Plasmon mode in an interacting electron gas; Thomas–Fermi approach to static screening; Friedel oscillations

V.M. STOJANOVIĆ

Thus far we discussed collective modes in Fermi gases with short-range interactions (charge-neutral Fermi systems!).

The most important example of an interacting Fermi gas are electrons in metals which interact through the long-ranged Coulomb interaction:

$$V(|\vec{r}_1-\vec{r}_2|)=\frac{e_0^2}{|\vec{r}_1-\vec{r}_2|}\Longrightarrow V_{\vec{q}}\propto\frac{4\pi}{|\vec{q}|^2}\,.$$

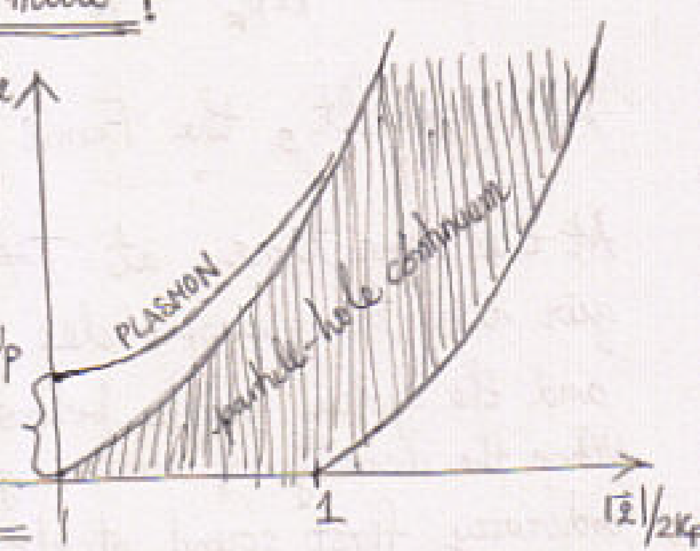
By making use of the condition

$$V_{\vec{q}}\,\mathrm{Re}\,\chi_0^R(\vec{q},\omega)=1\Longleftrightarrow\boxed{\mathrm{Re}\,\chi_0^R(\vec{q},\omega)=\frac{1}{V_{\vec{q}}}}\quad(**)$$

in the long-wavelength (small $\vec{q}$) regime we find that in the case of Coulomb interaction the zero sound is replaced by another collective mode which is gapped (as illustrated below) and is called plasmon mode!

By expanding $(**)$ for small $|\vec{q}|$ (but to 2nd order in $|\vec{q}|$!) one obtains the plasmon dispersion:

$$\boxed{\omega_{\vec{q}}=\omega_p\left\{1+\frac{3}{10}\left(\frac{|\vec{q}|v_F}{\omega_p}\right)^2+O(|\vec{q}|^4)\right\}}$$



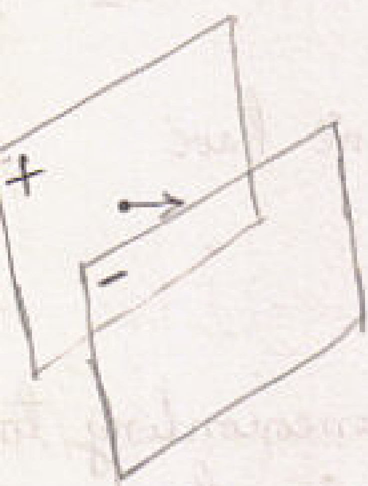
Here $\boxed{\omega_p=\sqrt{\frac{ne^2}{\varepsilon_0 m}}}$ is the plasma frequency.

In good metals, ω_p is rather large ($\sim 10\,eV$) !
Some typical values are listed here :

METAL	ω_p [eV]
Li	7.1
Na	5.7
K	3.7
Mg	10.6
Al	15.3

these values are measured experimentally!

<u>The plasma frequency</u> can be obtained already in <u>the classical picture</u> : consider a (negatively charged) electron gas in a positive charge-compensating background. When the electrons are shifted with respect to positively charged ions by the distance u, a polarization is created and accordingly an electric field.



The force acting on an individual electron is

$F = m\ddot{u} = -eE$, where the electric field E is given by

$$E = \frac{\sigma}{\varepsilon_0} = \frac{nue}{\varepsilon_0} \rightarrow$$

$$m\ddot{u} = -\frac{nue^2}{\varepsilon} \Leftrightarrow \boxed{\ddot{u} + \frac{ne^2}{\varepsilon m} u = 0}$$

Note that the "frequency squared" $= \frac{ne^2}{\varepsilon m}$ is precisely ω_p^2 !

