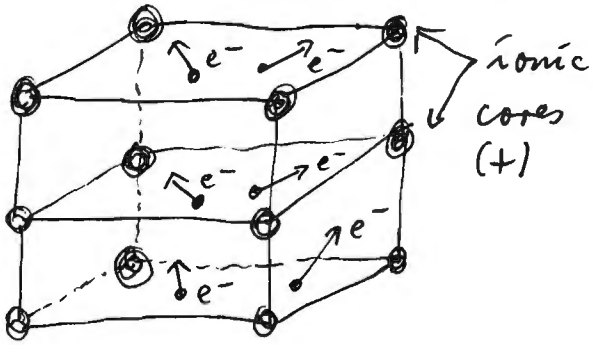
Ch. 5: The interacting electron gas

Ref: Fetter & Walecka, p. 21-31

Physical application: approximate treatment of metal or plasma.

metallic lattice

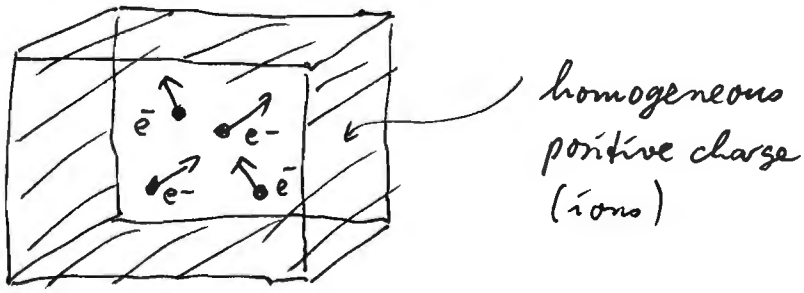


approximations

a) positive ionic cores much heavier than e^- ⇒ neglect ionic motion

b) treat ions as uniform positively charged background (not very realistic)

model problem



Steps in calculation

a) set up H in coordinate space, simplify

b) transform $H \rightarrow$ occupation # space ($\hat{H}$)

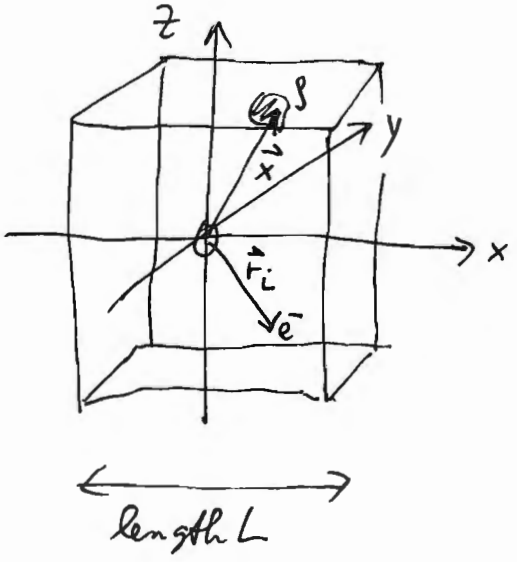
c) calculate g.s. energy per particle in 1st-order perturbation theory, using Wick's theorem

$$\frac{E_{g.s.}}{N} \approx \frac{1}{N} \langle \phi_0 | \hat{H} | \phi_0 \rangle$$ (ϕ_0: non-int. g.s.)

---

a) H in coordinate space

We consider a large cube of length L, with volume $V = L^3$, in the bulk medium.



notation:

electrons (e^-) at positions $\vec{r}_i$.

background charge (+) at position $\vec{x}$ is $\rho(\vec{x})$.

$$H = H_{el} + H_b + H_{el-b}$$

- H_{el}: interacting e^- gas
- H_b: uniform background (ions)
- H_{el-b}: interaction: e^- and (+) ions (background)

$$H_{el} = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2 \right) + \frac{1}{2} e^2 \sum_{\substack{i,j=1 \\ (i \neq j)}}^{N} \frac{e^{-\mu |\vec{r}_i - \vec{r}_j|}}{|\vec{r}_i - \vec{r}_j|}$$

Note: To avoid infinities in the theory due to ∞-range Coulomb int., we use a finite-range (screened) interaction of range

$$r_{cou} = \frac{1}{\mu} .$$

In the end, we will take the limit $r_{cou} \to \infty$, i.e. $\mu \to 0$.

The Coulomb self-energy of the positive background charge distribution is given by:

notation: $\rho(\vec{x}) = (+e)\, n(\vec{x})$

charge density — number density

$$H_b = \frac{1}{2} e^2 \int\int d^3x\, d^3x' \, \frac{n(\vec{x})\, n(\vec{x}')\, e^{-\mu |\vec{x} - \vec{x}'|}}{|\vec{x} - \vec{x}'|}$$

and the e^--background interaction is

$$H_{el\text{-}b} = -e^2 \sum_{i=1}^{N} \int d^3x \, \frac{n(\vec{x})\, e^{-\mu |\vec{x} - \vec{r}_i|}}{|\vec{x} - \vec{r}_i|}$$

$H_{el\text{-}b}$ has same form as H_b, but one needs to replace $(+e)\, n(\vec{x}')$ $\to \rho_{el}(\vec{x}') = \sum_{i=1}^{N} (-e)\, \delta(\vec{x}' - \vec{r}_i)$; furthermore, there is no factor $\frac{1}{2}$ in front, because this is an interaction energy, not a self-energy.

