

In the high density limit, the energy per electron is approximated by the sum of E_0 and E_1 given by Eqs. (66) and (88):

$$\frac{E}{N} \simeq \frac{E_0}{N} + \frac{E_1}{N} \quad \text{---- (89)}$$

where

$$\frac{E_0}{N} = \frac{e^2}{2a_0}\frac{1}{r_s^2}\frac{3}{5}\left(\frac{9}{4}\pi\right)^{\frac{2}{3}} \simeq \frac{e^2}{2a_0}\frac{2.21}{r_s^2} \quad \text{--- (90)}$$

$$\frac{E_1}{N} = -\frac{e^2}{2a_0}\frac{1}{r_s}\left(\frac{9\pi}{4}\right)^{\frac{1}{3}}\frac{3}{2\pi} \simeq -\frac{e^2}{2a_0}\frac{0.916}{r_s} \quad \text{--- (91)}$$

Thus,

$$\frac{E}{N} \underset{r_s \to 0}{=} \frac{e^2}{2a_0}\left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \cdots\cdots\right] \quad \text{--- (92)}$$

The minimum of $\frac{E}{N}$ with respect to r_s can be found as

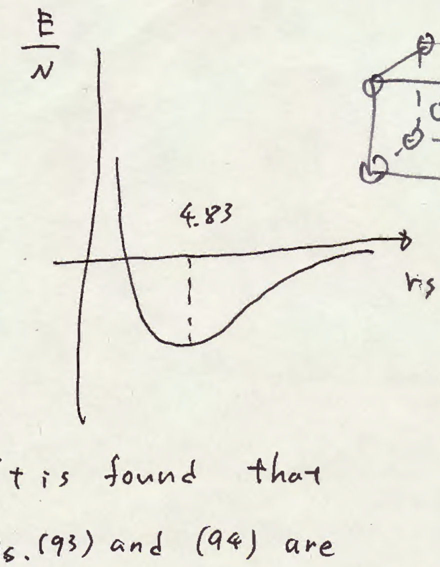
$$\frac{\partial}{\partial r_s}\left(\frac{E}{N}\right) = \frac{e^2}{2a_0}\left(2.21 \times (-2) \times r_s^{-3} - 0.916 \times (-1) \times r_s^{-2}\right) = 0$$

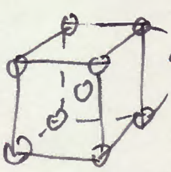
Fig. 4

$$-4.42 + 0.916\, r_s = 0 \quad \rightarrow \quad r_s = \frac{4.42}{0.916} = 4.83$$

$$\rightarrow \left(\frac{E}{N}\right)_{min} = -0.095 \times \left(\frac{e^2}{2a_0}\right)$$

$$= -1.29\ \text{eV} \quad \text{--- (93)}$$





4.225 Å

BCC

Sodium, Na

$$\rho = 2/4.225^3 = 2.852 \times 10^{-2}\ \text{Å}^{-3}$$

$$r_s = \frac{1}{a_0\left(\frac{4\pi}{3}\rho\right)^{\frac{1}{3}}}$$

$$= 3.93$$

$$\frac{E}{N} = -1.13\ \text{eV} \quad \text{--- (94)}$$

It is found that Eqs. (93) and (94) are in agrement.

E_0 and E_1 in terms of density $\rho = \frac{N}{V}$

It should be noted that $\frac{E_0}{N}$ and $\frac{E_1}{N}$ are the <u>kinetic</u> and <u>exchange</u> energies, respectively.

<u>Kinetic energy</u>

$$\frac{E_0}{N} = \frac{e^2}{2a_0} \frac{1}{r_s^2} \frac{3}{5} \left(\frac{9}{4} \pi \right)^{\frac{2}{3}} \quad \text{--- (95)}$$

<u>Exchange energy</u>

$$\frac{E_1}{N} = - \frac{e^2}{2a_0} \frac{1}{r_s} \left(\frac{9\pi}{4} \right)^{\frac{1}{3}} \frac{3}{2\pi} \quad \text{--- (96)}$$

Let us express $\frac{E_0}{N}$ and $\frac{E_1}{N}$ in terms of the eletron density $\rho = \frac{N}{V}$. Using Eqs. (44) and (46),

$$\rho = \frac{N}{V} = \frac{3}{4\pi} r_0^{-3} = \frac{3}{4\pi} (a_0 r_s)^{-3}$$

$$\longrightarrow \left(\frac{4\pi}{3} \rho \right)^{\frac{1}{3}} = \frac{1}{a_0 r_s} \longrightarrow \frac{1}{r_s} = a_0 \left(\frac{4\pi}{3} \rho \right)^{\frac{1}{3}} \quad \text{--- (97)}$$

Putting Eq. (97) into Eq. (95) an Eq. (96), we obtain

Kinetic energy

$$\frac{E_0}{N} = \frac{3e^2 a_0}{10} (3\pi^2)^{\frac{2}{3}} \rho^{\frac{2}{3}} \quad \text{--- (98)}$$

Exchange energy

$$\frac{E_1}{N} = - \frac{3e^2}{4} \left(\frac{3}{\pi} \right)^{\frac{1}{3}} \rho^{\frac{1}{3}} \quad \text{--- (99)}$$