## 8.5 Effects of interaction: the random phase approximation (RPA)

a perturbative approach fails in the attempt to describe the interacting electron gas. All orders must be included. Here we will adopt the random phase approximation within the jellium model and summarize the outcomes:

- renormalization of the Coulomb interaction (screening) which removes the divergence at $\vec{q}=0$
- converging expression for the ground state energy (not addressed here)
- screening of external potentials
- emerging of collective excitations (plasmons)

The starting point of the discussion is the polarizability which, in presence of interaction we evaluate using the equation of motion method:

$$\tilde{\chi}^R(\vec{q}, t-t') = -\frac{i}{\hbar}\Theta(t-t')\frac{1}{V}\langle[\hat{\rho}_{e,I}(\vec{q},t), \hat{\rho}_{e,I}(-\vec{q},t')]\rangle_0$$

For convenience, let us define the auxiliary correlator:

$$\chi^R(\vec{k}\vec{q}\sigma, t-t') = -\frac{i}{\hbar}\Theta(t-t')\langle[(a^+_{\vec{k}\sigma}a_{\vec{k}+\vec{q}\sigma})(t), \hat{\rho}_I(-\vec{q},t')]\rangle_0$$

Notice: - $\hat{\rho}$ is the particle density, not the charge density $\hat{\rho}_e$

- $$\tilde{\chi}^R(\vec{q}, t-t') = \frac{e^2}{V}\sum_{\vec{k}\sigma}\tilde{\chi}^R(\vec{k}\vec{q}\sigma, t-t')$$

We now proceed with the EOM on the auxiliary correlator $\tilde{\chi}^R(\vec{k}\vec{q}\sigma, t-t')$

$$i\hbar \partial_t \tilde{\chi}^R(\vec{k}\vec{q}\sigma, t-t') = \delta(t-t') \langle [ a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma} , \sum_{\vec{k}'\sigma'} a^+_{\vec{k}'\sigma'} a_{\vec{k}'-\vec{q}\sigma'} ](t) \rangle_0$$

$$+ \frac{i}{\hbar} \theta(t-t') \langle [[ \hat{H}_0 + \hat{V}_{ee}^{jellium} , a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma} ](t) , \hat{\rho}_I(\vec{q},t') ] \rangle_0$$

see (8.19b)

$$= \delta(t-t') \langle \hat{n}_{\vec{k}\sigma} - \hat{n}_{\vec{k}+\vec{q}\sigma} \rangle_0 + \frac{i}{\hbar} \theta(t-t') (\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}}) \langle [(a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma})(t), \hat{\rho}_I(\vec{q},t')]\rangle_0$$

$$+ \frac{i}{\hbar} \theta(t-t') \langle [ [ \hat{V}_{ee}^{jellium} , a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma} ](t) , \hat{\rho}_I(-\vec{q},t') ] \rangle_0 \qquad (8.22)$$

- The commutator with the single particle component of the Hamiltonian

$$\left[ \sum_{\vec{k}'\sigma'} \varepsilon_{\vec{k}'} a^+_{\vec{k}'\sigma'} a_{\vec{k}'\sigma'} , a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma} \right] = \sum_{\vec{k}'\sigma'} \varepsilon_{\vec{k}'} \Big\{ a^+_{\vec{k}'\sigma'} [ a_{\vec{k}'\sigma'} , a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma} ]$$

$$+ [ a^+_{\vec{k}'\sigma'} , a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma} ] a_{\vec{k}'\sigma'} \Big\} =$$

$$= \sum_{\vec{k}'\sigma'} \varepsilon_{\vec{k}'} \Big[ a^+_{\vec{k}'\sigma'} \underbrace{\{ a_{\vec{k}'\sigma'} , a^+_{\vec{k}\sigma} \}}_{\delta_{\sigma\sigma'} \delta_{\vec{k}\vec{k}'}} a_{\vec{k}+\vec{q}\sigma} - a^+_{\vec{k}\sigma} \underbrace{\{ a^+_{\vec{k}'\sigma'} , a_{\vec{k}+\vec{q}\sigma} \}}_{\delta_{\sigma\sigma'} \delta_{\vec{k}',\vec{k}+\vec{q}}} a_{\vec{k}'\sigma'} \Big]$$

$$= (\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}}) a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma}$$

