

In the preceding calculations, we treated the paramagnetic and diamagnetic effects separately. i.e., when computing Pauli paramagnetism we ignore the change in electron wavefunction due to the presence of the magnetic field  $H$ , and only considered the interaction of  $H$  with the intrinsic electron magnetic moment  $\mu_B$ . When computing Landau diamagnetism we ignored this interaction with the intrinsic moment, and considered only the effect of  $H$  on the eigenstates and hence the density of states.

Of course both effects are there simultaneously, so the total magnetic susceptibility of the free electron gas is therefore

$$\chi = \chi_P + \chi_L = \chi_P - \frac{1}{3} \chi_L = \frac{2}{3} \chi_P$$

Since  $\chi_P > 0$ , the net effect is paramagnetic.

For some more traditional calculations of Landau diamagnetism see:

Notes from AP Young UC Santa Cruz

<http://bartok.ucsc.edu/peter/231/magnetic-field/node5.html>

Pathria - "Statistical Mechanics", pgs 206 - 209

Landau + Lifshitz - "Statistical Mechanics v1", pgs 172 - 175

In real metals and doped semiconductors one does not necessarily find that the total  $\chi$  is paramagnetic. When we include effects of band structure, which causes the electron to behave as if it had an "effective" mass  $m^*$ , rather than its true free particle mass  $m$ , we can find that  $\chi$  can be either paramagnetic or diamagnetic.

The Pauli paramagnetic susceptibility was

$$\chi_p \sim g(E_F) = \frac{m k_F}{k^2 \pi^2} \quad \text{for free electrons}$$

For electrons in a periodic potential,  $\chi_p$  will go as  $\sim m^*$  rather than  $m$ , so

$$\chi_p \sim \frac{m^*}{m} \chi_{p \text{ free electron}}$$

The Landau diamagnetic susceptibility came from the Lorentz force on the electron in a magnetic field

$$\chi_L \sim \frac{e \vec{v}}{c} \times \vec{H}$$

where velocity  $v \sim \frac{dE_k}{dk} \sim \frac{1}{m}$  For electrons in a periodic potential we will then have  $v \sim \frac{1}{m^*}$

$$\text{so} \quad \chi_L \sim \frac{m}{m^*} \chi_{L \text{ free electron}}$$

So  $\frac{\chi_L}{\chi_p} \sim \left(\frac{m}{m^*}\right)^2 \frac{\chi_{L \text{ free}}}{\chi_{p \text{ free}}}$  Since we can have

$m^* \ll m$  in some materials, it is possible to have  $|X_L| \gg X_p$  and the material will have a ~~net~~ net diamagnetic response.

## The de Haas - van Alphen effect

At sufficiently low temperature and high magnetic field, so that  $\hbar\omega_c > k_B T$ , the oscillations due to the discrete Landau levels can be observed in measurements of magnetization  $M = -\frac{1}{V} \frac{\partial E}{\partial H}$ . These were first observed by de Haas and van Alphen in 1930 in magnetization measurements on Bi at 14.2°K. Similar oscillations are found in susceptibility  $\chi = \frac{\partial M}{\partial H}$ , conductivity (Shubnikov-de Haas effect), and many other quantities. Since we found that  $E_F$  has such oscillations, so  $g(E_F)$  will have such oscillations, hence we can easily see why many physical quantities also oscillate.

The period of oscillations is in the inverse magnetic field  $1/H$

$$\text{period is } \Delta X = 1 \Rightarrow \Delta \left( \frac{E_F^0}{\hbar\omega_c} \right) = 1 \quad \omega_c = \frac{eH}{mc}$$

since  $E_F^0$  is fixed while  $H$  varies, we have oscillations that are periodic in  $1/H$  with period

