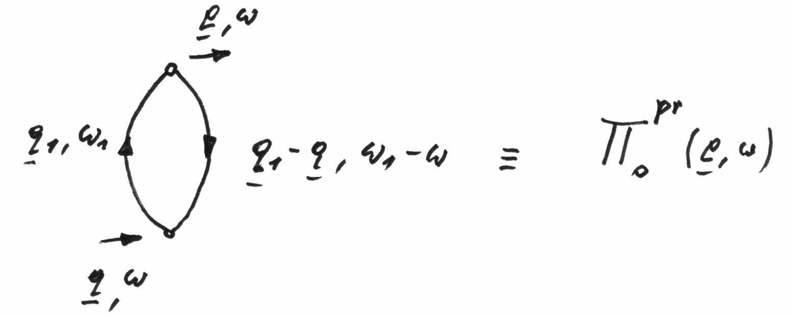
Summary Sec. 1.6:
The dielectric function of jellium in the RPA

Starting with the diagram that describes the simplest approximation[1] of a polarisation insertion into a bare Coulomb interaction line



and translating it into a mathematical formula, one obtains

$$\Pi_0^{pr}(\mathbf{q},\omega) = \left[\frac{i}{\hbar}\frac{(-1)}{(2\pi)^4}\right] \underbrace{\sum_\gamma \sum_\sigma \delta_{\gamma\sigma}}_{=2} \int d^3q_1 d\omega_1\, G^0(\mathbf{q}_1,\omega_1)\, G^0(\mathbf{q}_1 - \mathbf{q}, \omega_1 - \omega)\,.$$

After having used Cauchy's formula for the integration over ω_1, one gets the result

$$\begin{aligned}\Pi_0^{pr}(\mathbf{q},\omega) &= \frac{2}{\hbar(2\pi)^3}\int d^3k_1 \Theta(k_\mathrm{F} - k_1)\Theta(|\mathbf{k}_1 + \mathbf{q}| - k_\mathrm{F}) \\ &\quad\times\left[\frac{1}{\omega + \omega^0_{\mathbf{k}_1} - \omega^0_{\mathbf{k}_1+\mathbf{q}} + i\eta} - \frac{1}{\omega - \omega^0_{\mathbf{k}_1} + \omega^0_{\mathbf{k}_1+\mathbf{q}} - i\eta}\right].\end{aligned}$$

This wavevector-, frequency-dependent and complex polarisation function shall now be split into its real and imaginary part. This can be done by the frequently used formula

$$\frac{1}{\omega \pm i\eta} = P\,\frac{1}{\omega} \mp i\pi\delta(\omega)\ :$$

[1] Remember the names: "ring" or "bubble" approximation, or "random-phase approximation".

$$\Re\,\Pi_0^{pr}(\mathbf{q},\omega) = \frac{2}{\hbar(2\pi)^3} P \int d^3k_1 \Theta(k_{\rm F}-k_1)\Theta(|\mathbf{k}_1+\mathbf{q}|-k_{\rm F}) \times \left[\frac{1}{\omega+\omega^0_{\mathbf{k}_1}-\omega^0_{\mathbf{k}_1+\mathbf{q}}} - \frac{1}{\omega-\omega^0_{\mathbf{k}_1}+\omega^0_{\mathbf{k}_1+\mathbf{q}}}\right] ,$$

$$\Im\,\Pi_0^{pr}(\mathbf{q},\omega) = -\frac{2\pi}{\hbar(2\pi)^3} \int d^3k_1 \Theta(k_{\rm F}-k_1)\Theta(|\mathbf{k}_1+\mathbf{q}|-k_{\rm F}) \times \left[\delta(\omega+\omega^0_{\mathbf{k}_1}-\omega^0_{\mathbf{k}_1+\mathbf{q}}) + \delta(\omega-\omega^0_{\mathbf{k}_1}+\omega^0_{\mathbf{k}_1+\mathbf{q}})\right] .$$

By using the general relation between polarisation function Π^{pr} and dielectric function κ, one gets further

$$\kappa^{RPA}(\mathbf{q},\omega) = 1 - V(\mathbf{q})\,\Pi_0^{pr}(\mathbf{q},\omega) \equiv \kappa_1(\mathbf{q},\omega) + i\kappa_2(\mathbf{q},\omega)$$

with $\kappa_1(\mathbf{q},\omega)$ and $\kappa_2(\mathbf{q},\omega)$ as the real and the imaginary part of the dielectric function of jellium, respectively, in the *ring* or *random-phase* approximation.

