CHAPTER 6: THE INTERACTING ELECTRON GAS

In this chapter, we start the investigation of properties of the interacting electron gas, which can describe simple metals or semiconductors, for which either the presence of the ionic periodic potential can be neglected, or included in terms of effective mass.

Within the adiabatic approximation, the total electronic hamiltonian in the presence of the ion reads:

$$\hat{H}_{el} = \hat{T}_{el} + \hat{V}_{ee} + \hat{V}_{ei} + \hat{V}_{ii} =$$

$$= \sum_{\sigma} \int d\vec{r}\, \hat{\psi}_{\sigma}^{+}(\vec{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} + v_{ei}(\vec{r}) \right) \hat{\psi}_{\sigma}(\vec{r}) + \hat{V}_{ee} + \hat{V}_{ei} \qquad (6.1)$$

where $v_{ei}(\vec{r}) = -\sum_{\alpha\tau} \frac{Z_\tau e^2}{4\pi\varepsilon_0 |\vec{r} - \vec{R}_{\alpha\tau}|}$. Suppose we fully neglect the ion:

$$\hat{H}'_{el} = \hat{T}_{ee} + \hat{V}_{ee} = \sum_{\vec{k}\sigma} \frac{\hbar^2 k^2}{2m} \hat{a}^{+}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} + \frac{1}{2V} \sum_{\substack{\vec{k}\vec{k}' \\ \sigma\sigma'}} \sum_{\vec{q}} \tilde{v}_{ee}(\vec{q})\, \hat{a}^{+}_{\vec{k}+\vec{q}\sigma} \hat{a}^{+}_{\vec{k}'-\vec{q}\sigma'} \hat{a}_{\vec{k}'\sigma'} a_{\vec{k}\sigma} \qquad (6.2)$$

where $\tilde{v}_{ee}(\vec{q}) = \frac{e^2}{\varepsilon^{\circ} q^2}$ has an unphysical divergence at $|\vec{q}| = 0$. We can, first of all isolate the divergence and write:

$$\hat{V}_{ee} = \frac{1}{2V} \sum_{\substack{\vec{k}\vec{k}', \vec{q} \neq 0 \\ \sigma\sigma'}} \tilde{v}_{ee}(\vec{q})\, \hat{a}^{+}_{\vec{k}+\vec{q}\sigma} \hat{a}^{+}_{\vec{k}'-\vec{q}\sigma'} \hat{a}_{\vec{k}'\sigma'} \hat{a}_{\vec{k}\sigma} + \lim_{\vec{q} \to 0} \tilde{v}_{ee}(\vec{q}) \frac{\hat{N}_{el}(\hat{N}_{el} - 1)}{2V} \qquad (6.3)$$

The operatorial form of the diverging component stem from:

$$\sum_{\vec{k}\sigma\vec{k}'\sigma'} \hat{a}^{+}_{\vec{k}\sigma} \hat{a}^{+}_{\vec{k}'\sigma'} \hat{a}_{\vec{k}'\sigma'} \hat{a}_{\vec{k}\sigma} = -\sum_{\vec{k}\sigma\vec{k}'\sigma'} \hat{a}^{+}_{\vec{k}\sigma} \hat{a}^{+}_{\vec{k}'\sigma'} \hat{a}_{\vec{k}\sigma} \hat{a}_{\vec{k}'\sigma'}$$

$$= \sum_{\vec{k}\sigma\vec{k}'\sigma'} \left(\hat{a}^{+}_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} \hat{a}^{+}_{\vec{k}'\sigma'} \hat{a}_{\vec{k}'\sigma'} - a^{+}_{\vec{k}\sigma} \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'} \hat{a}_{\vec{k}'\sigma'} \right) = \hat{N}^2_{el} - \hat{N}_{el}$$

where $\hat{N}_{el} = \sum_{\vec{k}\sigma} \hat{n}_{\vec{k}\sigma}$.

6.1 The Jellium model

The unphysical divergence is removed by including the positively charged ionic background. The latter, not only provides the periodic potential for the electrons, but it further ensures charge NEUTRALITY.

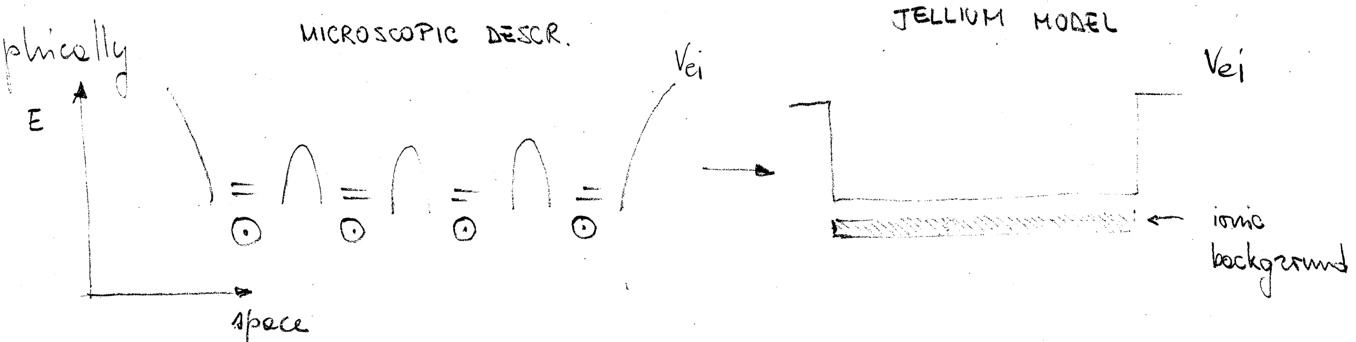
The (local) charge density is

$$e\tilde{\rho}(\vec r) = e\Big[\rho(\vec r) - \overbrace{\sum_{\alpha\tau} Z_\tau\, \delta(\vec r - \vec R_{\alpha\tau})}^{\rho_{ion}(\vec r) = \sum_\tau Z_\tau \rho_{ion,\tau}(\vec r)}\Big] \qquad e<0 \qquad (6.4)$$