$$\Delta \left( \frac{1}{H} \right) = \frac{\hbar}{E_F^0} \frac{e}{mc}$$

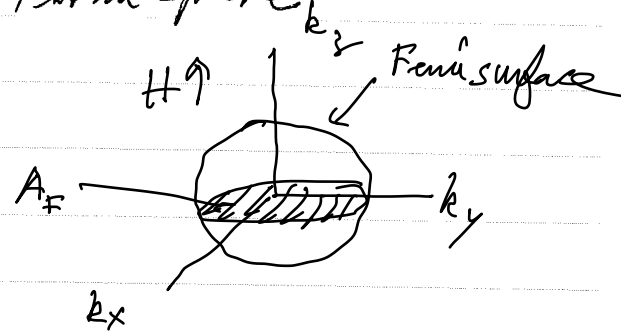
we can rewrite this as

$$\Delta\left(\frac{1}{H}\right) = \frac{\hbar^{2m}}{\hbar^2 k_F^2} \frac{e}{mc} = \frac{2e}{\hbar c k_F^2}$$

cross sectional area of the Fermi sphere

is  $A_F = \pi k_F^2$ , so

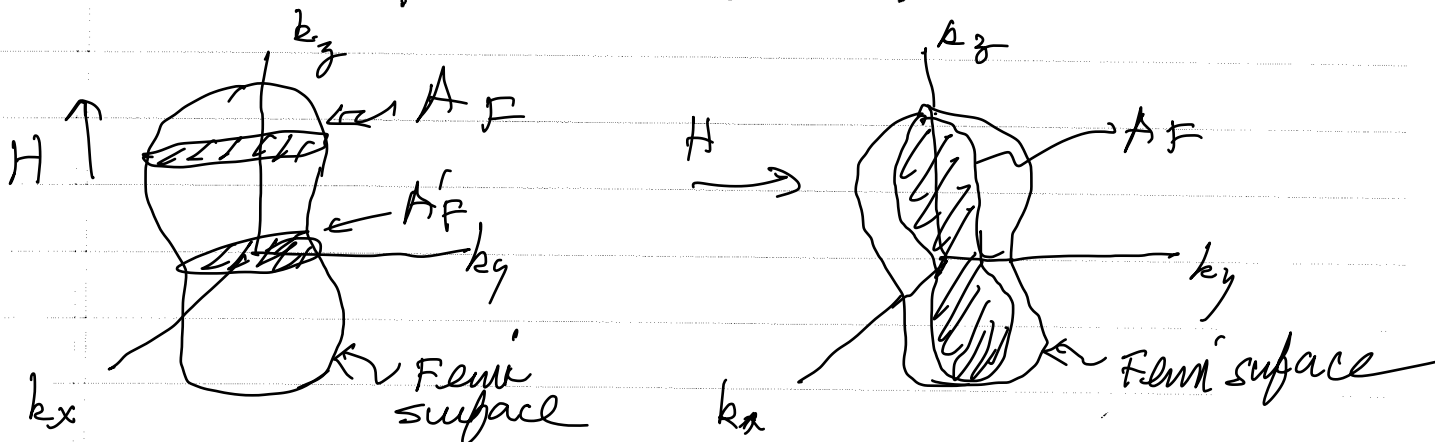
$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e}{\hbar c} \frac{1}{A_F}$$



The above turns out to be more generally true.

For electrons in a periodic potential (as opposed to our free electron model) the Fermi surface is not necessarily a sphere. Still the above relation holds where  $A_F$  is the <sup>extremal</sup> ~~maximal~~ cross sectional area of the Fermi surface perpendicular to the direction of the applied magnetic field. The de Haas-van Alphen effect thus became one of the methods for measuring the shape of the Fermi surface.

see Ashcroft + Mermin Chpt 14 for more details



## Screening and the dielectric function of the free electron gas

If an external electrostatic potential  $V(\vec{r})$  is applied to the electron gas, the average electron density will no longer be constant, as electrons will get attracted to the maximum of  $V$  (so that  $-eV$  is minimized).

If we write the new spatially varying electron density as

$$n(\vec{r}) = n + \delta n(\vec{r})$$

where  $n$  is the uniform density when  $V=0$ , then

$$\delta \rho = -e \delta n(\vec{r}) \text{ is called the "induced"}$$

charge density.