- The commutator with the jellium ee interaction of the Hamiltonian

$$\frac{1}{2V} \sum_{\vec{q}'\neq 0} \tilde{v}_{ee}(\vec{q}') [ \hat{\rho}_{\vec{q}'} \hat{\rho}_{-\vec{q}'} - \hat{N}_{el} , a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma} ]$$

where we have used the expression for the jellium model derived in (6.10). The commutator with $\hat{N}_{el}$ vanishes since $a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma}$ conserves the particle number. For the other part we obtain readily

$$\frac{1}{2V} \sum_{\vec{q}'\neq 0} \tilde{v}_{ee}(\vec{q}') \Big\{ \hat{\rho}_{\vec{q}'} [ \hat{\rho}_{-\vec{q}'} , a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma} ] + [ \hat{\rho}_{\vec{q}'} , a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma} ] \hat{\rho}_{-\vec{q}'} \Big\}$$

With the help of the definition of the density (5.25) and (8.19b)

$$\left[\hat{\rho}_{\pm\vec{q}'}, a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma}\right] = \sum_{\vec{k}_1\sigma_1} \left[a^+_{\vec{k}_1\sigma_1} a_{\vec{k}_1\pm\vec{q}'\sigma_1}, a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma}\right] =$$

$$= \sum_{\vec{k}_1\sigma_1} \left( a^+_{\vec{k}_1\sigma_1} a_{\vec{k}+\vec{q}\sigma} \delta_{\sigma_1\sigma} \delta_{\vec{k}_1\pm\vec{q}',\vec{k}} - a^+_{\vec{k}\sigma} a_{\vec{k}_1\pm\vec{q}'\sigma_1} \delta_{\sigma_1\sigma} \delta_{\vec{k}_1,\vec{k}+\vec{q}} \right)$$

$$= a^+_{\vec{k}\mp\vec{q}'\sigma} a_{\vec{k}+\vec{q}\sigma} - a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\pm\vec{q}'\sigma}$$

All together, the commutator with the jellium interaction Hamiltonian it is thus giving:

$$\frac{1}{2V} \sum_{\substack{\vec{q}'\neq 0 \\ \vec{k}'\sigma'}} \tilde{v}_{ee}(\vec{q}') \Big\{ a^+_{\vec{k}'\sigma'} a_{\vec{k}'+\vec{q}'\sigma'} \left( a^+_{\vec{k}+\vec{q}'\sigma} a_{\vec{k}+\vec{q}\sigma} - a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}-\vec{q}'\sigma} \right)$$

$$+ \left( a^+_{\vec{k}-\vec{q}'\sigma} a_{\vec{k}+\vec{q}\sigma} - a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}+\vec{q}'\sigma} \right) a^+_{\vec{k}'\sigma'} a_{\vec{k}'-\vec{q}'\sigma'} \Big\} \qquad (8.23)$$

At this point, by inserting (8.23) into (8.22) one would obtain a 6 operator correlation function, of which a new equation of motion should be derived. The chain of increasingly complicated correlators can be truncated by approximating (8.23) by its mean field version where only Hartree terms (the dominating ones in the second order perturbation theory)

$$\left[\tilde{V}^{\text{jellium}}_{ee}, a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}\sigma}\right] \approx \frac{1}{2V} \sum_{\substack{\vec{q}'\neq 0 \\ \vec{k}'\sigma'}} \tilde{v}_{ee}(\vec{q}') \Big\{ \langle a^+_{\vec{k}'\sigma'} a_{\vec{k}'+\vec{q}'\sigma'} \rangle \left( a^+_{\vec{k}+\vec{q}'\sigma} a_{\vec{k}+\vec{q}\sigma} - \right.$$

$$\left. - a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}-\vec{q}'\sigma} \right) + \left( a^+_{\vec{k}-\vec{q}'\sigma} a_{\vec{k}+\vec{q}\sigma} - a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}+\vec{q}'\sigma} \right) \langle a^+_{\vec{k}'\sigma'} a_{\vec{k}'-\vec{q}'\sigma'} \rangle$$

$$+ a^+_{\vec{k}'\sigma'} a_{\vec{k}'+\vec{q}'\sigma'} \left( \langle a^+_{\vec{k}+\vec{q}'\sigma} a_{\vec{k}+\vec{q}\sigma} \rangle - \langle a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}-\vec{q}'\sigma} \rangle \right) + \left( \langle a^+_{\vec{k}-\vec{q}'\sigma} a_{\vec{k}+\vec{q}\sigma} \rangle - \langle a^+_{\vec{k}\sigma} a_{\vec{k}+\vec{q}+\vec{q}'\sigma} \rangle \right)$$