Within the jellium model the ionic charge is supposed to be uniformly spread in space $\rho_{ion}(\vec r) \approx \frac{N_{el}}{V} = n_{el}$. We thus obtain

$$\rho^{jellium}(\vec r) \equiv \rho(\vec r) - n_e \qquad (6.5)$$

Graphically



In the total electronic Hamiltonian we obtain, correspondingly:

$$\hat H_{el} = \hat T_{el} + \hat V_{ee} + \hat V_{ei} + \hat V_{ii} \cong \hat T_{el} + \hat V_{ee} + \hat V_{ei}^{\,jellium} + \hat V_{ii}^{\,jellium}$$

$$\hat V_{ei} = -\frac{e^2}{4\pi\varepsilon_0}\int d\vec r \int d\vec r' \sum_j \delta(\vec r - \vec r_j) \sum_{\alpha\tau} Z_\tau\, \delta(\vec r' - \vec R_{\alpha\tau}) \frac{1}{|\vec r - \vec r'|} +$$

$$= -\frac{e^2}{4\pi\varepsilon_0}\int d\vec r \int d\vec r' \sum_\tau \hat\rho_{el}(\vec r)\, \hat\rho_{ion,\tau}(\vec r') \frac{Z_\tau}{|\vec r - \vec r'|}$$

$$\hat V_{ii} = \frac{1}{2}\int d\vec r\, d\vec r' \sum_\tau \sum_{\tau'} \hat\psi^\dagger_{ion,\tau}(\vec r)\, \hat\psi^\dagger_{ion,\tau'}(\vec r') \frac{Z_\tau Z_{\tau'} e^2}{4\pi\varepsilon_0 |\vec r - \vec r'|} \hat\psi_{ion,\tau'}(\vec r')\, \hat\psi_{ion,\tau}(\vec r)$$

But, in the jellium model $\sum_\tau Z_\tau \hat\rho_{ion,\tau}(\vec r) \cong \frac{\hat N_{el}}{V} \Rightarrow$ a UNIFORM density.

It follows immediately that.

$$\hat{V}_{ei} + \hat{V}_{ii} \cong -\frac{\hat{N}_{el}}{V}\int d\vec{r}\int d\vec{r}\,'\, \hat{\rho}_{el}(\vec{r})\,\frac{e^2}{|\vec{r}-\vec{r}\,'|} + \frac{1}{2}\frac{\hat{N}_{el}^2}{V^2}\int d\vec{r}\int d\vec{r}\,'\,\frac{e^2}{|\vec{r}-\vec{r}\,'|}$$

$$-\frac{\hat{N}_{el}}{V}\lim_{\vec{q}\to 0}\hat{\rho}_{el}(\vec{q})\,\tilde{v}_{ee}(\vec{q}) + \frac{1}{2}\frac{\hat{N}_{el}^2}{V}\lim_{\vec{q}\to 0}\tilde{v}_{ee}(\vec{q}) \qquad (6.6)$$

where in the last equality we have used the properties:

$$\int dx\, f(x) = \lim_{q\to 0}\tilde{f}(q)$$

$$\int dx\int dy\, f(x-y)\,g(y)\,e^{-iqx} = f(q)\,g(q) \qquad F[f*g] = F[f]\,F[g]$$

In the jellium model we can thus write:

$$\hat{H}_{el}^{jellium} = \hat{T}_{el} + \underbrace{\frac{1}{2V}\sum_{\substack{\vec{k}\sigma\,\vec{k}'\sigma' \\ \vec{q}\neq 0}}\tilde{v}_{ee}(\vec{q})\,\hat{a}^+_{\vec{k}+\vec{q}\sigma}\,\hat{a}^+_{\vec{k}'-\vec{q}\sigma'}\,\hat{a}_{\vec{k}'\sigma'}\,\hat{a}_{\vec{k}\sigma}}_{\hat{V}_{ee}^{jellium}} \qquad (6.7)$$

proof:

$$\hat{V}_{ee} + \hat{V}_{ei} + \hat{V}_{ii} - \hat{V}_{ee}^{jellium} =$$

$$= \lim_{\vec{q}\to 0}\tilde{v}_{ee}(\vec{q})\left[\frac{\hat{N}_{el}(\hat{N}_{el}-1)}{2V} - \frac{\hat{N}_{el}}{V}\hat{\rho}_{el}(\vec{q}) + \frac{\hat{N}_{el}^2}{2V}\right]$$

$$= \frac{1}{V}\lim_{\vec{q}\to 0}\tilde{v}_{ee}(\vec{q})\left[\frac{\hat{N}_{el}(\hat{N}_{el}-1)}{2} + \frac{\hat{N}_{el}^2}{2} - \hat{N}_{el}^2\right]$$

$$= -\lim_{q\to 0}\tilde{v}_{ee}(\vec{q})\,\frac{\hat{N}_{el}}{2V}$$

This last term can be neglected in the thermodynamic limit since it gives a negligible energy per particle.

e.g. $\hat{T}_{el} = \bar{\varepsilon}\,\hat{N}$ with $\bar{\varepsilon} = \left(\frac{4}{3}\pi k_F^3\right)^{-1} 4\pi\int_0^{k_F} dk\, k^2\,\frac{\hbar^2 k^2}{2m} = \frac{3}{5}\varepsilon_F$ (6.8)

has a finite energy per particle.