The analytical evaluation of the above integrals is rather tedious. This job has been done at first (1954) by the Danish physicist J. Lindhard. Here are the exact mathematical expressions of the Lindhard formulas:

Real part κ_1 of the dielectric function in RPA:

$$\kappa_1(q,\omega) = 1 + \frac{k_{FT}^2}{q^2} \times \left\{\frac{1}{2} + \frac{k_F}{4q}\left[\left(1 - \frac{\left(\omega - \frac{\hbar q^2}{2m}\right)^2}{q^2 v_0^2}\right) \ln\left|\frac{\omega - q v_0 - \hbar q^2/(2m)}{\omega + q v_0 - \hbar q^2/(2m)}\right| + \left(1 - \frac{\left(\omega + \frac{\hbar q^2}{2m}\right)^2}{q^2 v_0^2}\right) \ln\left|\frac{\omega + q v_0 + \hbar q^2/(2m)}{\omega - q v_0 + \hbar q^2/(2m)}\right|\right]\right\} .$$

Imaginary part κ_1 of the dielectric function in RPA:

$q \leq 2k_F$ **:**

$$\kappa_2(q,\omega) = \frac{\pi}{2}\frac{k_{FT}^2}{v_0}\frac{\omega}{q^3} \quad \text{for} \quad 0 \leq \omega \leq qv_0 - \frac{\hbar q^2}{2m},$$

$$\kappa_2(q,\omega) = \frac{\pi}{4}\frac{k_F k_{FT}^2}{q^3}\left[1 - \frac{\left(\omega - \frac{\hbar q^2}{2m}\right)^2}{q^2 v_0^2}\right] \quad \text{for}$$

$$qv_0 - \frac{\hbar q^2}{2m} \leq \omega \leq qv_0 + \frac{\hbar q^2}{2m} \quad ,$$

$$\kappa_2(q,\omega) = 0 \quad \text{else}\,.$$

$q \geq 2k_F$ **:**

$$\kappa_2(q,\omega) = \frac{\pi}{4}\frac{k_F k_{FT}^2}{q^3}\left[1 - \frac{\left(\omega - \frac{\hbar q^2}{2m}\right)^2}{q^2 v_0^2}\right] \quad \text{for}$$

$$-qv_0 + \frac{\hbar q^2}{2m} \leq \omega \leq qv_0 + \frac{\hbar q^2}{2m},$$

$$\kappa_2(q,\omega) = 0 \quad \text{else}\,.$$

These equations contain two constants which are defined as follows:

$$k_{FT}^2 = \frac{4me^2k_F}{\pi\hbar^2} \quad \text{Fermi-Thomas wavenumber}$$

$$v_0 = \frac{\hbar k_F}{m} \quad \text{Fermi velocity}$$

Due to the extraordinary important role of these functions in solid-state physics, their properties will now be discussed in some detail.

Properties of the dielectric function in the RPA:

Static limiting case:

$$\lim_{\omega\to 0}\kappa(q,\omega)=\kappa_1(q,0)+\underbrace{i\,\kappa_2(q,0)}_{\equiv 0}$$

and

$$\kappa_1(q,0)=1+\frac{k_{FT}^2}{2q^2}\left[1+\frac{k_F}{q}\left(1-\frac{q^2}{4k_F^2}\right)\ln|\frac{q+2k_F}{q-2k_F}|\right]\,.$$

The corresponding FT of the effective potential:

$$W(q,0)=\frac{4\pi e^2}{q^2\,\kappa_1(q,0)}\,.$$

Back to real space:

$$W(r)=\frac{1}{\Omega}\sum_{\mathbf{q}}\frac{4\pi e^2}{q^2\,\kappa_1(q,0)}\,\mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}}\,.$$

Easy to evaluate in the long wavelength limit

$$\kappa_1(q,0)\approx\kappa_1(q<<k_F,0)=1+\frac{k_{TF}^2}{q^2}\ :$$

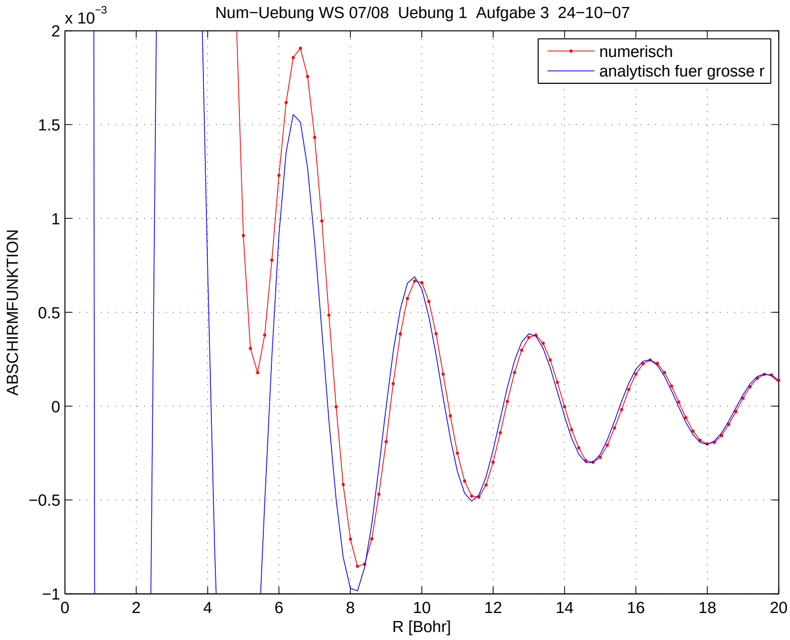
$$W(r)\approx\frac{1}{\Omega}\sum_{\mathbf{q}}\frac{4\pi e^2}{q^2+k_{TF}^2}\,\mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}}=\frac{e^2}{r}\,\mathrm{e}^{-k_{TF}r}.$$

This simple approximation reflects an important feature of the effective Coulomb potential: it is screened or shielded.