The induced charge density  $\delta \rho$  creates an "induced" electrostatic potential of its own,  $\delta V$ , given by,

$$-\nabla^2 \delta V = 4\pi \delta \rho \quad \text{Poisson's eqn for electrostatics}$$

So the total potential is then

$$V^{\text{tot}} = V + \delta V$$

Consider this in Fourier transform space

$V(\vec{k})$ ,  $V^{\text{tot}}(\vec{k})$ ,  $\delta V(\vec{k})$ ,  $\delta \rho(\vec{k})$  are the Fourier transforms of  $V(\vec{r})$ ,  $V^{\text{tot}}(\vec{r})$ ,  $\delta V(\vec{r})$ ,  $\delta \rho(\vec{r})$

$$\left. \begin{aligned} \psi \quad V(\vec{r}) &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} V(\vec{k}) \\ V(\vec{k}) &= \int d^3\vec{r} e^{-i\vec{k}\cdot\vec{r}} V(\vec{r}) \end{aligned} \right\} \text{etc.}$$

The dielectric function  $\epsilon(\vec{k})$  is then defined by

$$V^{\text{tot}}(\vec{k}) = \frac{V(\vec{k})}{\epsilon(\vec{k})}$$

[ In your EM course you probably saw the dielectric constant  $\epsilon$ , defined by  $D = \epsilon E$ . Here we generalize this to spatially varying situations by defining  $\epsilon(\vec{k})$ . The limit  $\epsilon(k \rightarrow 0)$  is the uniform dielectric constant you saw in EM.

Recall  $D$  is the field produced by the "free" charge, i.e. the charge external to the material itself, while  $E$  includes the fields due to the polarized charges that make up the material.

Hence  $\vec{E} = -\vec{\nabla} V^{\text{tot}}$ , while  $\vec{D} = -\vec{\nabla} V$  the applied potential ]

$$\text{Now } -\nabla^2 \delta V = 4\pi \delta \rho$$

$$\Rightarrow k^2 \delta V(\vec{k}) = 4\pi \delta \rho(\vec{k})$$

$$\delta V(\vec{k}) = \frac{4\pi}{k^2} \delta \rho(\vec{k})$$

$$V^{\text{tot}}(\vec{k}) = V(\vec{k}) + \delta V(\vec{k}) = V(\vec{k}) + \frac{4\pi}{k^2} \delta \rho(\vec{k})$$

$$\text{so } V(\vec{k}) = V^{\text{tot}}(\vec{k}) - \frac{4\pi}{k^2} \delta \rho(\vec{k})$$

$$\frac{V(\vec{k})}{V^{\text{tot}}(\vec{k})} = \varepsilon(\vec{k}) = 1 - \frac{4\pi}{k^2} \frac{\delta \rho(\vec{k})}{V^{\text{tot}}(\vec{k})}$$

We now need to find what is the  $\delta \rho$  that is induced in the presence of a  $V^{\text{tot}}$ .

(Note: the electrons see not just the applied potential  $V$ , but also the induced potential  $\delta V$ . Hence, when considering the behavior of an isolated electron, it sees the total potential  $V^{\text{tot}} = V + \delta V$ , where  $\delta V$  describes the interaction of the electron under consideration with all the other electrons. This is an example of a mean field approximation — we will approximate the interaction of an electron with all other electrons via the average electrostatic potential  $\delta V$  created by the other electrons.)



To compute  $sp$  we assume  $V(\vec{r})$  is slowly varying so that the system is in local equilibrium at every position  $\vec{r}$ . This approx is good for getting the small  $\hbar$  limit of  $\epsilon(\hbar)$ .

Then the probability to have an electron with wave vector  $\hbar$  at position  $\vec{r}$  is given by the Fermi function

$$f(\hbar, \vec{r}) = \frac{1}{e^{(\epsilon_{\hbar} - eV^{tot}(\vec{r}) - \mu)/k_B T} + 1}$$

$$= f^0(\hbar; \mu + eV^{tot}(\vec{r}))$$

where  $f^0(\hbar; \mu) = \frac{1}{e^{(\epsilon_{\hbar} - \mu)/k_B T} + 1}$  is the equilibrium distribution when  $V=0$ .