Notice: To keep all expressions in (6.3) - (6.7) meaningfull alway consider the Yukawa potential: $v_{ee}(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\frac{e^{-\alpha|\vec{r}|}}{|\vec{r}|} \Rightarrow \lim_{\vec{q}\to 0} \tilde{v}_{ee}(\vec{q}) = \frac{e^2}{\varepsilon_0 \alpha^2}$. The limit $\alpha \to 0$ can be safely taken as last step.

- $$\hat{\rho}^{\text{jellium}}(\vec{r}) = \hat{\rho}(\vec{r}) - \frac{\hat{N}_{el}}{V} = \frac{1}{V}\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}} \underbrace{\sum_{\vec{k}\sigma} \hat{a}^+_{\vec{k}\sigma}\hat{a}_{\vec{k}+\vec{q}\sigma}}_{\hat{\rho}_{\vec{q}}} - \frac{1}{V}\sum_{\vec{k}\sigma}\hat{a}^+_{\vec{k}\sigma}\hat{a}_{\vec{k}\sigma} =$$
$$= \frac{1}{V}\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}} \underbrace{\hat{\rho}_{\vec{q}}\,(1-\delta_{\vec{q},0})}_{\rho^{\text{jellium}}_{\vec{q}}} \qquad (6.9)$$

- $$\hat{V}^{\text{jellium}}_{ee} = \frac{1}{2V}\sum_{\vec{q}\neq 0}\sum_{\substack{\vec{k}\sigma \\ \vec{k}'\sigma'}} \tilde{v}_{ee}(\vec{q})\, \hat{a}^+_{\vec{k}+\vec{q}\sigma}\hat{a}^+_{\vec{k}'-\vec{q}\sigma'}\hat{a}_{\vec{k}\sigma'}\hat{a}_{\vec{k}\sigma} =$$
$$= \frac{1}{2V}\sum_{\substack{\vec{q}\neq 0\\ \vec{k}\sigma \\ \vec{k}'\sigma'}} \tilde{v}_{ee}(\vec{q}) \left(\hat{a}^+_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}\sigma}\, a^+_{\vec{k}'-\vec{q}\sigma'}a_{\vec{k}'\sigma'} - a^+_{\vec{k}+\vec{q}\sigma}a_{\vec{k}'\sigma'}\,\delta_{\sigma\sigma'}\delta_{\vec{k}'-\vec{q},\vec{k}}\right)$$
$$= \frac{1}{2V}\sum_{\vec{q}\neq 0}\tilde{v}_{ee}(\vec{q})\left(\hat{\rho}_q\hat{\rho}_{-q} - \hat{N}_{el}\right) \qquad (6.10)$$

6.2 Energy scales

The fundamental question it is now under which conditions is the Coulomb interaction weak/strong with respect to the kinetic energy

i) $\frac{V}{N_{el}} \equiv \frac{4}{3}\pi r_0^3 = \frac{1}{n_e}$ is the average volume occupied by 1 electron

ii) Assuming that the electrons interacts predominantly with its nearest neighbours, one obtains a POTENTIAL ENERGY PER PARTICLE
$$\varepsilon_{pot} \approx \frac{e^2}{4\pi\varepsilon_0 r_0} \propto n_e^{1/3} \qquad (6.11)$$

iii) KINETIC ENERGY PER PARTICLE (ground state energy of free electron gas)
$$\varepsilon_{kin} \overset{(6.8)}{=} \frac{3}{5}\frac{\hbar^2}{2m}k_F^2 = \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2 n_e)^{2/3} \propto n_e^{2/3} \qquad (6.12)$$

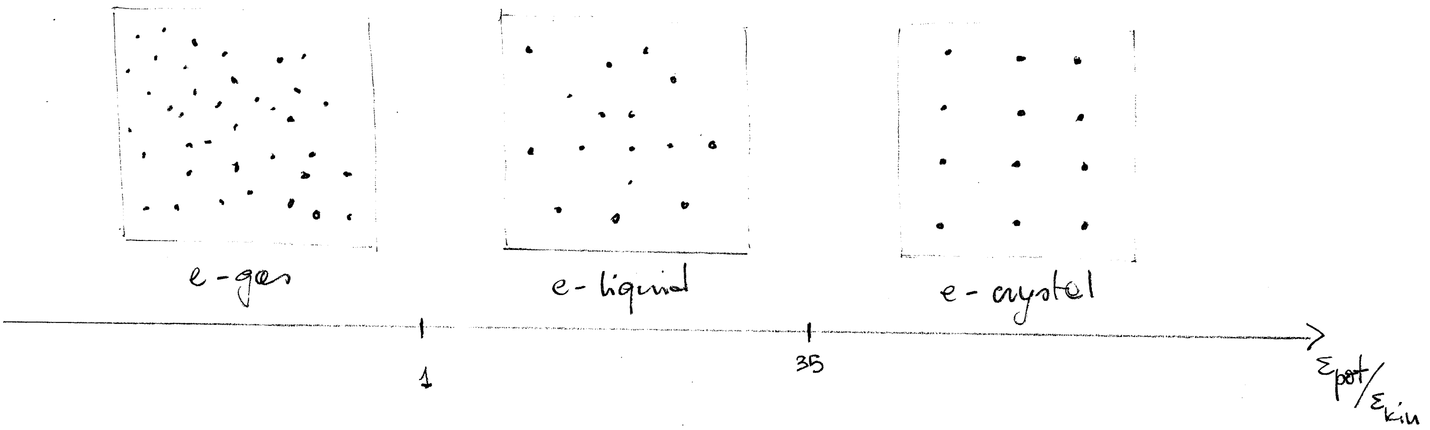
where in (6.12) we have used the fact that:

$$N_{el} = V \frac{1}{(2\pi)^3} \sum_{\sigma} \int d\vec{k}\, f(\varepsilon_{\vec{k}}) \overset{T=0}{=} V \frac{1}{\pi^2} \int_0^{k_F} dk\, k^2 = \frac{V k_F^3}{3\pi^2} \Rightarrow k_F = (3\pi^2 n_e)^{1/3}.$$

iv) $$\frac{\varepsilon_{pot}}{\varepsilon_{kin}} \propto \frac{n_e^{1/3}}{n_e^{2/3}} = n_e^{-1/3} \xrightarrow[n_e \to \infty]{} 0,$$

The importance of the e-e interaction DIMINISHES as the density INCREASES. (effect of the Pauli exclusion principle!)

(6.13)



v) A parameter used to define the RATIO of the two energy scales is provided by the dimensionless density parameter r_s:

$$r_s \equiv \frac{r_0}{a_0} = \frac{r_0}{\frac{4\pi\varepsilon_0 \hbar^2}{m e^2}} = \frac{e^2}{4\pi\varepsilon_0 r_0} \frac{m r_0^2}{\hbar^2} \approx \frac{\varepsilon_{pot}}{\varepsilon_{kin}} \quad \left(= \frac{\varepsilon_{pot}}{\varepsilon_{kin}} \underbrace{\frac{3}{10} \left| \frac{9\pi}{4} \right|^{2/3}}_{\cong 1.105} \right) \qquad (6.14)$$

$a_0 = 0.05$ nm is the Bohr radius

Most metals lie in intermediate coupling regime:

metal	Li	Na	K	Cu	Be	Al	Sn	Pb
r_s	3.2	3.9	4.9	2.7	1.9	2.1	2.2	2.3

The question is now how to treat e-e interactions?

1. Landau's Fermi liquid theory: • Is the realm of the intermediate coupling regimes. It gives an understanding of why a theory of weakly interacting fermions, is able to describe most of the properties of metals, despite $r_s \sim O(1)$

2. Perturbation theory: • First order in $V_{ee}^{jellium}$ is convergent and gives reasonably good results
• Second order: collapses due to divergent integrals

3. Mean field methods: Appealing but sometimes introduce spurious effects or break fundamental conservation laws.

4. Quantum field theoretical methods: Methods that cure the divergences in the perturbation theory.

6.3 Electron-electron interaction in perturbation theory

The starting point of the discussion is the jellium Hamiltonian (6.7):

$$\hat{H}_{el}^{jellium} = \hat{T}_{el} + \hat{V}_{ee}^{jellium}$$

We wish to evaluate the ground state energy per particle ε_G of the interacting system in perturbation theory

■ 0^{th} order

$$\varepsilon_G^{(0)} = \langle FS | \hat{T}_{el} | FS \rangle / N_{el} = \frac{3}{5} \varepsilon_F = 1.105 \frac{\varepsilon_{pot}}{r_s} = \frac{2.21}{r_s^2} Ry \qquad (6.15)$$

where $|FS\rangle$ stands for the Fermi sea $|FS\rangle = \prod_{|\vec{k}| \leq k_F, \sigma} a^+_{\vec{k}\sigma} |0\rangle$

$$1 Ry = \frac{e^2}{8\pi\varepsilon_0 a_0} = 13.6 \text{ eV}$$

■ 1^{st} order

$$\varepsilon_G^{(1)} = \langle FS | \hat{V}_{ee}^{jellium} | FS \rangle / N_{el} =$$

$$= \frac{1}{2VN_{el}} \sum_{\vec{q} \neq 0} \sum_{\substack{\vec{k}\sigma \\ \vec{k}'\sigma'}} \tilde{v}_{ee}(\vec{q}) \langle FS | \hat{a}^+_{\vec{k}+\vec{q}\sigma} \hat{a}^+_{\vec{k}'-\vec{q}\sigma'} \hat{a}_{\vec{k}'\sigma'} \hat{a}_{\vec{k}\sigma} | FS \rangle \qquad (6.16)$$

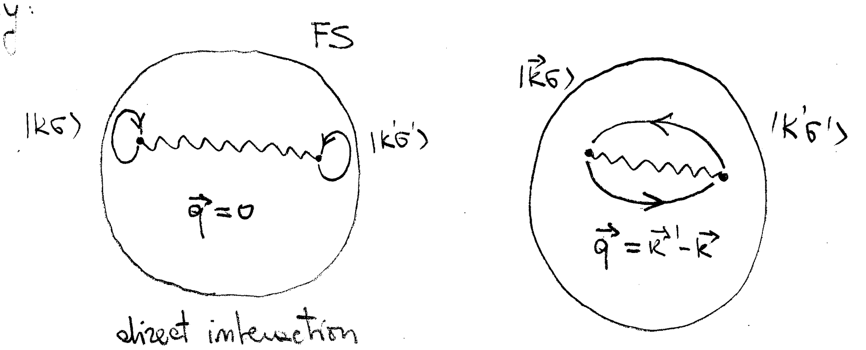
The matrix element in eq. (6.16) is evaluated as follows

i) The annihilation operators $a_{\vec{k}\sigma}$, and $a_{\vec{k}'\sigma'}$ give a non-zero result only if $|\vec{k}| < k_F$ and $|\vec{k}'| < k_F$

ii) The projection on the Fermi sea $\langle FS|$ requires that the creators $\hat{a}^+_{\vec{k}+\vec{q}\sigma}$ and $\hat{a}^+_{\vec{k}'-\vec{q}\sigma'}$ reconstruct $|FS\rangle$.