Without the *long wavelength limit*, the Fourier series can be reduced to

$$W(r)=\left(\frac{e^2}{r}\right)\underbrace{\frac{2}{\pi}\int_0^\infty dq\,\frac{\sin(qr)}{q\kappa_1(q,0)}}_{F(r)}\,.$$

A numerical evaluation of the screening function $F(r)$:



Analytically, the above Fourier integral can be solved at least for the limit of large radii [see J. Friedel, Nuovo Cimento, Suppl. **7**,287 (1958)]:

$$W(r \to \infty) \propto \frac{\cos(2k_F r)}{r^3} \, .$$

The screening of the effective potential is not *exponentially* but *oscillatory* with a wavelength of π/k_F. Such Friedel oscillations have often been experimentally observed, e.g. in *Nuclear Magnetic resonance* (NMR) and *scanning tunneling microscope* (STM) measurements.

Dynamical limiting case:

Before we discuss this limit of the RPA dielectric function, we refer once more to the relation

$$W(\mathbf{q},\omega) = \frac{V(\mathbf{q})}{\kappa(\mathbf{q},\omega)}$$

that describes the FT of the *effective interaction potential*.

Obviously, the influence of the polarisation effect on the effective potential is largest if one has

$$\kappa(\mathbf{q},\omega) = 0\,.$$

Now to the *long wavelength limit* which leads to the result

$$\lim_{q\to 0} \kappa(q,\omega) = \kappa_1(0,\omega) + \underbrace{i\,\kappa_2(0,\omega)}_{\equiv 0}$$

with

$$\kappa_1(0,\omega) = 1 - \frac{k_{FT}^2 v_0^2}{3}\frac{1}{\omega^2}\,.$$

From that, one easily gets the resonance frequency

$$\omega_{res}(q=0) = \frac{k_{FT}v_0}{\sqrt{3}} = \ldots = \left(\frac{4\pi e^2}{m}\right)^{1/2}\sqrt{n_e}\,. \qquad (1)$$

long wavelength limit means that one has a long-range polarisation effect of the electron gas, i.e., a huge number of particles takes part on this process: this is called a

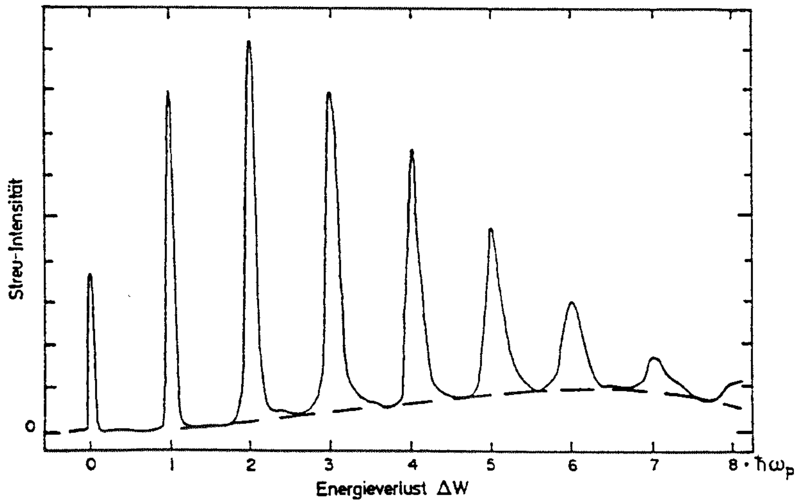
collective excitation of the electron gas

which behaves similar to a classical plasma: therefore, the *resonance frequency* is more frequently called the plasma frequency:

$$\omega_{res}(q=0) = \omega_p(0)\,.$$

The real existence of such *plasma oscillations* in crystalline media can be proved by energy loss experiments where one measures the energy loss of particles penetrating material foils.

Ever if the incoming particles are in resonance with the electronic plasma, i.e., if their kinetic energy is a multiple of $\hbar\omega_p$, the energy loss spectrum will show marking peaks:



Energy loss spectrum of 20 keV electrons penetrating an Al foil of 2080 Angstrom [Marton, Simpson, Fowler, and Swanson (1962)].

From a quantitative evaluation of these experimental data one gets for Al a plasma excitation energy of 15.3 eV. This value agrees nicely with the corresponding theoretical result based on Eq. (1) $\rightarrow$ 15.8 eV.

Apart from these limits, is it of course necessary and fruitful to investigate the full, i.e., wavevector <u>and</u> frequency dependent dielectric function κ^{RPA}, and according to the previous discussions, we are mainly interested in the zeros of this function on the complex ω plane:

$$\kappa(\mathbf{q}, \omega = \nu - i\gamma) = 0 \,.$$

You surely remember the very similar situation when we treated the theory of the selfenergy $\Sigma(\mathbf{q}, \omega)$.

Provided that the condition $|\gamma| << |\nu|$ is fulfilled, the above equation separates into

$$\kappa_1(\mathbf{q}, \nu) = 0 \qquad \text{and} \quad \gamma = \kappa_2(\mathbf{q}, \nu) \left(\frac{\partial \kappa_1}{\partial \omega} \right)_{\nu}^{-1} \,.$$

Interpretation:

- Collective excitations of the electron gas happen at energies $\hbar\nu(\mathbf{q})$ where $\nu(\mathbf{q})$ mean the real roots of the real part of the dielectric function. Consequently, $\hbar\nu(\mathbf{q})$ is called the dispersion relation of these excitations.