$$a^+_{\vec{k}'\sigma'} a_{\vec{k}'-\vec{q}'\sigma'} \Big\} + \text{constant}$$

If now we assume a translationally invariant mean field parameter $\langle a^\dagger_{\vec k\sigma} a_{\vec k'\sigma'}\rangle = \delta_{\vec k\vec k'}\delta_{\sigma\sigma'}\bar n_{\vec k}$ one obtains

$$\left[\tilde V^{\text{jellium}}_{ee},\ a^\dagger_{\vec k\sigma} a_{\vec k+\vec q\sigma}\right] \approx \frac{1}{2V}\sum_{\vec k'\sigma'} \tilde v_{ee}(\vec q)\Big[a^\dagger_{\vec k'\sigma'} a_{\vec k'+\vec q\sigma'}\left(\bar n_{\vec k+\vec q} - \bar n_{\vec k}\right) +$$

$$\left(\bar n_{\vec k+\vec q} - \bar n_{\vec k}\right) a^\dagger_{\vec k'\sigma'} a_{\vec k'+\vec q\sigma'}\Big] =$$

$$= \frac{1}{V}\sum_{\vec k'\sigma'} \tilde v_{ee}(\vec q)\left(\bar n_{\vec k+\vec q} - \bar n_{\vec k}\right) a^\dagger_{\vec k'\sigma'} a_{\vec k'+\vec q\sigma'} + \text{const.} \qquad (8.24)$$

If we return now to the equation of motion for the correlator $\tilde\chi^R(\vec k\vec q\sigma, t-t')$ we obtain:

$$i\hbar\,\partial_t \tilde\chi^R(\vec k\vec q\sigma, t-t') = +\delta(t-t')\left(\bar n_k - \bar n_{\vec k+\vec q}\right) + \left(\varepsilon_{\vec k+\vec q} - \varepsilon_{\vec k}\right)\tilde\chi^R(\vec k\vec q\sigma, t-t')$$

$$-\left(\bar n_{\vec k+\vec q} - \bar n_{\vec k}\right)\frac{\tilde v_{ee}(\vec q)}{V}\sum_{\vec k'\sigma'}\tilde\chi^R(\vec q\vec k'\sigma', t-t') \qquad (8.25)$$

By transforming (8.25) into the frequency domain: $\partial_t \to -i(\omega+i\eta)$
$\delta(t-t') \to 1$

$$\tilde\chi^R(\vec k\vec q\sigma,\omega) = \frac{\bar n_k - \bar n_{\vec k+\vec q}}{\hbar\omega - (\varepsilon_{\vec k+\vec q} - \varepsilon_{\vec k}) + i\eta}\left(1 + \frac{\tilde v_{ee}(\vec q)}{V}\sum_{\vec k'\sigma'}\tilde\chi^R(\vec q\vec k'\sigma',\omega)\right)$$

Finally, by operating on both sides with $\frac{e^2}{V}\sum_{\vec k\sigma}$ we obtain an equation for the charge-density correlator

$$\boxed{\tilde\chi^R_{RPA}(\vec q,\omega) = \tilde\chi^R_0(\vec q,\omega) + \tilde\chi^R_0(\vec q,\omega)\,\tilde u_{ee}(\vec q)\,\tilde\chi^R_{RPA}(\vec q,\omega)} \qquad (8.26)$$

(8.26) is a recursive equation which indicates how the interacting polarizability can be written as a geometrical series of the interaction

$$\tilde{\chi}^R_{RPA} = \tilde{\chi}^R_0 \sum_{n=0}^{\infty} \left( \tilde{u}_{ee}(q) \tilde{\chi}^R_0 \right)^n$$

with the simple non perturbative solution:

$$\tilde{\chi}^R_{RPA}(\vec{q},\omega) = \frac{\tilde{\chi}^R_0(\vec{q},\omega)}{1 - \tilde{\chi}^R_0(\vec{q},\omega)\,\tilde{u}_{ee}(\vec{q})} \qquad (8.27)$$

(8.27) has profound consequences in the theory of the interacting electron gas.

