PLASMA OSCILLATIONS AND SCREENING IN HEG

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1. Plasma oscillations

In 1930 Rudberg made the first systematic measurements of the energy distribution of 50-400 eV electrons scattered from the surfaces of a number of metals. He found peaks which occurred at fixed energy intervals from the peak of elastically scattered electrons, irrespective of the primary bombarding energy or the scattering angle.
In 1933 Wood noticed that thin layers of alkali metals turn from reflecting fo transparent when illuminated by light from visible to UV [1].
Ruthemann extended Rudberg's measurements to electrons transmitted through thin films of various materials [3], finding energy losses at fixed energy intervals. Measurements of electron energy losses in vapours of a number of materials confirmed the known atomic transitions, but showed no correlation with the energy losses in the solid state [5].
The loss spectrum is made up of combinations of 15-ev and 7-ev losses, though the various reported loss values differ considerably. There have been a number of attempts to explain the origin of the loss lines in aluminum and other materials.

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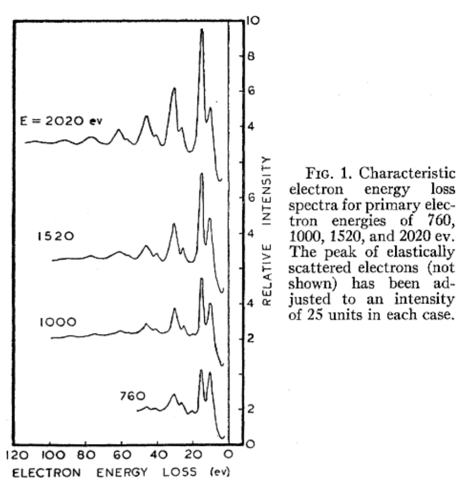

Figure 1. Energy losses in Aluminum (from [8]). For Al, $\hbar\omega_{pl} = 15.8$eV assuming 3 free electrons per atom.

The plasma oscillation theory bt David Bohm and David Pines[1] in 1953 [6] yielded a satisfactory understanding of the loss mechanism. The energy losses are due to collective excitation of the conduction electrons, the magnitude of the elementary loss being given by $\hbar\omega_{pl}$, where

$$\omega_{pl} = \sqrt{\frac{4\pi e^2 n}{m}}$$

is the plasma oscillation frequency, n is the density of free electrons in the material. Note that it does not depend on Planck's constant. Subsequently, Murray Gell-Mann and Keith Brueckner showed that the approximation used by Bohm and Pines (RPA) can be derived from a summation of leading-order chain Feynman diagrams in a dense electron gas [7].

2. Dielectric function

For a homogeneous system the *retarded* generalized dielectric function is

$$\epsilon^{\mathsf{R}}(\mathbf{k},\omega) = 1 - v(\mathbf{k})\Pi^{\star\mathsf{R}}(\mathbf{k},\omega) \tag{1}$$

In linear response, a perturbation $\varphi(x)$ coupled to the density causes a density variation

$$\delta n(\mathbf{x},t) = \int \frac{d^3k}{(2\pi)^3}\int \frac{d\omega}{2\pi} e^{i\mathbf{k}\cdot\mathbf{x}-i\omega t}\frac{\Pi^{\star\mathsf{R}}(\mathbf{k},\omega)}{\epsilon^{\mathsf{R}}(\mathbf{k},\omega)}\varphi(\mathbf{k},\omega) \tag{2}$$

Irrespective of the form of the external field, the response of the system is enhanced in the vicinity of zeros of the dielectric function close to the real axis. Such zeros are associated to *collective excitations* of the system, such as plasmons for the electron gas, or zero sound in ^{3}He.
Since $\Pi^{\mathsf{R}} = \Pi^{\star\mathsf{R}}/\epsilon^{\mathsf{R}}$, a zero of ϵ^{R} is a pole of Π^{R}, and poles occur in the lower half $\omega-$plane. Therefore, if $\omega_1(\mathbf{k}) + i\omega_2(\mathbf{k})$ is a zero of ϵ^{R} then it is always $\omega_2(\mathbf{k}) < 0$.
If such a zero exists and is simple, $\omega(\mathbf{k}) = \omega_1(\mathbf{k}) + i\omega_2(\mathbf{k})$, the polarization has (Laurent) expansion

$$\Pi^{\mathsf{ret}}(\mathbf{k},\omega) = \frac{Z(\mathbf{k})}{\omega-\omega(\mathbf{k})} + \text{analytic term}$$