Now, assume uniform background charge

$$n(\vec{x}) \longrightarrow \frac{N}{L^3} = \frac{N}{V}$$

$$H_b = \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \int d^3x \int d^3x' \, \frac{e^{-\mu|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} =$$

$$= \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \int d^3x \int d^3x' \, \frac{e^{-\mu z}}{z} \qquad \text{with} \quad \boxed{z \overset{\text{def}}{=} |\vec{x}-\vec{x}'|}$$

$= \int d^3z$, for uniform medium!

Instead of integrating over all $\vec{x}'$, we can integrate over all $z = |\vec{x}-\vec{x}'|$, for fixed $\vec{x}$, due to translational invariance of the uniform background charge. Using spherical coordinates:

$$\int d^3z \longrightarrow \int z^2 dz \int d\Omega_z$$

$$H_b = \frac{1}{2} e^2 \left(\frac{N}{V}\right)^2 \underbrace{\int d^3x}_{=V} \underbrace{\int d\Omega_z}_{=4\pi} \underbrace{\int_0^\infty dz \, z^{\not 2} \left(\frac{e^{-\mu z}}{\not z}\right)}_{= 1/\mu^2} =$$

$$= \frac{1}{2} e^2 \frac{N^2}{V^2} V 4\pi \frac{1}{\mu^2} \Rightarrow \boxed{H_b = \frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}}$$

In a similar way, we can calculate H_{el-b} for uniform $n(\vec{x}) = N/V$:

$$\boxed{H_{el-b}} = -e^2 \left(\frac{N}{V}\right) \underbrace{\sum_{i=1}^{N}}_{\text{yields another factor } N} \int d^3x \, \frac{e^{-\mu|\vec{x}-\vec{r}_i|}}{|\vec{x}-\vec{r}_i|} \longrightarrow \boxed{-e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}}$$

The total Hamiltonian in coordinate repr. becomes

$$H = \underbrace{-\frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}}_{= H_b + H_{el-b} \;=\; \text{constant?}} + \underbrace{\sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2\right) + \frac{1}{2} e^2 \sum_{\substack{i,j=1 \\ (i \neq j)}}^{N} \frac{e^{-\mu|\vec{r}_i - \vec{r}_j|}}{|\vec{r}_i - \vec{r}_j|}}_{= H_{el}}$$

The constant 1st term diverges in the "physical" limit $\mu \to 0$. No reason to worry; we will show below that $V_{e\text{-}e^-}$ contains a term which will cancel this infinity!

---

b) $\hat{H}$ in occupation number space

Like in the theory of the free Fermi gas, we use the s.p. basis (ch. 2, p. 7):

$$\varphi_{\vec{k}\lambda}(\vec{x}) = \underbrace{L^{-3/2}}_{\| \; V^{-1/2}} e^{i\vec{k}\cdot\vec{x}} \eta_\lambda^{s=\frac{1}{2}}$$

↑ spinor ($\lambda = \pm\frac{1}{2}$ or $\uparrow\downarrow$)

$$\searrow \quad \hat{H} = \underbrace{-\frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}}_{\text{constant, unchanged}} + \hat{T}^{(1)} + \hat{V}^{(2)}_{e\text{-}e^-}$$

The 1-body kin. energy operator is the same as for free Fermi gas (ch. 3, p. 11):

$$\hat{T}^{(1)} = \sum_{\vec{k},\lambda} \frac{\hbar^2 \vec{k}^2}{2m} \hat{n}_{\vec{k}\lambda}$$

($\hat{n}_{\vec{k}\lambda}$: electron number operator)

and the 2-body potential operator has the form (see notes ch. 2, p. 28):

$$\hat{V}^{(2)}_{e\text{-}e\text{-}} = \frac{1}{2} \sum_{\vec{k}_1 \ldots \vec{k}_4} \sum_{\lambda_1 \ldots \lambda_4} \langle \vec{k}_1 \lambda_1, \vec{k}_2 \lambda_2 | v_{ee} | \vec{k}_3 \lambda_3, \vec{k}_4 \lambda_4 \rangle$$

$$\times \hat{c}^{+}_{\vec{k}_1 \lambda_1} \hat{c}^{+}_{\vec{k}_2 \lambda_2} \hat{c}_{\vec{k}_4 \lambda_4} \hat{c}_{\vec{k}_3 \lambda_3} .$$

note sequence!