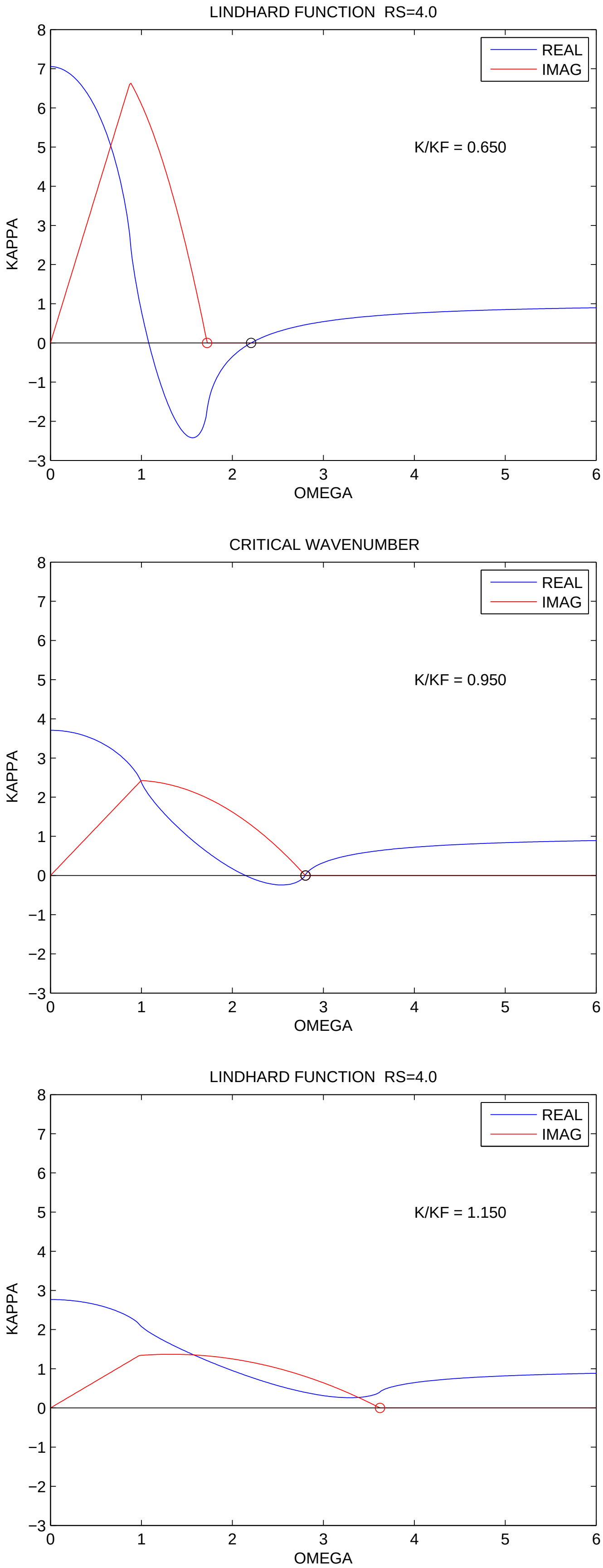
- Usually, collective excitations of the electron gas have damping factors γ proportional to the imaginary part of the dielectric function.

- If a collective excitation with energy $\hbar\nu(\mathbf{q})$ simultaneously fulfills both equations

  $$\kappa_1(\mathbf{q}, \nu) = 0 \qquad \text{and} \quad \kappa_2(\mathbf{q}, \nu) = 0 \,,$$

  we call this an undamped plasmonic excitation.

- In the framework of quantum mechanics, these two aspects, namely (i) the existence of an energy-momentum dispersion and (ii) a finite lifetime of the excited state, make it reasonable to interprete these collective excitations of the electron gas as quasiparticles named plasmons.



Real and imaginary parts of the dielectric function of jellium in the RPA as a function of ω. $q/k_F = 0.650$, 0.950, and 1.150.

Interpretation:

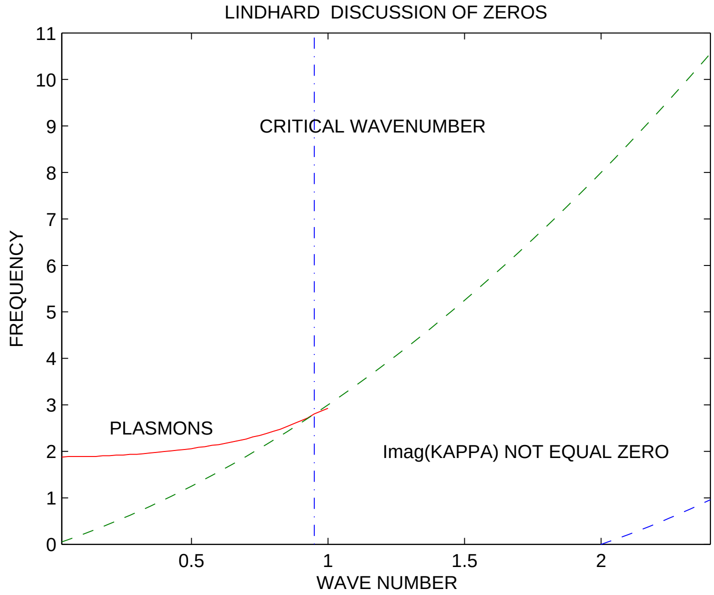
- $\boxed{q/k_F = 0.650}$ The real part of the Lindhard function has a zero point at ≈ 2.2. At this point, the imaginary part of κ is also zero:
  All conditions of an undamped plasmon excitation are fulfilled.