i) Recall the expression of the dielectric constant (8.16b)

$$\tilde{\varepsilon}^{-1}(\vec{q},\omega) = 1 + \tilde{u}_{ee}(\vec{q})\,\tilde{\chi}^R(\vec{q},\omega) = \frac{1}{1 - \tilde{\chi}^R_0(\vec{q},\omega)\,\tilde{u}_{ee}(\vec{q})}$$

in the limit $\omega = 0$ $\vec{q} \to 0$ we have proven that $\tilde{\chi}^R_0(\vec{q},0) \xrightarrow{52b} -e^2 d(\varepsilon_F) =$

$$= -e^2 \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{\frac{\hbar^2 k_F^2}{2m}} = -e^2 \frac{1}{\cancel{2}\pi^{\cancel{2}}} \frac{\cancel{2}m}{\hbar^2} k_F \frac{4\cancel{\pi}\varepsilon_0}{4\pi\varepsilon_0} = -\frac{me^2}{4\pi\varepsilon_0\hbar^2} \frac{4}{\pi} k_F = -\frac{4}{\pi} \frac{k_F}{a_0} \varepsilon_0$$

We thus obtain

$$\tilde{\varepsilon}^{-1}(\vec{q},0) \xrightarrow[\vec{q}\to 0]{} \frac{1}{1 + \frac{4}{\pi}\frac{k_F}{a_0}\frac{1}{q^2}} = \frac{1}{1 + \frac{k_{TF}^2}{q^2}}$$

where we have defined the Thomas-Fermi momentum $k_{TF} = \sqrt{\frac{4 k_F}{\pi a_0}}$

The corresponding screened Coulomb interaction thus reads:

$$\tilde{v}^s_{ee}(\vec{q}) = \frac{\tilde{v}_{ee}(\vec{q})}{\tilde{\varepsilon}(\vec{q},0)} \approx \frac{e^2}{\varepsilon_0(k_{TF}^2 + q^2)} \to v^s(r) = \frac{e^{-r k_{TF}}}{4\pi\varepsilon_0 r} \qquad (8.28)$$

Thus the theory cures the divergence of the Coulomb potential and predicts a screening which increases with the density of states at the Fermi energy.

In the same way one obtains a screening of the static external potentials.

ii) The appearance of <u>new collective excitations</u> is obtained by considering the comparison between the Lehmann representation of a correlator and the polarizability $\chi^R$. The excitations of the unperturbed system correspond to the poles (the zeros of the denominator) of the imaginary part of the correlator. We rewrite first (8.27) as:

$$\tilde{\chi}^R_{RPA}(\vec{q},\omega) = \tilde{\chi}^R_0 \frac{1}{1-\tilde{u}_{ee}\,\mathrm{Re}\,\tilde{\chi}^R_0 - i\tilde{u}_{ee}\,\mathrm{Im}\,\tilde{\chi}^R_0} =$$

$$= \tilde{\chi}^R_0 \frac{1-\tilde{u}_{ee}\,\mathrm{Re}\,\tilde{\chi}^R_0 + i\tilde{u}_{ee}\,\mathrm{Im}\,\tilde{\chi}_0}{\left(1-\tilde{u}_{ee}\,\mathrm{Re}\,\tilde{\chi}^R_0\right)^2+\left(\tilde{u}_{ee}\,\mathrm{Im}\,\tilde{\chi}^R_0\right)^2}$$

* In the region in which $\mathrm{Im}\,\tilde{\chi}^R_0$ has poles, the same happens to $\mathrm{Im}\,\tilde{\chi}^R_{RPA}$ => the electron-holes excitation discussed for the non interacting electron gas are still present in the new theory.
* In the region in which $\mathrm{Im}\,\tilde{\chi}^R_0 = 0$ we have (we have to reintroduce $\eta = 0^+$)

$$-\mathrm{Im}\,\tilde{\chi}^R_{RPA}(\vec{q},\omega) = \lim_{\eta\to 0^+} \frac{\eta}{\left(1-\tilde{u}_{ee}\,\mathrm{Re}\,\tilde{\chi}_0\right)^2+\eta^2} = \pi\,\delta\left(1-\tilde{u}_{ee}\,\mathrm{Re}\,\tilde{\chi}^R_0\right)$$