The 2-body potential matrix element is

$$\langle \ldots | v_{ee} | \ldots \rangle = e^2 \int d^3x_1 \int d^3x_2 \, \varphi^{+}_{\vec{k}_1 \lambda_1}(\vec{x}_1) \, \varphi^{+}_{\vec{k}_2 \lambda_2}(\vec{x}_2)$$

$$\times \frac{e^{-\mu |\vec{x}_1 - \vec{x}_2|}}{|\vec{x}_1 - \vec{x}_2|} \varphi_{\vec{k}_3 \lambda_3}(\vec{x}_1) \, \varphi_{\vec{k}_4 \lambda_4}(\vec{x}_2) .$$

Each plane wave contains a normal. factor $V^{-1/2}$, and the spinor parts are orthonormal (Kronecker δ-s):

$$\langle \ldots | v_{ee} | \ldots \rangle = \frac{e^2}{V^2} \underbrace{\eta^{+}_{\lambda_1}(1) \, \eta_{\lambda_3}(1)}_{= \delta_{\lambda_1 \lambda_3}} \underbrace{\eta^{+}_{\lambda_2}(2) \, \eta_{\lambda_4}(2)}_{= \delta_{\lambda_2 \lambda_4}} \times$$

$$\times \int d^3x_1 \int d^3x_2 \, e^{i(-\vec{k}_1 + \vec{k}_3)\cdot \vec{x}_1} \, e^{-i(-\vec{k}_2 + \vec{k}_4)\cdot \vec{x}_2} \, \frac{e^{-\mu |\vec{x}_1 - \vec{x}_2|}}{|\vec{x}_1 - \vec{x}_2|}$$

Substitution: $\vec{y} = \vec{x}_1 - \vec{x}_2$, $\vec{x} = \vec{x}_2$. Again, we shift origin of integration because of translational invariance of system.

$$\int d^3x_2 \int d^3x_1 \rightarrow \int d^3x \int d^3y :$$

$$\langle \ldots | v_{ee} | \ldots \rangle = \frac{e^2}{V^2} \delta_{\lambda_1 \lambda_3} \delta_{\lambda_2 \lambda_4} \underbrace{\int d^3x \, e^{-i(\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4)\cdot \vec{x}}}_{= V \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4}}$$

$$\times \underbrace{\int d^3y \, e^{i(\vec{k}_3 - \vec{k}_1)\cdot \vec{y}} \, \frac{e^{-\mu y}}{y}}_{= \text{F.T. of Yukawa potential} = 4\pi \left[(\vec{k}_1 - \vec{k}_3)^2 + \mu^2 \right]^{-1}}$$

The $e^- e^-$ interaction in occupation # space becomes

$$\hat{V}^{(2)}_{e^-e^-} = \frac{e^2}{2V^2} \sum_{\vec{k}_1 \vec{k}_2 \vec{k}_3 \vec{k}_4} \sum_{\lambda_1 \lambda_2 \lambda_3 \lambda_4} \delta_{\lambda_1 \lambda_3} \delta_{\lambda_2 \lambda_4} \cdot V \cdot \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4}$$

$$\times \frac{4\pi}{(\vec{k}_1 - \vec{k}_3)^2 + \mu^2} \hat{c}^+_{\vec{k}_1 \lambda_1} \hat{c}^+_{\vec{k}_2 \lambda_2} \hat{c}_{\vec{k}_4 \lambda_4} \hat{c}_{\vec{k}_3 \lambda_3} .$$

$\downarrow$

Define momentum transfer $\boxed{\hbar \vec{q} = \hbar (\vec{k}_1 - \vec{k}_3)}$.

Because of momentum conservation contained in the Kronecker delta above

$$\delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4} \rightarrow \boxed{\vec{k}_1 + \vec{k}_2 \overset{!}{=} \vec{k}_3 + \vec{k}_4} \quad (*)$$

the sum over 4 momenta can be reduced to a triple sum.
We define the new momenta

$$\boxed{\vec{k}, \vec{p}, \vec{q}}$$

via the transformation equations

$$\vec{k}_1 = \vec{k} + \vec{q}, \quad \vec{k}_2 = \vec{p} - \vec{q}, \quad \vec{k}_3 = \vec{k}, \quad \vec{k}_4 = \vec{p}$$

which ensures the momentum conservation $(*)$. We find for $\hat{V}$:

$$\boxed{\hat{V}^{(2)}_{e^-e^-} = \frac{e^2}{2V} \sum_{\vec{k}, \vec{p}, \vec{q}} \sum_{\lambda_1 \lambda_2} \frac{4\pi}{\vec{q}^2 + \mu^2} \hat{c}^+_{\vec{k}+\vec{q}, \lambda_1} \hat{c}^+_{\vec{p}-\vec{q}, \lambda_2} \hat{c}_{\vec{p} \lambda_2} \hat{c}_{\vec{k} \lambda_1}}$$

We separate the last eq. into a term with no momentum transfer ($|\vec{q}| = 0$) and a term involving finite momentum transfer ($|\vec{q}| \neq 0$):

$$\boxed{\hat{V}^{(2)}_{e^-e^-} = \hat{V}^{(2)}_{e^-e^-}(q=0) + \hat{V}^{(2)}_{e^-e^-}(q \neq 0)}.$$