- $\boxed{q/k_F = 0.950}$ At *the critical value of* q, the zero point of $\Re\kappa$ coincides with the end point of the region of ω where $\Im\kappa > 0$:
  This is the situation where the region of the undamped plasmon excitations ends.

- $\boxed{q/k_F = 1.150}$ In the region of q smaller but near to the critical value, one observes more or less strongly damped plasmon excitations.

- In the region where q is significantly larger than the critical value, the damping of the plasmon excitations is so strong that one cannot further call that a <u>collective</u> excitation: in fact, the plasmon degenerates into many two-particle (electron-hole) creations and annihilations.

These important consequences can be better overlooked in the next diagram:



Regions of electron-hole scattering and of undamped plasmon excitations in the $\{\mathbf{q};\omega\}$ space, according to Lindhard's formula.

- The dashed lines indicating the region where $\Im\kappa(\mathbf{q},\omega) > 0$ are given by the expressions

$$\frac{\hbar q^2}{2m} + qv_0 \qquad \text{and} \qquad \frac{\hbar q^2}{2m} - qv_0\,.$$

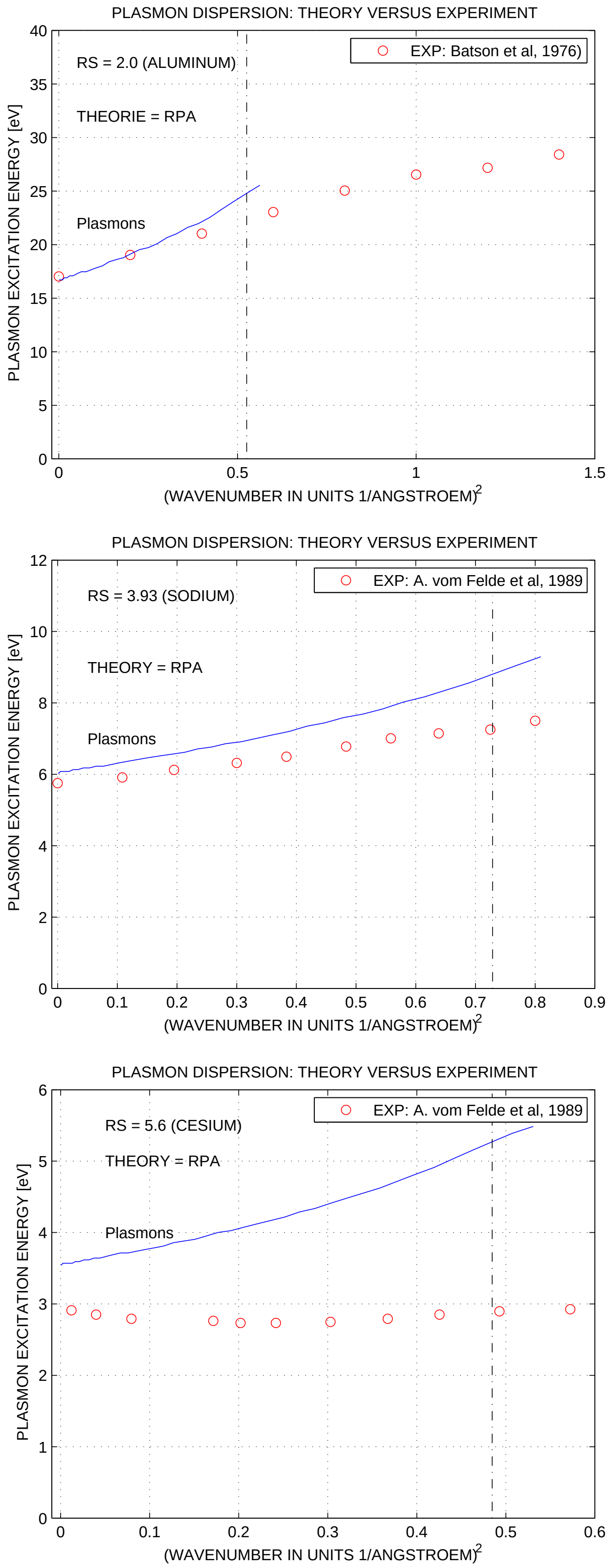
  This region is dominated by more or less strongly damped plasmon excitations or electron-hole scattering processes.

- Only outside this region, undamped collective excitations may appear. The corresponding excitation energies and their dependence on the wave vector $\mathbf{q}$ are also shown in the above diagram (the red curve named "PLASMONS"). The corresponding dispersion relation is given by

$$\omega_p(q) = \omega_p(0)\left(1 + \frac{9}{10}\frac{q^2}{k_{\mathrm{TF}}^2} + \cdots\right)\,,$$

  where $\omega_p(0)$ means the *resonance frequency* which has been previously discussed.

This plasmon dispersion can be measured by inelastic X-ray spectroscopy.