The pole contribution of the integral is evaluated with the residue theorem for $t > 0$:

$$\delta n_{pole}(\mathbf{x},t) = -i\int \frac{d\mathbf{k}}{(2\pi)^3} A(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}-i\omega_1(\mathbf{k})t-|\omega_2(\mathbf{k})|t}$$

It is a superposition of waves with dispersion $\omega = \omega_1(\mathbf{k})$, that decay in time with characteristic time $|\omega_2(\mathbf{k})|^{-1}$, with amplitude $Z(\mathbf{k})\varphi(\mathbf{k},\omega_1(\mathbf{k}))$.
The collective mode is long-lived if $|\omega_2| \ll \omega_1$. A linear expansion in ω_2 of the complex equation $\epsilon^{\mathsf{R}}(\mathbf{k},\omega_1+i\omega_2) = 0$ gives two real equations:

$$1 - v(\mathbf{k})\,\mathrm{Re}\,\Pi^\star(\mathbf{k},\omega_1(\mathbf{k})) = 0 \tag{3}$$

$$\omega_2(\mathbf{k}) = -\frac{\mathrm{Im}\Pi^{\star\mathsf{R}}(\mathbf{k},\omega)}{\frac{\partial}{\partial\omega}\mathrm{Re}\Pi^\star(\mathbf{k},\omega)}\Big|_{\omega=\omega_1(\mathbf{k})} \tag{4}$$

For the electron gas, the leading term is $\omega = \omega_{pl}$. The density variation is a standing wave $\delta n_{pole}(\mathbf{x},t) = A(\mathbf{x})e^{-i\omega_{pl}t}$.

[1] D.Pines (1924–2018) obtained his PhD with D.Bohm at Princeton in 1951, with the thesis "The role of plasma oscillations in electron interactions".

Exercise 2.1. *Show that the residue is*

$$Z(\mathbf{k}) = \frac{1}{v(\mathbf{k})} \frac{1}{\frac{\partial}{\partial\omega}\epsilon^R(\mathbf{k}, \omega_1(\mathbf{k}))}$$

2.1. **Poles and dielectric function in RPA.** We reproduce the evaluations in [9] in RPA. Eq.(3) is solved in the region

$$\omega > \frac{\hbar q^2}{2m} + \frac{\hbar k_F q}{m}$$

where $\mathrm{Im}\Pi^{(0)}(q,\omega) = 0$ and $\omega_2(q) = 0$. At the microscopic scale $q > k_F$, HEG is no longer a valid description, while it is universal for small q.

$$0 = 1 - v(\mathbf{q})\frac{2}{\hbar}\int \frac{d\mathbf{p}}{(2\pi)^3}\theta(k_F - p)\frac{2(\omega_{|\mathbf{p}+\mathbf{q}|} - \omega_p)}{\omega^2 - (\omega_{|\mathbf{p}+\mathbf{q}|} - \omega_p)^2}$$

With $k_F > p$ it is $\omega > (\omega_{|\mathbf{p}+\mathbf{q}|} - \omega_p)$ in the region. We expand in geometric series:

$$\begin{aligned}
0 &= 1 - v(\mathbf{q})\frac{4}{\hbar\omega^2}\int \frac{d\mathbf{p}}{(2\pi)^3}\theta(k_F - p)\left[(\omega_{|\mathbf{p}+\mathbf{q}|} - \omega_p) + \frac{(\omega_{|\mathbf{p}+\mathbf{q}|} - \omega_p)^3}{\omega^2} + \dots\right] \\
&= 1 - v(\mathbf{q})\frac{4}{\hbar\omega^2}\int \frac{d\mathbf{p}}{(2\pi)^3}\theta(k_F - p)\left[\frac{\hbar q^2}{2m} + \frac{\hbar\mathbf{q}\cdot\mathbf{p}}{m} + + \frac{1}{\omega^2}\left(\frac{\hbar q^2}{2m} + \frac{\hbar\mathbf{q}\cdot\mathbf{p}}{m}\right)^3 + \dots\right]
\end{aligned}$$