The first term can be simplified as follows

$$\hat{V}^{(2)}_{e^-e^-}(q=0) = \frac{e^2}{2V} \sum_{\vec{k},\vec{p}} \sum_{\lambda_1,\lambda_2} \frac{4\pi}{\mu^2} \hat{c}^+_{\vec{k}\lambda_1} \hat{c}^+_{\vec{p}\lambda_2} \hat{c}_{\vec{p}\lambda_2} \hat{c}_{\vec{k}\lambda_1}.$$

Using anticommutation relations for $\hat{c}, \hat{c}^+$ we find (using shorthand notation)

$$c_1^+ c_2^+ c_2 c_1 = -c_1^+ c_2^+ c_1 c_2 = -c_1^+ (\delta_{12} - c_1 c_2^+) c_2 =$$

$$= -c_1^+ c_2 \delta_{12} + (c_1^+ c_1)(c_2^+ c_2) = -\hat{n}_1 \delta_{12} + \hat{n}_1 \hat{n}_2$$

Insert this above:

$$\hat{V}^{(2)}_{e^-e^-}(q=0) = -\frac{e^2}{2V} \frac{4\pi}{\mu^2} \underbrace{\sum_{\vec{k},\lambda_1} \hat{n}_{\vec{k}\lambda_1}}_{=\hat{N}} + \frac{e^2}{2V} \frac{4\pi}{\mu^2} \underbrace{\sum_{\vec{k},\lambda_1} \hat{n}_{\vec{k}\lambda_1}}_{=\hat{N}} \underbrace{\sum_{\vec{p},\lambda_2} \hat{n}_{\vec{p}\lambda_2}}_{=\hat{N}}$$

$$\rightarrow \boxed{\hat{V}^{(2)}_{e^-e^-}(q=0) = -\frac{e^2}{2V} \frac{4\pi}{\mu^2} \hat{N} + \frac{e^2}{2V} \frac{4\pi}{\mu^2} \hat{N}^2}$$

In normal quantum many-body theory, the total particle number N is always fixed, and we may replace the number operator $\hat{N}$ by its eigenvalue N:

$$\hat{N} \rightarrow N.$$

We now combine all terms of the Hamiltonian:

$$\hat{H} = \underbrace{-\frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}}_{\hat{H}_0 + \hat{H}_{el-b}} + \sum_{\vec{k},\lambda} \frac{\hbar^2 \vec{k}^2}{2m} \hat{n}_{\vec{k}\lambda} \underbrace{- \frac{e^2}{2V} \frac{4\pi}{\mu^2} N + \frac{e^2}{2V} \frac{4\pi}{\mu^2} N^2}_{\hat{V}_{ee}(q=0)}$$

$$+ \hat{V}_{ee}(q \neq 0),$$

where

$$\hat{V}_{ee}(q\neq 0) = \frac{e^2}{2V} \sum_{\vec{k},\vec{p}} \sum_{\vec{q}\neq 0} \sum_{\lambda_1,\lambda_2} \frac{4\pi}{\vec{q}^2} \hat{c}^{+}_{\vec{k}+\vec{q},\lambda_1} \hat{c}^{+}_{\vec{p}-\vec{q},\lambda_2} \hat{c}_{\vec{p}\lambda_2} \hat{c}_{\vec{k}\lambda_1}$$

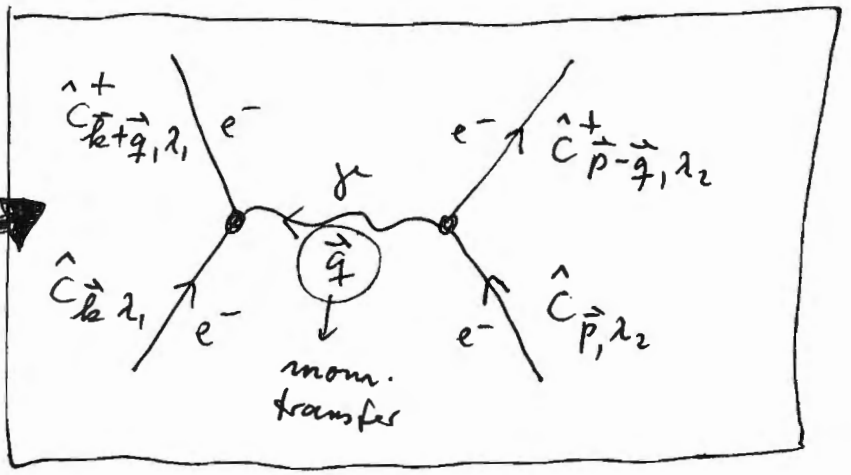
denotes the electron-electron Coulomb interaction for finite momentum transfer; here we have taken the physical limit $\mu \to 0$. We see that the constant energy of $(\hat{H}_0 + \hat{H}_{e-b})$ cancels against the 2nd term of $V_{ee}(q=0)$. The remaining term in $\hat{V}_{ee}(q=0)$ vanishes in the proper physical limit, as we will now demonstrate: It represents an energy per particle of

$$\frac{E}{N} = -\frac{e^2}{2V}\frac{4\pi}{\mu^2} = \frac{-e^2}{2L^3}\frac{4\pi}{\mu^2} = -\frac{e^2 2\pi}{L}\left(\frac{r_{coul}}{L}\right)^2$$