Plasmon dispersion curves in aluminum, sodium, and cesium. Comparison between theory and inelastic X-ray spectroscopy measurements.

Interim result:

<u>Remember:</u> The simplest approximation of the selfenergy of an electron gas is the real and frequency-independent exchange approximation

$$\hbar\Sigma^{pr}(\mathbf{k}) = \frac{i}{(2\pi)^4}\int d^3q d\omega_1\, V(\mathbf{q})\, \mathrm{e}^{i(\omega-\omega_1)\eta}\, G^0(\mathbf{k}-\mathbf{q},\omega-\omega_1)\,.$$

The next step of the theoretical description of Σ^{pr} is self-evident:

Reset the bare Coulomb potential $V(\mathbf{q})$ in the above equation by the effective interaction potential $W(\mathbf{q},\omega_1)$.

Consequently, one obtains the dynamical selfenergy function

$$\hbar\Sigma^{pr}(\mathbf{k},\omega) = \frac{i}{(2\pi)^4}\int d^3q d\omega_1\, W(\mathbf{q},\omega_1)\, \mathrm{e}^{i(\omega-\omega_1)\eta}\, G^0(\mathbf{k}-\mathbf{q},\omega-\omega_1)\,. \tag{2}$$

Including the random-phase approximation

$$W(\mathbf{q},\omega_1) \approx W^{RPA}(\mathbf{q},\omega_1) = \frac{V(\mathbf{q})}{\kappa^{RPA}(\mathbf{q},\omega_1)}\,,$$

one yields

$$\hbar\Sigma^{(RPA)pr}(\mathbf{k},\omega) = \frac{i}{(2\pi)^4}\int d^3q\, V(\mathbf{q}) \int \frac{d\omega_1}{\kappa^{RPA}(\mathbf{q},\omega_1)}\, \mathrm{e}^{i(\omega-\omega_1)\eta}\, G^0(\mathbf{k}-\mathbf{q},\omega-\omega_1)\,.$$

- Due to the fact that $\kappa(\mathbf{q},\omega_1)$ is both frequency-dependent and complex, the dynamical selfenergy has these properties, too, what means that the corresponding quasiparticles have finite lifetimes.

- The mathematical evaluation of $\Sigma^{(RPA)pr}(\mathbf{k},\omega)$ is the next topic of this lecture.

  However, in order to be able to perform such a calculation, we have to learn some more details about the dielectric function κ.

Summary 1.7: Time-ordered and retarded response functions

- Response functions are functions which *answer* to perturbations of the system to be investigated, e.g., they describe how an electron gas reacts on a penetrating particle.
- Typical response functions treated in our context are

$$\Sigma(\mathbf{q},\omega) \qquad \Pi(\mathbf{q},\omega) \qquad \kappa(\mathbf{q},\omega) \qquad \frac{1}{\kappa(\mathbf{q},\omega)}$$

- Time-ordered functions are functions which have been derived from Green's functions including the *time-ordering operator* $\hat{T}$.

The most important object in connection with *effective interaction potentials* is the inverse of the dielectric function

$$\frac{1}{\kappa(\mathbf{q},\omega)}$$

which has been extensively discussed in the previous sections.

However, depart from a derivation of this function from a Dyson equation, there exists another independent theoretical access to this quantity, by means of time-dependent perturbation theory.

A detailed description of such procedure would overstress the intentions of this lecture, but can be found in many textbooks:

D. Pines, *The Many-Body Problem*, Benjamin, Reading, 1962, p. 235ff,

D. Pines, *Elementary Excitations in Solids*, Benjamin, New York, 1964, p. 121ff.

The result of such a calculation reads

$$\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^T = 1+\frac{4\pi e^2}{\hbar q^2}\sum_n |\,(\hat{\rho}_\mathbf{q})_{n0}\,|^2 \left\{\frac{1}{\omega-\omega_{n0}+i\eta} - \frac{1}{\omega+\omega_{n0}-i\eta}\right\}, \tag{3}$$

where "T" means time-ordered.

Evidently, the above exact result is not directly useful for a numerical evaluation, because it contains several unknown quantities, e.g. $|(\hat{\rho}_{\mathbf{q}})_{n0}|^2$, the matrix element of the *density fluctuation operator* $\hat{\rho}_{\mathbf{q}}$ with respect to the unperturbed states $< n|$ and $|0>$ of the interacting electron gas with its excitation energies $\omega_{n0} = (E_n - E_0)/\hbar$.

Nevertheless, Eq. (3) is useful for some general statements about response functions, especially about $1/\kappa$:

- The function $1/\kappa$ is not analytical, neither in the upper nor in the lower ω half-plane.