$$\Rightarrow \begin{cases} \vec{q} = 0 & \text{excluded in the jellium Hamiltonian} \\ \text{or} & \\ \vec{q} = \vec{k}' - \vec{k} & \sigma' = \sigma \end{cases}$$

Graphically:



direct interaction
excluded in jellium

$$\langle FS| \hat{V}_{ee}^{\text{jellium}} |FS\rangle = \delta_{\vec{k},\vec{k}'-\vec{q}}\, \delta_{\sigma\sigma'} \langle FS| \hat{a}^+_{\vec{k}+\vec{q}\sigma} \hat{a}^+_{\vec{k}\sigma} \hat{a}_{\vec{k}+\vec{q}\sigma} \hat{a}_{\vec{k}\sigma} |FS\rangle \overset{\vec{q}\neq 0}{=}$$

$$= -\delta_{\vec{k},\vec{k}'-\vec{q}}\, \delta_{\sigma\sigma'} \langle FS| \hat{n}_{\vec{k}+\vec{q}\sigma} \hat{n}_{\vec{k}\sigma} |FS\rangle \tag{6.17}$$

And correspondingly:

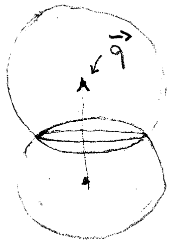
$$\varepsilon_G^{(1)} = -\frac{1}{2VN_e} \sum_{\vec{q}\neq 0} \sum_{\vec{k}\sigma} \tilde{v}_{ee}(\vec{q})\, \Theta(k_F - |\vec{k}+\vec{q}|)\, \Theta(k_F - |\vec{k}|)$$

By converting $\vec{k}$ and $\vec{q}$ sums into integrals:

$$\varepsilon_G^{(1)} = -\frac{2}{2VN_{el}} \frac{V^2}{(2\pi)^6} \int d\vec{q}\, \tilde{v}_{ee}(\vec{q}) \left(1 - \frac{V}{(2\pi)^3}\delta(\vec{q})\right) \int d\vec{k}\, \Theta(k_F - |\vec{k}+\vec{q}|)\, \Theta(k_F - |\vec{k}|)$$

For a given $\vec{q}$, the integration volume is the overlap volume of 2 spheres of radius k_F shifted by $\vec{q}$. $\Rightarrow 0 < |\vec{q}| < 2k_F$

The integral is independent of the direction of $\vec{q}$ and, for fixed $\vec{q}$ (for fixing the ideas taken in the z direction) it is most easily solved in cylindrical coordinates



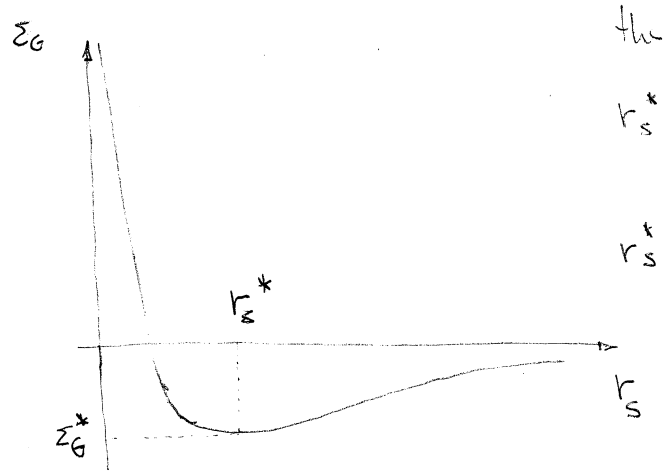
$$\varepsilon_G^{(1)} = -\frac{\overset{\text{spin}}{\cancel{2}}}{\cancel{2}\cancel{V}N_{el}}\,\frac{e^2}{4\pi\varepsilon_0}\,\frac{V^{\cancel{2}}}{\underset{2\pi^3}{(2\pi)^6}}\,\overset{q\text{-solid angle}}{4\pi}\int_0^{2k_F} dq\,\cancel{q^2}\,\overset{\frac{4\pi\varepsilon_0\tilde{v}(\vec{q})}{e^2}}{\frac{\cancel{4\pi}}{\cancel{q^2}}}\cdot\overset{\text{reflex. symmetry}}{\cancel{2}}\int_{q/2}^{k_F} dk_z\,\cancel{\pi}\left(k_F^2-k_z^2\right)$$

$$= -\frac{e^2}{4\pi\varepsilon_0}\,\frac{V}{N_{el}}\,\frac{1}{2\pi^3}\int_0^{2k_F} dq\left[k_F^2\left(k_F-\frac{q}{2}\right)-\frac{k_F^3}{3}+\frac{q^3}{24}\right] =$$

$$= -\frac{e^2}{4\pi\varepsilon_0}\,\frac{V}{N_{el}}\,\frac{1}{2\pi^3}\left(k_F^3\,2k_F - k_F^2\,\frac{\cancel{4}k_F^2}{\cancel{4}} - \frac{2k_F^4}{3} + \frac{\overset{4}{\cancel{16}}\,k_F^4}{\cancel{4}\cdot\underset{6}{\cancel{24}}}\right) = -\frac{e^2}{4\pi\varepsilon_0}\,\frac{V}{N_{el}}\,\frac{k_F^4}{2\pi^3} \approx -\frac{0.916}{r_s}\,Ry$$

$$\left(\sqrt[3]{\frac{12}{\pi^4}}\right) \qquad (6.18)$$

$$\Rightarrow \quad \varepsilon_G = \varepsilon_G^{(0)} + \varepsilon_G^{(1)} = \left(\frac{2.211}{r_s^2} - \frac{0.916}{r_s}\right) Ry \qquad (6.19)$$