with $r_{coul} = 1/\mu$ = range of Coulomb force. We now take the limit $L \to \infty$, $r_{coul} \to \infty$ in such a way that $(r_{coul}/L) \ll 1$, i.e. the range of the Coulomb repulsion between 2 electrons is much smaller than the size L of the bulk material. In this case, the term vanishes, and the system Hamiltonian becomes

$$\hat{H} = \underbrace{\sum_{\vec{k},\lambda} \frac{\hbar^2\vec{k}^2}{2m} \hat{n}_{\vec{k}\lambda}}_{\equiv \hat{T}^{(1)}} + \hat{V}^{(2)}_{ee}(q\neq 0)$$

$\hat{V}_{ee}(q\neq 0)$ may be represented by a "Feynman-like" diagram; virtual photon exchange, photon propagator $\propto \frac{1}{\vec{q}^2}$.



c) Ground state energy in 1st-order perturbation theory

In 1st-order perturbation theory (see Shankar, QM, ch. 17) we may replace the exact (= interacting) ground state by the non-interacting g.s. of the free Fermi gas:

$$E_{g.s.} = \langle g.s. | \hat{H} | g.s. \rangle \overset{\text{perturb.}}{\approx} \langle \phi_0 | \hat{H} | \phi_0 \rangle$$

($|g.s.\rangle$: interacting; $|\phi_0\rangle$: non-int.)

In this approximation, the g.s. energy becomes

$$\boxed{E_{g.s.} \approx \underbrace{\langle \phi_0 | \hat{T}^{(1)} | \phi_0 \rangle}_{\overset{\text{def}}{=} E_0} + \underbrace{\langle \phi_0 | \hat{V}_{ee}^{(1)}(q \neq 0) | \phi_0 \rangle}_{\overset{\text{def}}{=} E_1}}$$

We have already calculated the energy E_0 for the free Fermi gas and found (ch. 3, p. 13):

$$\boxed{\frac{E_0}{N} = \frac{3}{5} E_F, \quad E_F = \frac{p_F^2}{2m} \text{ with } p_F = \hbar k_F = \hbar (3\pi^2 \rho_0)^{1/3}}$$

Using the expression for $\hat{V}_{ee}(q \neq 0)$ on p. 9, we get for the interaction energy E_1:

$$E_1 = \frac{e^2}{2V} \sum_{\vec{k},\vec{p}} \sum_{\vec{q} \neq 0} \sum_{\lambda_1, \lambda_2} \frac{4\pi}{q^2} \langle \phi_0 | \hat{c}^+_{\vec{k}+\vec{q},\lambda_1} \hat{c}^+_{\vec{p}-\vec{q},\lambda_2} \cdot \hat{c}_{\vec{p}\lambda_2} \hat{c}_{\vec{k}\lambda_1} | \phi_0 \rangle$$

This expression may be evaluated using Wick's theorem result (ch. 4, p. 14):

$$\left.\begin{aligned} \langle \phi_0 | \hat{c}_\alpha^+ \hat{c}_\beta^+ \hat{c}_\delta \hat{c}_\gamma | \phi_0 \rangle &= \rho_{\delta\beta}\cdot\rho_{\gamma\alpha} - \rho_{\delta\alpha}\cdot\rho_{\gamma\beta} \\ \text{with} \quad \rho_{\beta\alpha} &= \theta(\varepsilon_F - \varepsilon_\alpha)\,\delta_{\alpha\beta}. \end{aligned}\right\}$$

In our case, the quantum numbers are

$$\alpha = (\vec{k}+\vec{q}, \lambda_1) \quad \beta = (\vec{p}-\vec{q}, \lambda_2) \quad \delta = (\vec{p}, \lambda_2) \quad \gamma = (\vec{k}, \lambda_1)$$

$$\rightarrow \underline{\langle \phi_0 | \hat{c}^+_{\vec{k}+\vec{q},\lambda_1} \hat{c}^+_{\vec{p}-\vec{q},\lambda_2} \hat{c}_{\vec{p}\lambda_2} \hat{c}_{\vec{k}\lambda_1} | \phi_0 \rangle =}$$

$$= \rho_{\vec{p},\lambda_2;\,\vec{p}-\vec{q},\lambda_2}\cdot\rho_{\vec{k},\lambda_1;\,\vec{k}+\vec{q},\lambda_1} - \rho_{\vec{p},\lambda_2;\,\vec{k}+\vec{q},\lambda_1}\cdot\rho_{\vec{k},\lambda_1;\,\vec{p}-\vec{q},\lambda_2} =$$

$$= \underbrace{\delta_{\vec{p},\vec{p}-\vec{q}}}_{=\delta_{\vec{q},\vec{0}}}\cdot\delta_{\lambda_2\lambda_2}\cdot\underbrace{\theta(\varepsilon_F-\varepsilon_p)}_{\text{"}1}\cdot\underbrace{\delta_{\vec{k},\vec{k}+\vec{q}}}_{=\delta_{\vec{q},\vec{0}}}\cdot\delta_{\lambda_1\lambda_1}\cdot\underbrace{\theta(\varepsilon_F-\varepsilon_k)}_{\text{"}1}$$