Integrals with odd powers of $(\mathbf{p}\cdot\mathbf{q})$ vanish by parity. We confine to the first two terms in q. The leading integral is the volume of the Fermi sphere. $\frac{4}{3}\pi k_F^3/(2\pi)^3 = n/2$, where n is the uniform density:

$$\begin{aligned}
0 &= 1 - v(\mathbf{q})\frac{4}{\hbar\omega^2}\left[\frac{\hbar q^2}{2m}\frac{n}{2} + \frac{3}{\omega^2}\frac{\hbar q^2}{2m}\left(\frac{\hbar}{m}\right)^2 q_i q_j \int \frac{d\mathbf{p}}{(2\pi)^3}\theta(k_F - p)p_i p_j + \dots\right] \\
&= 1 - v(\mathbf{q})\frac{n}{\omega^2}\frac{q^2}{m}\left[1 + \frac{2}{n}\frac{1}{\omega^2}\frac{\hbar^2 q^2}{m^2}\frac{4\pi}{(2\pi)^3}\frac{k_F^5}{5} + \dots\right]
\end{aligned}$$

Note the disappearance of $\hbar$ in the leading term.

• The Coulomb potential is special for the cancellation of q^2 in the leading term. The result is:

$$\omega(q) = \omega_{pl} + \frac{3}{10}\frac{v_F^2}{\omega_{pl}}q^2 + \dots \tag{5}$$

The RPA expression of the dielectric function at small q is:

$$\epsilon_{\mathsf{RPA}}(q,\omega) = 1 - \frac{\omega_{pl}^2}{\omega^2}\left[1 + \frac{3}{5}\frac{v_F^2}{\omega^2}q^2 + \dots\right]$$

• Zero sound in ^{3}He (see [9]). The potential is short ranged and radial. For small q: $v(\mathbf{q}) = \int d\mathbf{x} v(x) e^{-i\mathbf{q}\cdot\mathbf{x}} \approx v_0[1 - \frac{1}{6}a^2 q^2 + ...]$ where $a^2 = \int d\mathbf{x} v(r) r^2/v_0$ measures the range of the potential. The equation $\epsilon = 0$ at leading term now is:

$$0 = 1 - v_0\frac{n}{m}\frac{q^2}{\omega^2}$$

The equation has solution if $v_0 > 0$ (repulsive potential) and the dispersion relation is wave-like: $\omega(q) = (\sqrt{v_0 n/m})q$. It is necessary, for the density wave to propagate that its velocity is $\sqrt{v_0 n/m} > v_F$.

3. Screening in HEG

An impurity with charge Ze is placed in $\mathbf{x}=0$ in the HEG. The perturbation is $\hat V = -Ze^2\int d\mathbf{x}\hat n(\mathbf{x})/|\mathbf{x}|$. The electrons respond to the perturbation and screen the charge. We look at the equilibrium density in presence of the charge. The field $\varphi(\mathbf{k},\omega) = -Z(4\pi e^2/k^2)2\pi\delta(\omega)$ is inserted in eq.(2):

$$\delta n(\mathbf{x}) = -Z\int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \frac{4\pi e^2 \Pi^{\star\mathsf{R}}(\mathbf{k},0)}{k^2 - 4\pi e^2\Pi^{\star\mathsf{R}}(\mathbf{k},0)} \tag{6}$$

In HEG the polarization depends on k. The angular integrals are done first:

$$\begin{aligned}\delta n(r) &= -2\pi Z\int_0^\infty \frac{k^2dk}{(2\pi)^3}\frac{4\pi e^2\Pi^{\star\mathsf{R}}(\mathbf{k},0)}{k^2-4\pi e^2\Pi^{\star\mathsf{R}}(\mathbf{k},0)}\frac{e^{ikr}-e^{-ikr}}{ikr}\\ &= -\frac{Z}{4\pi^2 ir}\int_{-\infty}^{+\infty} kdk\,\frac{4\pi e^2\Pi^{\star\mathsf{R}}(\mathbf{k},0)}{k^2-4\pi e^2\Pi^{\star\mathsf{R}}(\mathbf{k},0)}e^{ikr}\end{aligned}$$