The electron gas is stable when the e-interaction is turned on

$r_s^* = 4.83 \quad \varepsilon^* = -0.095\ Ry = -1.29\ eV$

(1st order in V_{ee}^{jelli})

$r_s^* = 3.96 \quad \varepsilon^* = -0.083\ Ry = -1.13\ eV$

(exp. on Na)

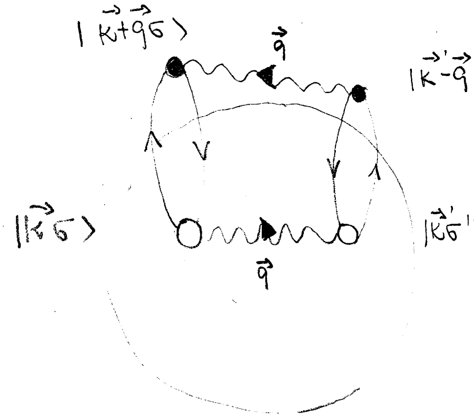
r_s^* is the average electron distance in units of a_0 at which the energy per particle shows a minimum. The corresponding energy is ε_G^*.

One can try to improve the result and go to the next order.

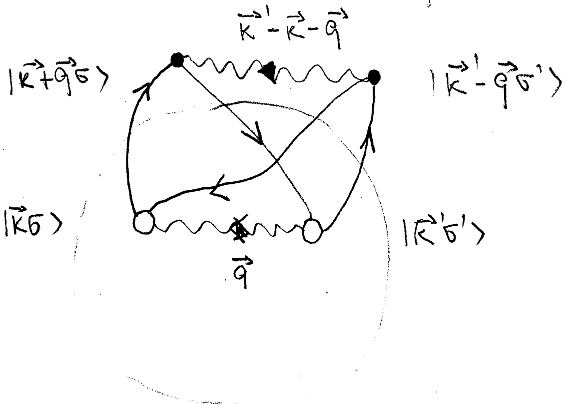
■ <u>2nd order</u> This contribution, however DIVERGES!

$$\mathcal{E}_G^{(2)} = \frac{1}{N_{el}} \sum_{|\nu\rangle \neq |FS\rangle} \frac{\langle FS| \hat{V}_{ee}^{jellium} |\nu\rangle\langle\nu| \hat{V}_{ee}^{jellium} |FS\rangle}{E^{(0)} - E_\nu} = \mathcal{E}_{dir}^{(2)} + \mathcal{E}_{exc}^{(2)} \tag{6.20}$$

$|\nu\rangle \neq |FS\rangle$ means that in the intermediate state $|\nu\rangle$ electrons have been created outside the Fermi sea. $\Rightarrow$ $|\vec{k}'-\vec{q}|$ and $|\vec{k}+\vec{q}|$ are larger than k_F.



DIRECT INT. PROCESS



EXCHANGE INT. PROCESS

Due to the $\langle FS|$ operation the holes in the Fermi sea should be refilled at the end of the process. If the excited electrons are put back in the same state they were taken out we have a DIRECT process. If instead they are exchanged we have an EXCHANGE process. (

The divergence arise from the <u>direct</u> process. The constraint $|\nu\rangle \neq |FS\rangle$ yields:

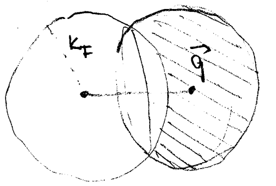
$$|\nu\rangle = \theta(|\vec{k}+\vec{q}| - k_F)\,\theta(|\vec{k}'-\vec{q}| - k_F)\,\theta(k_F - |\vec{k}'|)\,\theta(k_F - |\vec{k}'|)\; \hat{a}^+_{\vec{k}+\vec{q}\sigma}\,\hat{a}^+_{\vec{k}'-\vec{q}\sigma'}\,\hat{a}_{\vec{k}'\sigma'}\,\hat{a}_{\vec{k}\sigma}|$$

$$\mathcal{E}_{dir}^{(2)} = \frac{1}{4V^2 N_{el}} \sum_{\vec{q}\neq 0} \sum_{\substack{\vec{k}\vec{k}' \\ \sigma\sigma'}} \frac{\tilde{V}_{ee}^2(\vec{q})}{E^{(0)} - E_\nu}\, \theta(|\vec{k}+\vec{q}| - k_F)\,\theta(|\vec{k}'-\vec{q}| - k_F)\,\theta(k_F - |\vec{k}|)\,\theta(k_F - |\vec{k}'|)$$

We count the power of $\vec{q}$ at small $\vec{q}$.