$$- \delta_{\vec{p},\vec{k}+\vec{q}}\cdot\delta_{\lambda_2\lambda_1}\cdot\underbrace{\theta(\varepsilon_F-\varepsilon_p)}_{=\theta(k_F-p)}\cdot\underbrace{\delta_{\vec{k},\vec{p}-\vec{q}}}_{\equiv\delta_{\vec{p},\vec{k}+\vec{q}}}\cdot\delta_{\lambda_2\lambda_1}\underbrace{\theta(\varepsilon_F-\varepsilon_k)}_{=\theta(k_F-k)}$$

Note that this <u>matrix element</u> is to be <u>inserted</u> into the expression for $V_{ee}(q\neq 0)$ on page 9, or for <u>E_1 on p. 10</u>:

$$E_1 = \frac{e^2}{2V}\sum_{\vec{k},\vec{p}}\sum_{\vec{q}\neq 0}\sum_{\lambda_1,\lambda_2}\frac{4\pi}{q^2}\langle\phi_0|\hat{c}^+\hat{c}^+\hat{c}\,\hat{c}|\phi_0\rangle$$

Therefore the <u>first term</u> <u>$\propto \delta_{\vec{q},\vec{0}}$</u> does <u>not contribute</u> and we are left with

$$E_1 = \frac{e^2}{2L^3}\sum_{\vec{k},\vec{p}}\sum_{\vec{q}\neq 0}\sum_{\lambda_1,\lambda_2}\frac{4\pi}{q^2}\left[-\delta_{\vec{p},\vec{k}+\vec{q}}\,\delta_{\lambda_2\lambda_1}\,\theta(k_F-p)\,\theta(k_F-k)\right]$$

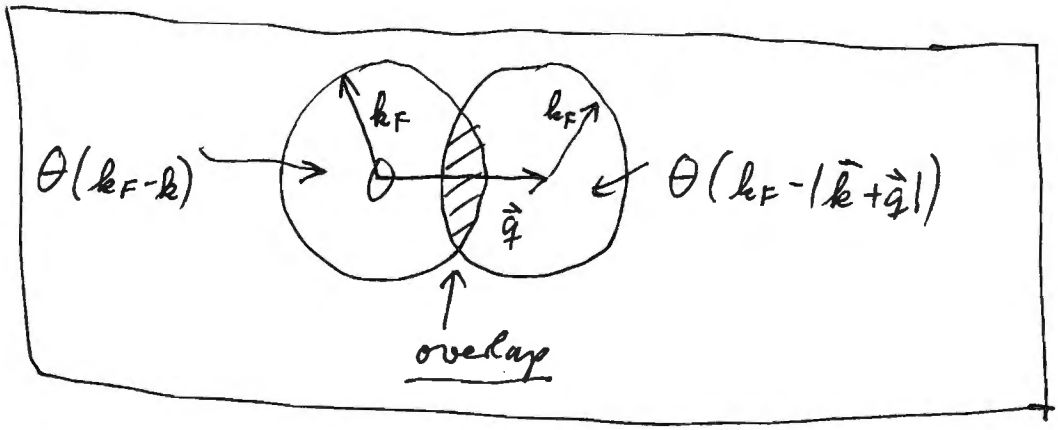
Rearranging the factors:

$$E_1 = -\frac{e^2}{2L^3}\underbrace{\left(\sum_{\lambda_1\lambda_2}\delta_{\lambda_2\lambda_1}\right)}_{=\left(\sum_{\lambda_1}1\right)=2}\sum_{\vec{k}}\sum_{\vec{q}\neq\vec{0}}\frac{4\pi}{q^2}\underbrace{\left[\sum_{\vec{p}}\delta_{\vec{p},\vec{k}+\vec{q}}\,\theta(k_F-p)\right]}_{=\theta(k_F-|\vec{k}+\vec{q}|)}\theta(k_F-k)$$

$$E_1 = -\frac{e^2}{\chi L^3}\cdot\chi\sum_{\vec{k}}\sum_{\vec{q}\neq 0}\frac{4\pi}{q^2}\,\theta(k_F-|\vec{k}+\vec{q}|)\,\theta(k_F-k) \xrightarrow[\text{large } L]{\text{see ch. 3, p. 12}}$$

$$E_1 = -\frac{e^2}{L^3}\left(\frac{L^3}{(2\pi)^3}\int d^3k\right)\left(\frac{L^3}{(2\pi)^3}\int_{(q\neq 0)} d^3q\right)\frac{4\pi}{q^2}\,\underbrace{\theta(k_F-|\vec{k}+\vec{q}|)}_{\text{Fermi spheres}}\,\theta(k_F-k)$$

This integral involves the overlap between two "Fermi spheres" in momentum space, with radius k_F:



See Fetter & Walecka, p. 28, fig. 3.1

For the interaction energy per particle one obtains, after calculating the overlap (details see FW, p. 28):

$$\boxed{\frac{E_1}{N} = -\frac{3}{4\pi}e^2 k_F}$$

Question: E_1 is part of the electron-electron interaction (for $|\vec{q}|\neq 0$). How can it be negative? Shouldn't it be repulsive (+ sign)?