Thomas-Fermi approach to static screening

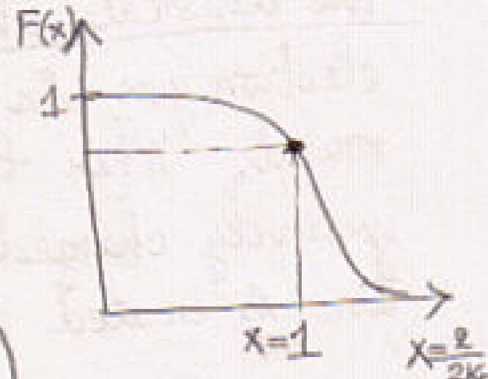
The RPA dielectric function is given by

$$\boxed{\varepsilon^{RPA}(\vec{q},\omega) = 1 - V_q \chi_0^R(\vec{q},\omega)}.$$

If we limit ourselves to the screening of a static external electric field or a static field of a charged impurity then it is sufficient to consider its $\omega = 0$ version:

$$\boxed{\varepsilon^{RPA}(\vec{q},\omega=0) = 1 + \frac{q_{TF}^2}{q^2} F\left(\frac{q}{2k_F}\right)},$$

where $F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right|$



and $\boxed{q_{TF}^2 = \frac{6\pi e_0^2 n}{\varepsilon_F}}$.

(q_{TF} is the Thomas-Fermi wavenumber.)

In the long-wavelength limit ($x \ll 1$) we have

$$\boxed{\varepsilon^{RPA}(\vec{q},0) \approx 1 + \frac{q_{TF}^2}{q^2}}$$

$\Rightarrow$ the total electrostatic potential V_{tot} corresponding to an external potential $V_{ext} \propto \frac{4\pi}{q^2}$ is given by

$$V_{tot} = \frac{V_{ext}}{\varepsilon^{RPA}(\vec{q},0)} \approx \frac{V_{ext}}{1 + \frac{q_{TF}^2}{q^2}}$$

$\Rightarrow$ if $V_{ext} \propto \frac{4\pi}{q^2}$, we obtain

$$V_{tot} \simeq \frac{4\pi}{q^2 + q_{TF}^2}$$

In real space, the last potential corresponds to

$$V_{tot}(r) \propto \frac{e^{-q_{TF} r}}{r} = \frac{e^{-\frac{r}{q_{TF}^{-1}}}}{r}, \text{ i.e.,}$$

this is a Yukawa-type potential with the decay length q_{TF}^{-1}, the Thomas-Fermi screening length.

From the definition of q_{TF} it can be concluded that q_{TF} is of the same order of magnitude as k_F (Fermi momentum) and that in typical metals q_{TF}^{-1} is of the order of 5Å! Interestingly, this is of the same order as the interatomic distance!

Thus we conclude that static external electric field cannot penetrate into a metal deeper than certain distance which is of the order of the interatomic one!

The reason for this is very efficient screening by the electrons of the host metal.

The fact that $E \approx 0$ inside of a metal was widely used in electrostatics, but we have now provided a microscopic mechanism.

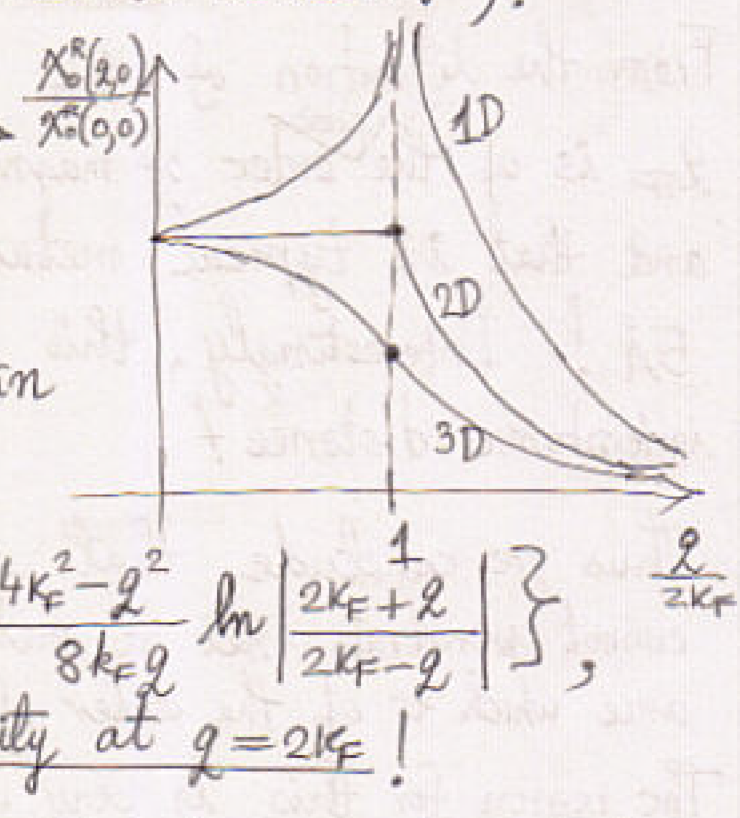
Q: What is the distribution of the induced charge around an impurity placed inside a metal?

Assume that the impurity has charge Ze.