* $\tilde{V}_{ee}^2(\vec{q}) \propto \frac{1}{q^4}$
* $E^{(0)} - E_\nu \propto k^2 + k'^2 - (\vec{k}+\vec{q})^2 - (\vec{k}'-\vec{q})^2 \propto q$ when $q \to 0$
* $\sum_{\vec{k}} \ldots \theta(|\vec{k}+\vec{q}| - k_F)\,\theta(k_F - |\vec{k}|) \propto q$ when $q \to 0$

The last proportionality can be readily seen since the shadowed volume is calculated as:



$$V_{sh} = \frac{4}{3}\pi k_F^3 - 2\cdot\pi \int_{\frac{q}{2}}^{k_F} dk_z \left(k_F^2 - k_z^2 \right)$$

$$= \frac{4}{3}\pi k_F^3 - 2\pi \left[k_F^2 \left(k_F - \frac{q}{2} \right) - \frac{k_F^3}{3} + \frac{q^3}{24} \right]$$

$$= \cancel{\frac{4}{3}\pi k_F^3} - \cancel{\frac{4}{3}\pi k_F^3} + \pi k_F^2 q - \frac{\pi q^3}{12} = \pi k_F^2 q + o(q)$$

We obtain thus an integrand:

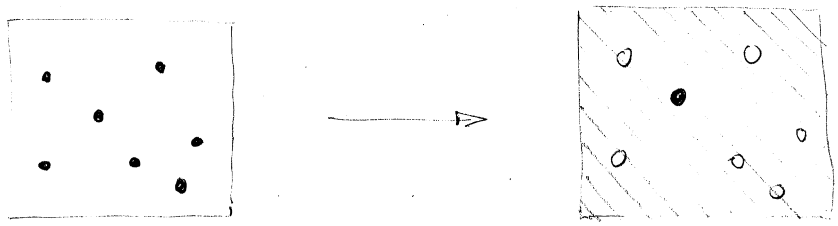
$$\varepsilon^{(2)}_{dir} \propto \int_0^{q_{max}} dq \; q^2 \frac{1}{q^4} \frac{1}{q} qq = \int_0^{q_{max}} dq \frac{1}{q} = \ln q_{max} - \ln q \Big|_0 \quad \text{divergent !}$$

The exchange process is not singular at low momenta.

$$\tilde{v}_{ee}^{\,2}(\vec{q}) \longrightarrow \tilde{v}_{ee}(\vec{q})\, \tilde{v}_{ee}(|\vec{k}' - \vec{k} - \vec{q}|) \propto \frac{1}{q^2} \quad \text{for } q \to 0$$

The physics of interacting particles is typically complicated, because the dynamics of the individual particle depends on the state of all the other ones. Example: correlated e-gas. We expect that the probability to find two electrons in close proximity is small due to the strong repulsive interaction.

In this lecture we study what happens when we include correlations ON AVERAGE. The effect of all the other particles is included as a field generated by a mean density, leaving a single particle problem. (which is solvable)



7.1 Basic concepts of mean-field theory

Consider two kinds of particles described by the operators $\hat{a}_\mu$, $\hat{b}_\nu$, respectively and

i) Assume that only interactions between particles of different kind are relevant:

$$\hat{H} = \hat{H}_0 + \hat{V}_{int}$$

where

$$\hat{H}_0 = \sum_\nu \varepsilon_\nu \hat{a}^+_\nu \hat{a}_\nu + \sum_\mu \varepsilon_\mu \hat{b}^+_\mu \hat{b}_\mu$$

$$\hat{V}_{int} = \sum_{\nu\nu'\mu\mu'} v_{\nu\mu\mu'\nu'} \hat{a}^+_\nu \hat{b}^+_\mu \hat{b}_{\mu'} \hat{a}_{\nu'} \qquad (7.1)$$

ii) Suppose that we expect, based on physical arguments, that the density operators $\hat{a}^+_\nu \hat{a}_{\nu'}$ and $\hat{b}^+_\mu \hat{b}_{\mu'}$ deviate only little from their average values $\langle \hat{a}^+_\nu \hat{a}_{\nu'} \rangle$ and $\langle \hat{b}^+_\mu \hat{b}_{\mu'} \rangle$

One defines the deviations:

$$\delta\hat{A}_{\nu\nu'} = \hat{a}^{+}_{\nu}\hat{a}_{\nu'} - \langle \hat{a}^{+}_{\nu}\hat{a}_{\nu'}\rangle \qquad \delta\hat{B}_{\mu\mu'} = \hat{b}^{+}_{\mu}\hat{b}_{\mu'} - \langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle$$

and obtains, for the interaction Hamiltonian:

$$\hat{V}_{int} = \sum_{\nu\nu'\mu\mu'} v_{\nu\mu\mu'\nu'}\Big[\underbrace{\hat{a}^{+}_{\nu}\hat{a}_{\nu'}\langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle + \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\langle a^{+}_{\nu}a_{\nu'}\rangle - \langle \hat{a}^{+}_{\nu}\hat{a}_{\nu'}\rangle\langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle}_{\text{simple particle operators}}$$

$$+ \underbrace{\delta\hat{A}_{\nu\nu'}\delta\hat{B}_{\mu\mu'}}_{\substack{\text{neglected in}\\ \text{mean field}}}\Big]$$

proof:

$$\hat{V}_{int} = \sum_{\nu\nu'\mu\mu'} v_{\nu\mu\mu'\nu'}\left[\delta\hat{A}_{\nu\nu'} + \langle \hat{a}^{+}_{\nu}\hat{a}_{\nu'}\rangle\right]\left[\delta\hat{B}_{\mu\mu'} + \langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle\right]$$

$$= \sum_{\nu\nu'\mu\mu'} v_{\nu\mu\mu'\nu'}\left[\delta\hat{A}_{\nu\nu'}\langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle + \delta\hat{B}_{\mu\mu'}\langle a^{+}_{\nu}\hat{a}_{\nu'}\rangle + \langle \hat{a}^{+}_{\nu}\hat{a}_{\nu'}\rangle\langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle + \delta\hat{A}_{\nu\nu'}\delta\hat{B}_{\mu\mu'}\right]$$

$$= \sum_{\nu\nu'\mu\mu'} v_{\nu\mu\mu'\nu'}\left[\hat{a}^{+}_{\nu}\hat{a}_{\nu'}\langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle + \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\langle \hat{a}^{+}_{\nu}\hat{a}_{\nu'}\rangle - \langle \hat{a}^{+}_{\nu}\hat{a}_{\nu'}\rangle\langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle + \delta\hat{A}_{\nu\nu'}\delta\hat{B}_{\mu\mu'}\right]$$