In RPA, the static limit of the Lindhard function is:

$$\Pi^{(0)}(k,0) = -\frac{mk_F}{\pi^2\hbar^2} g\left(\frac{k}{k_F}\right)$$

$$\delta n(r)_{\mathsf{RPA}} = \frac{Z}{4\pi^2 ir}\int_{-\infty}^{+\infty} kdk\,\frac{k_{\mathsf{TF}}^2 g(k/k_F)}{k^2+k_{\mathsf{TF}}^2 g(k/k_F)}e^{ikr}$$

For "large" r the phase rapidly oscillates, and one expects that the main contribution of the integral arises for small k. The drastic simplification is to approximate $g(k/k_F)=g(0)=1$. This is the Thomas-Fermi approximation. The integral is easily calculated:

$$\delta n(r)_{\mathsf{TF}} \approx \frac{Z}{4\pi^2 ir}\int_{-\infty}^{+\infty} kdk\,\frac{k_{\mathsf{TF}}^2}{k^2+k_{\mathsf{TF}}^2}e^{-ikr} = \frac{Z}{2\pi}k_{\mathsf{TF}}\frac{e^{-k_{\mathsf{TF}}r}}{r}$$

The screening is very efficient and occurs on a scale of few k_F^{-1}. The exponential decay is not correct, albeit a good approximation in realistic situation. The function g has singular derivative in $k=2k_F$. For large r a more accurate evaluation gives:

$$\delta n(r)_{\mathsf{RPA}} \approx Z\frac{C}{r^3}\cos(2k_F r)$$

with a constant C (see [9]). The impurity is surrounded by "Friedel oscillations", i.e. regions at regular distances of decaying negative and positive charge densities. They were predicted by Friedel in 1952. (see Crommie, M., Lutz, C. and Eigler, D. Imaging standing waves in a two-dimensional electron gas. Nature 363, 524–527 (1993).)

3.1. **Dielectric function of HEG.**

In linear response, the variation of the electron charge density (the induced charge density) in response to the perturbation caused by the electrostatic potential of an external charge density $\rho^{ext}(\mathbf{x},t)$ is:

$$-e\delta n(x) = \frac{e^2}{\hbar}\int d_4x' D^{\mathsf{ret}}(x,x')\int d_4x''\frac{\delta(t'-t'')}{|\mathbf{x}'-\mathbf{x}''|}\rho^{ext}(x'')$$

If the unperturbed electron system is invariant for space translations, the retarded function depends on $x-x'$. In Fourier space, the induced charge is:

$$\delta\rho^{ind}(\mathbf{k},\omega) = \Pi^{\mathsf{ret}}(\mathbf{k},\omega)\frac{4\pi e^2}{\mathbf{k}^2}\rho^{ext}(\mathbf{k},\omega)$$

The Maxwell equation div$\mathbf{E} = 4\pi(\rho^{ext} + \rho^{ind})$ now is:

$$\begin{aligned} i\mathbf{k}\cdot\mathbf{E}(\mathbf{k},\omega) =& 4\pi\left[1 + \Pi^{\mathsf{ret}}(\mathbf{k},\omega)\frac{4\pi e^2}{\mathbf{k}^2}\right]\rho^{ext}(\mathbf{k},\omega) \\ =& 4\pi\frac{1}{1 - v(\mathbf{k})\Pi^{\star\mathsf{ret}}(\mathbf{k},\omega)}\rho^{ext}(\mathbf{k},\omega) \\ =& 4\pi\frac{1}{\epsilon^{\mathsf{ret}}(\mathbf{k},\omega)}\rho^{ext}(\mathbf{k},\omega) \end{aligned}$$

This is compared with the Maxwell equation $i\mathbf{k}\cdot\mathbf{D}(\mathbf{k},\omega) = 4\pi\rho^{ext}(\mathbf{k},\omega)$.

Simple approximate expressions for the dielectric functions [10, 12] are:

$$\epsilon_{TF}(q) = 1 + \frac{q_{TF}^2}{q^2} \qquad \left(q_{TF}^2 = \frac{6\pi e^2 n_0}{E_F}\right) \qquad \text{(Thomas-Fermi)} \tag{7}$$

$$\epsilon_{RPA}^{\mathsf{ret}}(q,\omega) = 1 - \frac{4\pi e^2}{q^2}\Pi^{(0)\mathsf{ret}}(q,\omega) \qquad \text{(Lindhard)} \tag{8}$$

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