- Separating Eq. (3) in its real and imaginary parts by means of

$$\frac{1}{\omega \pm i\eta} = P\,\frac{1}{\omega} \mp i\pi\,\delta(\omega)$$

  leads to

$$\Re\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^T = 1 + P\,\frac{4\pi e^2}{\hbar q^2}\sum_n |\,(\hat{\rho}_{\mathbf{q}})_{n0}\,|^2 \left\{\frac{1}{\omega - \omega_{n0}} - \frac{1}{\omega + \omega_{n0}}\right\}$$

  and

$$\Im\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^T = -\frac{4\pi^2 e^2}{\hbar q^2}\sum_n |\,(\hat{\rho}_{\mathbf{q}})_{n0}\,|^2 \left\{\delta(\omega - \omega_{n0}) + \delta(\omega + \omega_{n0})\right\}\ .$$

- These results immediately reflect the relation

$$\left(\frac{1}{\kappa(\mathbf{q},-\omega)}\right)^T = \left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^T\ .$$

- An extremely important equation can be derived from an extended version of Eq. (3):

$$\begin{aligned}\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^T &= 1 + \frac{4\pi e^2}{\hbar q^2}\int_0^\infty d\sigma \sum_n \delta(\sigma - \omega_{n0})\,|\,(\hat{\rho}_{\mathbf{q}})_{n0}\,|^2 \\ &\times \left\{\frac{1}{\omega - \sigma + i\eta} - \frac{1}{\omega + \sigma - i\eta}\right\}\ .\end{aligned}$$

If this expression is combined with $\Im(1/\kappa)$ for positive frequencies,

$$\Im\left(\frac{1}{\kappa(\mathbf{q},\sigma)}\right)^T = -\frac{4\pi^2 e^2}{\hbar q^2}\sum_n |\,(\hat{\rho}_\mathbf{q})_{n0}\,|^2\,\delta(\sigma-\omega_{n0})\,,$$

one gets

$$\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^T = 1+\frac{1}{\pi}\int_0^\infty d\sigma\,\Im\left(\frac{1}{\kappa(\mathbf{q},\sigma)}\right)^T\left\{\frac{1}{\sigma-\omega-i\eta}+\frac{1}{\sigma+\omega-i\eta}\right\}. \tag{4}$$

What goes wrong with this result?

Remember: "Time-ordered" means that - in the Green's function - both cases $t > t'$ and $t < t'$ are accepted, provided that the order of the two Heisenberg field operators is suitable chosen.

Such time-ordered functions are powerful tools for doing calculations,

BUT - for answer functions - they have a severe deficiency:

they violate the principle of causality.

If this principle is taken into account, time-dependent perturbation theory obtains - instead of Eq. (3) - the so-called retarded version of $1/\kappa$:

$$\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^R = 1+\frac{4\pi e^2}{\hbar q^2}\sum_n |\,(\hat{\rho}_\mathbf{q})_{n0}\,|^2\left\{\frac{1}{\omega-\omega_{n0}+i\eta}-\frac{1}{\omega+\omega_{n0}+i\eta}\right\}.$$

- This retarded function (R) has all its poles on the lower half-plane of ω:
  it is analytical on the whole upper half-plane.

- A corresponding analysis of this function as for its time-ordered counterpart leads to

$$\left(\frac{1}{\kappa(\mathbf{q},-\omega)}\right)^R = \left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^{R*} \tag{5}$$

- and further to

$$\Re\left(\frac{1}{\kappa(\mathbf{q},-\omega)}\right)^R = \Re\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^T$$

and

$$\Im\left(\frac{1}{\kappa(\mathbf{q},-\omega)}\right)^R = \mathrm{sign}(\omega)\,\Im\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^T .$$

- The corresponding relation to Eq. (4) reads

$$\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^R = 1+\frac{1}{\pi}\int_0^\infty d\sigma\,\Im\left(\frac{1}{\kappa(\mathbf{q},\sigma)}\right)^R \left\{\frac{1}{\sigma-\omega-i\eta}+\frac{1}{\sigma+\omega+i\eta}\right\} .$$

From this equation, it follows immediately

$$\Re\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^R = 1+\frac{1}{\pi}P\int_0^\infty d\sigma\,\Im\left(\frac{1}{\kappa(\mathbf{q},\sigma)}\right)^R \left\{\frac{1}{\sigma-\omega}+\frac{1}{\sigma+\omega}\right\} .$$

and - using the relation (5)

$$\Re\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^R = 1+\frac{1}{\pi}P\int_{-\infty}^\infty d\sigma\,\Im\left(\frac{1}{\kappa(\mathbf{q},\sigma)}\right)^R \frac{1}{\sigma-\omega} . \tag{6}$$

This important connection between the real and the imaginary part of a response function is called the

relation of Kramers and Kronig.

Without derivation: There is also a complementary Kramers-Kronig relation that reads

$$\Im\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^R = \frac{1}{\pi}P\int_{-\infty}^{+\infty} d\sigma\left[1-\Re\left(\frac{1}{\kappa(\mathbf{q},\sigma)}\right)^R\right]\frac{1}{\sigma-\omega} .$$

Consequences of the principle of causality:

- Retarded response functions are analytical on the (complex) upper half-plane of ω.

- Real and imaginary parts of response functions are connected via the Relation of Kramers and Kronig.