To obtain the correct answer it will not be sufficient to use the long-wavelength form of the static RPA dielectric function. In fact, behavior of $\varepsilon^{RPA}(\vec{q},0)$ at $q=2k_F$ will be of crucial importance. Note that $2k_F$ is the diameter of the Fermi surface!

Interestingly, $\chi_0^R(\vec{q},0)$ and therefore $\varepsilon^{RPA}(\vec{q},0)$ has singularities at $q=2k_F$ in all dimensions (they become more drastic as the dimension is reduced!).

static Lindhard function in different dimensions



As regards the corresponding dielectric function, which in 3D reads

$$\varepsilon^{RPA}(\vec{q},0)=1+\frac{q_{TF}^2}{q^2}\left\{\frac{1}{2}+\frac{4k_F^2-q^2}{8k_Fq}\ln\left|\frac{2k_F+q}{2k_F-q}\right|\right\},$$

it has a logarithmic singularity at $q=2k_F$!

Consider the induced charge distribution that corresponds to a point charged impurity at the origin (its charge distribution is $\boxed{\rho_{ext}(\vec{r})=Ze\delta(\vec{r})}$).

F.T. of $\rho_{ext}(\vec{r})$

$$\Rightarrow \rho_{ind}=\rho_{tot}-\rho_{ext}=\int\frac{d^3\vec{q}}{(2\pi)^3}\left\{\frac{1}{\varepsilon(q)}-1\right\}\rho_{\vec{q}}^{ext}\,e^{i\vec{q}\cdot\vec{r}}$$

By switching to the spherical coordinates and doing the integration over the azimuthal angle (which yields a factor of 2π!)

We obtain

$$\rho_{ind} = \frac{Ze}{(2\pi)^2} \int_0^{+\infty} dq\, q^2 \left\{ \frac{1}{\varepsilon(q)} - 1 \right\} \underbrace{\int_0^{\pi} d\theta \sin\theta\, e^{iqr\cos\theta}}_{= \int_{-1}^{1} e^{iqrx} dx \,=\, \frac{e^{iqr} - e^{-iqr}}{iqr} \,\equiv\, \frac{2\sin(qr)}{qr}}$$

and further

$$\rho_{ind} = -\frac{Ze}{2\pi^2} \int_0^{\infty} dq\, q \frac{\varepsilon(q)-1}{\varepsilon(q)} \frac{\sin(qr)}{r} \text{, that is}$$

$$\boxed{\rho_{ind} = -\frac{Ze}{r} \int_0^{+\infty} g(q) \sin(qr)\, dq} \text{, with}$$

$$\boxed{g(q) \equiv \frac{q}{2\pi^2} \frac{\varepsilon(q)-1}{\varepsilon(q)}}.$$

Since $g(q)$ is a rather complicated function, the integral for ρ_{ind} is difficult to compute exactly. We will be interested in its asymptotic spatial dependence.

By noting that $g(q)$ vanishes for both $q \to 0$ and $q \to \infty$ and doing two consecutive integration by parts we obtain

$$\rho_{ind} \cong \frac{Ze}{r^3} \int_0^{+\infty} g''(q) \sin(qr)\, dq$$

where $g(q) \propto \frac{C}{q - 2k_F}$ is <u>singular around $q = 2k_F$</u> !

The most important contribution to the above integral stems from the neighburhood of $q = 2k_F$, i.e., from $q \in (2k_F - \Delta, 2k_F + \Delta)$

$$\Downarrow$$

$$\varrho_{ind}(r) \approx \frac{Ze}{r^3} C \int_{2k_F-\Delta}^{2k_F+\Delta} \frac{\sin(qr)}{q - 2k_F} \, dq \quad (r \to \infty)$$

Note that $\sin(qr) = \sin[(q-2k_F)r + 2k_F r] =$

$$= \sin((q-2k_F)r) \cos(2k_F r) + \cos[(q-2k_F)r] \sin(2k_F r)$$

and that $\dfrac{\cos[(q-2k_F)r]}{q-2k_F}$ is an <u>odd function</u> around $q = 2k_F$; thus it yields zero when integrated over a symmetric interval!

$$\Longrightarrow \quad \varrho_{ind}(r) \approx \frac{Ze}{r^3} C \int_{2k_F-\Delta}^{2k_F+\Delta} dq \frac{\sin[(q-2k_F)r]}{q-2k_F} \cos(2k_F r)$$

$$\Longleftrightarrow \quad \varrho_{ind}(r) \approx ZeC \frac{\cos(2k_F r)}{r^3} \int_{-\Delta}^{\Delta} \frac{\sin x}{x} dx$$

$\boxed{x = (q-2k_F)r}$

This integral yields finite value even for $\Delta \to \infty$: $\int_{-\infty}^{+\infty} \frac{\sin x}{x} dx = \frac{\pi}{2}$

$$\Longrightarrow \quad \boxed{\varrho_{ind}(r) \propto \frac{\cos(2k_F r)}{r^3}}$$

Friedel oscillations!