=> there are new possible excitations with a dispersion which solve the implicit equation

$$1-\tilde{u}_{ee}\,\mathrm{Re}\,\tilde{\chi}^R_0 = 0 \qquad (8.29)$$

Since $\tilde{\varepsilon}_{RPA}(\vec{q},\omega) = 1 - \tilde{u}_{ee}(\vec{q})\tilde{\chi}^R_0(\vec{q},\omega)$, the combined condition $\mathrm{Im}\,\tilde{\chi}^R_0 = 0$ and $1 - \tilde{u}_{ee}(\vec{q})\mathrm{Re}\,\tilde{\chi}^R_0(\vec{q},\omega) = 0$ implies the vanishing of the dielectric function. Consequently an infinitesimally small external perturbation $\phi_{ext}(\vec{q},\omega)$ can lead to a finite $\phi_{tot}(\vec{q},\omega)$. The associated excitations are long lived modes of the system!

In order to solve (8.29) we make use of the approximated Lindhard function:

$$\mathrm{Re}\,\tilde{\chi}^R_0(\vec{q},\omega) \simeq \frac{n_e}{m}\frac{q^2}{\omega^2}\left[1 + \frac{3}{5}\left(\frac{q v_F}{\omega}\right)^2\right] e^2$$

valid in the regime $\begin{cases} v_F q \ll \omega \\ q \ll k_F \\ k_B T \ll \varepsilon_F \end{cases}$

$$0 = 1 - \tilde{u}_{ee}(\vec{q})\,\mathrm{Re}\,\tilde{\chi}^R_0(\vec{q},\omega) = 1 - \frac{1}{\varepsilon_0 \cancel{q^2}}\frac{n_e}{m}\frac{\cancel{q^2}}{\omega^2}\left[1 + \frac{3}{5}\left(\frac{q v_F}{\omega}\right)^2\right] e^2$$

Which delivers the dispersion relation

$$\begin{cases} \omega^2 = \omega_p^2\left[1 + \frac{3}{5}\left(\frac{q v_F}{\omega}\right)^2\right] \quad \text{or} \\ \omega \approx \omega_p + \frac{3}{10}\frac{v_F^2}{\omega_p} q^2 \end{cases} \tag{8.30}$$

where we have introduced the plasma frequency $\omega_p \equiv \sqrt{\frac{n_e e^2}{m\varepsilon_0}}$. If we renormalize the energies to the Fermi energy and $q$ to the Fermi momentum

$$\frac{\hbar\omega}{\varepsilon_F} \approx \sqrt{r_s}\; 1.36 + \frac{1}{\sqrt{r_s}}\, 1.28\, \frac{q^2}{k_F^2}$$

where we have used the fact that

$$\frac{\hbar\omega_p}{\varepsilon_F} = \hbar\sqrt{\frac{n_e e^2}{m\varepsilon_0}}\cdot\frac{2m}{\hbar^{2}k_F^2} = \sqrt{\frac{k_F^3}{3\pi^2}\,\frac{4me^2}{\hbar^2 k_F^4\varepsilon_0}} = \sqrt{\frac{16}{3\pi}\,\frac{me^2}{4\pi\varepsilon_0\hbar^2}\,\frac{1}{k_F}} =$$

$$= \sqrt{\frac{16}{3\pi}}\sqrt{\frac{1}{a_0 k_F}} = \sqrt{\frac{16}{3\pi}}\left(\frac{4}{9\pi}\right)^{1/6}\sqrt{r_s} = 1.36\sqrt{r_s}$$

$$\hbar\frac{3}{10}\frac{v_F^2}{\omega_p}q^2\cdot\frac{2m}{\hbar^2k_F^2} = \frac{3}{5}\,\frac{\hbar^2k_F^2}{m^2}\sqrt{\frac{m\varepsilon_0}{n_e e^2}}\cdot\frac{\cancel{2m}}{\hbar}\,\frac{q^2}{k_F^2} = \frac{3}{5}\sqrt{\frac{\hbar^2k_F^4\, m\varepsilon_0\, 3\pi^2\, 4}{k_F^3\, m^2\, e^2\, 4}}\;\frac{q^2}{k_F^2}$$

$$= \frac{3}{5}\sqrt{\frac{3\pi}{4}}\sqrt{k_F a_0}\;\frac{q^2}{k_F^2} = \frac{3}{5}\sqrt{\frac{3\pi}{4}}\left(\frac{9\pi}{4}\right)^{1/6}\frac{1}{\sqrt{r_s}}$$

Recalling the spectrum of the particle-hole excitations