Answer: Remember, we split up $\hat{V}_{ee}$ into 2 parts:

$$\langle \phi_0 | \hat{V}_{ee} | \phi_0 \rangle = \underbrace{\langle \phi_0 | \hat{V}_{ee}(q=0) | \phi_0 \rangle}_{= + \frac{e^2}{2V} \frac{4\pi}{\mu^2} N^2} + \underbrace{\langle \phi_0 | V_{ee}(q \neq 0) | \phi_0 \rangle}_{\text{"exchange energy"}}.$$

"direct" energy (p.8) (positive)

("exchange energy" (negative))

The "direct" part of $V_{ee}(q=0)$ cancels out the electrostatic energies of $(H_b + H_{el-b})$, see p.8, which reflect the electric neutrality of the total system. The remaining term $(q \neq 0)$ is known as the "exchange energy" which arises from the evaluation of the matrix element

$$\langle \phi_0 | \hat{c}^{+}_{k+\vec{q},\lambda_1} \hat{c}^{+}_{p-\vec{q},\lambda_2} \hat{c}_{p\lambda_2} \hat{c}_{k\lambda_1} | \phi_0 \rangle$$

via Wick's theorem using anticommutation relations for the $\hat{c}, \hat{c}^{+}$. Therefore, the negative sign of the exchange energy is ultimately due to the antisymmetry of the many-particle electron wave function (fermionic system)!!

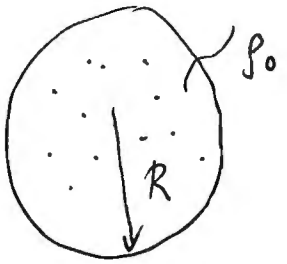
Hence, the total g.s. energy per particle, in 1st-order perturbation theory, is:

$$\boxed{\frac{E_{g.s.}(k_F)}{N} = \frac{E_0}{N} + \frac{E_1}{N} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} - \frac{3}{4\pi} e^2 k_F}$$

We have already established that $k_F = k_F(\rho_0) = (3\pi^2 \rho_0)^{1/3}$.

So, we could express

$$\frac{E_{g.s.}(\rho_0)}{N} = \ldots$$



The density of a large sphere with radius R is

$$\rho_0 = \frac{N}{V} = \frac{N}{\frac{4\pi}{3}R^3}.$$

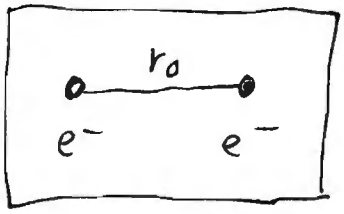
In order for ρ_0 to be a constant, we must have

$$R^3 \propto N \quad \text{or} \quad R = r_0 N^{1/3} \quad \text{(like in nucleus!)}.$$

Indeed in this case, we get

$$\boxed{\rho_0 = \frac{3N}{4\pi R^3} = \frac{3\cancel{N}}{4\pi r_0^3 \cancel{N}} = \frac{3}{4\pi r_0^3}} \quad (*)$$

where the radius parameter r_0 may be identified with the average distance r_0 between the electrons



$$\searrow \quad k_F = \left(3\pi^2 \rho_0\right)^{1/3} \overset{(*)}{=} \left(\frac{9\pi^2}{4\pi r_0^3}\right)^{1/3}$$

$$\Rightarrow \boxed{k_F(r_0) = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_0}}$$

Finally, the textbook introduces the dimensionless distance parameter

$$\boxed{r_s \overset{\text{def}}{=} \frac{r_0}{a_0}} \quad \text{with } a_0 = 0.529 \times 10^{-10}\,\text{m} = \text{Bohr radius}$$

and expresses the energies in units of

$$\boxed{\text{Ry} = \text{Rydberg} = \frac{e^2}{2a_0} = 13.6\,\text{eV}}$$

A straightforward calculation yields

$$\boxed{\frac{E_{g.s.}(r_s)}{N} = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} \quad [\text{Rydberg}]}$$