Summarizing:

$$\hat{V}_{MF} = \sum_{\nu\nu'\mu\mu'} v_{\nu\mu\mu'\nu'}\left[\hat{a}^{+}_{\nu}\hat{a}_{\nu'}\langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle + \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\langle a^{+}_{\nu}a_{\nu'}\rangle - \langle \hat{a}^{+}_{\nu}\hat{a}_{\nu'}\rangle\langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle\right] \tag{7.2}$$

Looking to (7.2) we can formulate the mean field procedure in a different way. For an interaction being the product of 2 operators $\hat{A}$ and $\hat{B}$

$$\hat{H}_{AB} = \hat{A}\hat{B} \Rightarrow \hat{H}_{MF,AB} = \langle\hat{A}\rangle\hat{B} + \hat{A}\langle\hat{B}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle$$

The last term is introduced to ensure the correct averaging $\langle \hat{H}_{MF,AB}\rangle = \langle\hat{A}\rangle\langle\hat{B}\rangle$ which derives from $\hat{A}$ and $\hat{B}$ being uncorrelated.

$$\Rightarrow \langle \hat{V}_{in}\rangle \simeq \langle \hat{V}_{MF}\rangle = \sum_{\nu\nu'\mu\mu'} v_{\nu\mu\mu'\nu'}\langle \hat{a}^{+}_{\nu}\hat{a}_{\nu'}\rangle\langle \hat{b}^{+}_{\mu}\hat{b}_{\mu'}\rangle \tag{7.3}$$

The fundamental question is a procedure to calculate averages. Two equivalent methods exist:

1. The average $\langle \hat{a}^+_\nu \hat{a}_{\nu'} \rangle$ has to be found selfconsistently

Let us define $\bar{n}^a_{\nu\nu'} \equiv \langle \hat{a}^+_\nu \hat{a}_{\nu'} \rangle$ and $\bar{n}^b_{\mu\mu'} \equiv \langle \hat{b}^+_\mu \hat{b}_{\mu'} \rangle$. The mean field Hamiltonian depends on $\bar{n}^a$ and $\bar{n}^b$. The average is understood with respect to the mean field Hamiltonian:

$$\begin{cases} \bar{n}^a_{\nu\nu'} = \dfrac{1}{Z_{MF}} \mathrm{Tr}\left[e^{-\beta \hat{H}_{MF}(\{\bar{n}^a_{\nu\nu'}, \bar{n}^b_{\mu\mu'}\})} \hat{a}^+_\nu \hat{a}_{\nu'} \right] \\ \bar{n}^b_{\mu\mu'} = \dfrac{1}{Z_{MF}} \mathrm{Tr}\left[e^{-\beta \hat{H}_{MF}(\{\bar{n}^a_{\nu\nu'}, \bar{n}^b_{\mu\mu'}\})} \hat{b}^+_\mu \hat{b}_{\mu'} \right] \end{cases} \quad (7.4)$$

with $Z_{MF} = \mathrm{Tr}[e^{-\beta \hat{H}_{MF}}]$

The equations (7.4) are a set of coupled non-linear equations in the average density operators $\bar{n}^a_{\nu\nu'}$, $\bar{n}^b_{\mu\mu'}$.

2. Variational principle

$\bar{n}^a_{\nu\nu'}$ and $\bar{n}^b_{\mu\mu'}$ are minimizing the free energy F_{MF} associated to the mean-field Hamiltonian.

$$0 = \frac{\partial}{\partial \bar{n}^a_{\nu\nu'}} F_{MF} = \frac{\partial}{\partial \bar{n}^a_{\nu\nu'}} \left(-\frac{1}{\beta} \ln Z_{MF} \right) = \frac{1}{Z_{MF}} \mathrm{Tr}\left[e^{-\beta \hat{H}_{MF}} \frac{\partial}{\partial \bar{n}^a_{\nu\nu'}} \hat{H}_{MF} \right]$$

$$= \frac{1}{Z_{MF}} \mathrm{Tr}\left[e^{-\beta \hat{H}_{MF}} \sum_{\mu\mu'} v_{\nu\mu\mu'\nu'} \left(\hat{b}^+_\mu \hat{b}_{\mu'} - \bar{n}^b_{\mu\mu'} \right) \right]$$

$$= \sum_{\mu\mu'} v_{\nu\mu\mu'\nu'} \left(\langle \hat{b}^+_\mu \hat{b}_{\mu'} \rangle_{MF} - \bar{n}^b_{\mu\mu'} \right). \quad (7.5)$$

Analogously for $0 = \dfrac{\partial}{\partial \bar{n}^b_{\mu\mu'}} F_{MF}$

The equations above prove the equivalence of the 2 approaches, since the minimization of F_{MF} reproduces (7.4).