Summary 1.8:
Importance and application of Eq. (4)

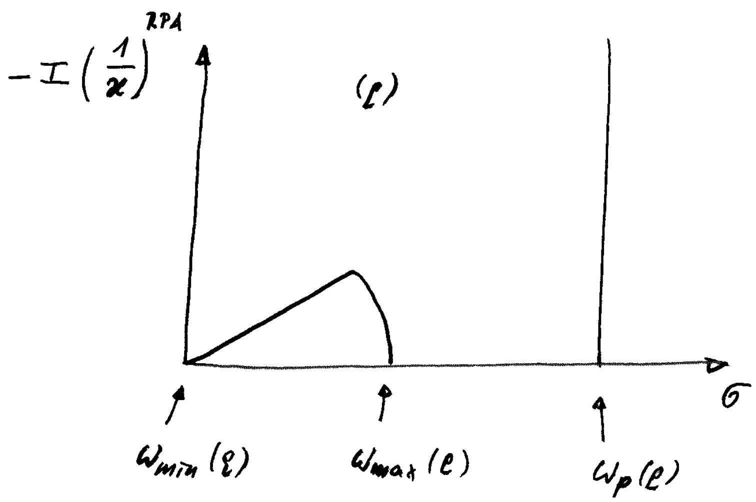
$$\left(\frac{1}{\kappa(\mathbf{q},\omega)}\right)^T = 1+\frac{1}{\pi}\int_0^\infty d\sigma\,\Im\left(\frac{1}{\kappa(\mathbf{q},\sigma)}\right)^T \left\{\frac{1}{\sigma-\omega-i\eta}+\frac{1}{\sigma+\omega-i\eta}\right\}.$$

Many calculations in solid-state physics contain effective dynamical potentials and require the evaluation of ω integrals which are often performed by using Cauchy's formula. By doing so, the residua of the function under the integral have to be calculated; this procedure is often complicated by the difficult singularity system of functions like $1/\kappa(\mathbf{q},\omega_1+i\omega_2)$.

This work is extraordinarily simplified by the use of Eq. (4) where the "pole situation" on the complex ω plane is described by two simple terms.

The prize for this advantage is the appearence of an additional integration along the positive real σ axis. The integrand contains the imaginary part of $1/\kappa$, and this function is generally quite a "well-behaved function" of σ. Therefore, a numerical evaluation of the σ integration is in many cases an easy task.

The properties of the function $\Im(1/\kappa)$ in the RPA



Sketch of the imaginary part of $\Im(1/\kappa)$ as a function of σ.

As you already know, the function $\Im\left(\frac{1}{\kappa(q,\sigma)}\right)$ consists of two contributions: the continuum part for

$$\omega_{min}(q) \leq \sigma \leq \omega_{max}(q)$$

and the (undamped) plasmapole part at $\sigma = \omega_p(q)$ with the property

$$\Re(1/\kappa) = \Im(1/\kappa) = 0\,.$$

Writing

$$\kappa(q,\sigma) = \kappa_1(q,\sigma) + i\kappa_2(q,\sigma)\,,$$

one gets

$$\Im\left(\frac{1}{\kappa(q,\sigma)}\right) = -\frac{\kappa_2(q,\sigma)}{\kappa_1^2(q,\sigma)+\kappa_2^2(q,\sigma)}\,. \tag{7}$$

This function is well-behaved in the *continuum region*.

The (undamped) plasmon zero has the properties

$$\kappa_1(q,\omega_p(q)) = 0 \qquad \text{and} \qquad \kappa_2(q,\sigma) \equiv 0 \quad (\text{around } \omega_p).$$

<u>Mathematical procedure:</u>

$\kappa_2(q,\sigma)$ is reset by $\kappa_2(q,\sigma) = \eta$ with $\eta > 0$,
and $\kappa_1(q,\sigma)$ is *linearly* Taylor expanded at $\sigma = \omega_p(q)$:

$$\kappa_1(q,\sigma) \approx \underbrace{\kappa_1(q,\omega_p(q))}_{=0} + \underbrace{\left[\frac{\partial}{\partial\sigma}\kappa_1(q,\sigma)\right]_{\omega_p(q)}}_{=\kappa_1'(q)} (\sigma - \omega_p(q))\;.$$

Including this into Eq. (7), one gets for the
plasmapole contribution (P)

$$\Im\left(\frac{1}{\kappa(q,\sigma)}\right)_P \approx \lim_{\eta\to 0}\frac{(-\eta)}{\left[\kappa_1'(q)\,(\sigma-\omega_p(q))\right]^2+\eta^2}\,.$$

This limit is one of the numeral ways to represent Dirac's delta distribution, and one gets as an approximation of $\Im(1/\kappa)$ for the plasmapole region

$$\Im\left(\frac{1}{\kappa(q,\sigma)}\right)_P \approx -\frac{\pi}{\kappa_1'(q)}\,\delta\left(\sigma-\omega_p(q)\right)\;.$$

Combining this with Eq. (7) reads

$$\Im\left(\frac{1}{\kappa(q,\sigma)}\right) \approx \underbrace{-\left(\frac{\kappa_2(q,\sigma)}{\kappa_1^2(q,\sigma)+\kappa_2^2(q,\sigma)}\right)}_{\omega_{min}(q)\leq\sigma\leq\omega_{max}(q)} - \frac{\pi}{\kappa_1'(q)}\,\delta\left(\sigma-\omega_p(q)\right)\,.$$

Remember:

- According to Lindhard's results, one has

  $$\omega_{min} = \max\left(0, -qv_0 + \frac{\hbar q^2}{2m}\right) \qquad \text{and} \qquad \omega_{max} = qv_0 + \frac{\hbar q^2}{2m}\,.$$

- The plasmapole term is only existing as long as the condition

  $$\omega_{max}(q) < \omega_p(q)$$

  holds.