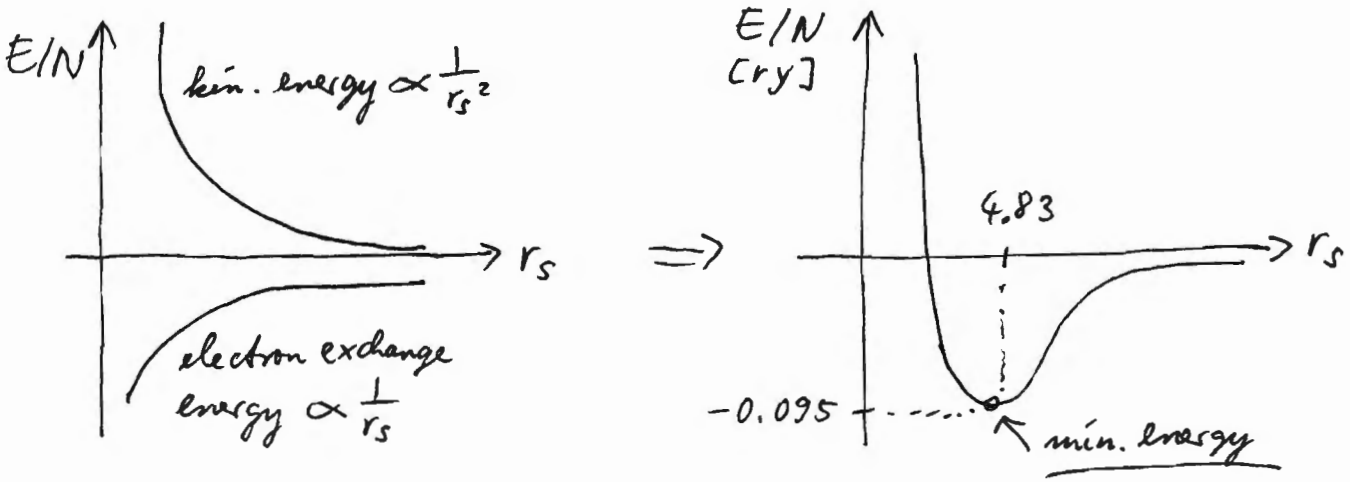
Comment on validity of 1st-order pert. theory

Valid if the interaction (2nd-term) is small compared to the first (kin. energy), which is true in the limit

$$\text{electron distance } r_s \to 0 \iff \rho_0 \to \text{large}$$

So, our results are good in the high-density limit!

Plot of our result



Minimum system energy is obtained for

$$(r_s)_{min} = 4.83, \quad \text{with } (E_{g.s.}/N)_{min} = -0.095\,ry = -1.29\,eV$$

Summary: The metal has a negative g.s. energy per particle, i.e. the system is bound. Note that the binding arises entirely from $\hat{V}_{ee}(q \neq 0)$, i.e. from the electron exchange energy which is negative because of antisym. relations for fermion operators $\hat{c}, \hat{c}^+$. This means that the binding of metals cannot be understood classically!!!

Comparison to exp. data

Even though this model is relatively crude (replacement of ionic cores by uniform background charge), it explains exp. data for metallic sodium under typical lab conditions rather well:

> Exp: $(r_s)_{min} = 3.96$, $(E_{g.s.}/N)_{min} = -1.13\,eV$.

Note: binding energy of metal = heat of vaporization.
One can also calculate pressure and bulk modulus (see FW, p.30).

Proof that bound state exists (Rayleigh-Ritz principle)

Even though our perturbative treatment is only justified in the high-density limit of the electron gas ($r_s \to 0$), we can use the Rayleigh-Ritz variational principle (see Shankar, QM, ch.16) to prove the existence of a bound ground state, because

$$E_{g.s.} = \langle g.s. | \hat{H} | g.s. \rangle \leq \langle \phi_0 | \hat{H} | \phi_0 \rangle \leq 0.$$

($|g.s.\rangle$: exact; $|\phi_0\rangle$: arbitrary normalized state (here: non-int. g.s.))

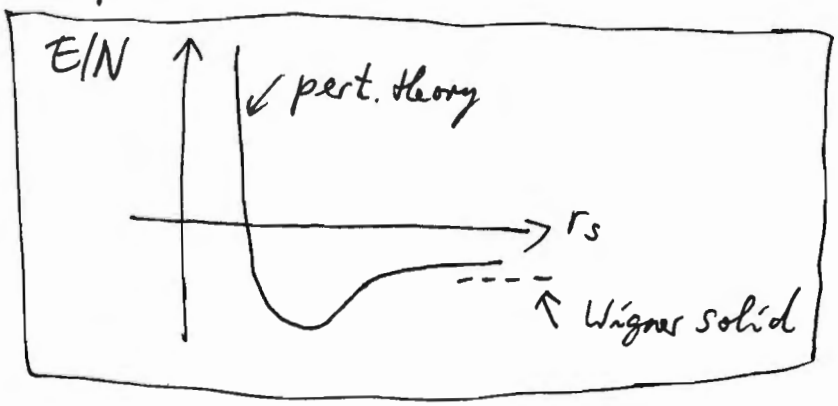
This implies that the exact g.s. energy lies below our perturbative result, i.e. there is definitely a bound state (with negative energy).

Further improvements of this theory

1) one improvement is to use Green's function (= propagator) techniques (see FW, chapter 3) and to sum up higher-order terms in the "proper self-energy" using Feynman diagrams (see FW, sections 12 for $T=0$ and section 30 for $T \neq 0$). These higher-order terms are called the correlation energy.

2) Further theoretical progress requires that one must replace the homogeneous background charge by the ionic cores.

3) Low-density limit ($r_s \to \infty$): in 1938, Wigner has shown that in the low-density limit the electrons crystallize into a "Wigner solid" which has lower energy than our perturbative result:



see FW, fig. 3.2