So the effect of  $V^{tot}(\vec{r})$  can be viewed as if there is now a spatially varying chemical potential  $\mu + eV^{tot}(\vec{r})$  (this is sometimes called the electro-chemical potential)

Then

$$sp(\vec{r}) = -e \int \frac{d^3k}{4\pi^3} \left[ f^0(\hbar; \mu + eV^{tot}(\vec{r})) - f^0(\hbar; \mu) \right]$$

↑

includes factor

$\times 2$  for spin degeneracy

expand in small  $eV^{\text{tot}} \ll \mu \approx \epsilon_F$

$$\begin{aligned}\delta p(\vec{r}) &= -e \int \frac{d^3k}{4\pi^3} \frac{\partial f^0}{\partial \mu} eV^{\text{tot}}(\vec{r}) \\ &= -e^2 V^{\text{tot}}(\vec{r}) \frac{\partial}{\partial \mu} \int \frac{d^3k}{4\pi^3} f^0(\vec{k})\end{aligned}$$

$$= -e^2 V^{\text{tot}}(\vec{r}) \frac{\partial M}{\partial \mu}$$

equilibrium density  $n(\mu)$  as function of chemical pot  $\mu$ .

~~$\frac{\delta p(\vec{r})}{V^{\text{tot}}(\vec{r})}$~~

So also  $\delta p(\vec{k}) = -e^2 V^{\text{tot}}(\vec{k}) \frac{\partial M}{\partial \mu}$

$$\frac{\delta p(\vec{k})}{V^{\text{tot}}(\vec{k})} = -e^2 \left( \frac{\partial M}{\partial \mu} \right)$$

So dielectric function is

$$\epsilon(\vec{k}) = 1 - \frac{4\pi}{k^2} \frac{\delta p(\vec{k})}{V^{\text{tot}}(\vec{k})}$$

$$\epsilon(\vec{k}) = 1 + \frac{4\pi e^2}{k^2} \frac{\partial M}{\partial \mu}$$

This is called the Thomas-Fermi dielectric function, and it can be written in the form

$$\epsilon(\vec{k}) = 1 + k_0^2/k^2 \quad k_0^2 \equiv 4\pi e^2 \frac{\partial M}{\partial \mu}$$

where  $1/k_0$  is called the screening length

Before considering the physical consequences of  $\epsilon(\vec{k})$  as above, let's first compute  $k_0$ .

As  $T \rightarrow 0$ ,  $\mu \rightarrow \epsilon_F$  the Fermi energy. Now  $\epsilon_F$  is defined by

$$M = \int_0^{\epsilon_F} d\epsilon g(\epsilon) \Rightarrow \frac{\partial M}{\partial \epsilon_F} = g(\epsilon_F)$$

↑  
density of states

For a free electron gas,  $g(\epsilon_F) = \frac{3}{2} \frac{M}{\epsilon_F}$

$$\text{So } k_0^2 = 4\pi e^2 g(\epsilon_F) = \frac{6\pi e^2 M}{\epsilon_F}$$

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We can compare this to what one would get using classical Boltzmann statistics for the electrons, instead of the quantum Fermi-Dirac statistics. Then, the probability distribution for an electron with momentum  $\hbar\vec{k}$  would be

$$f(\vec{k}, \vec{r}) = C e^{-\frac{(\epsilon_k - eV^{\text{tot}}(\vec{r}))}{k_B T}}$$

↑  
normalization constant

expand for small  $eV^{\text{tot}}$

$$f(\vec{k}, \vec{r}) \approx c e^{-\epsilon_k/k_B T} \left[ 1 + \frac{eV^{\text{tot}}(\vec{r})}{k_B T} \right]$$
$$= f^0(k) \left[ 1 + \frac{eV^{\text{tot}}(\vec{r})}{k_B T} \right]$$

$$S_f(\vec{r}) = -e \int \frac{d^3k}{4\pi^3} \left[ f(\vec{k}, \vec{r}) - f^0(k) \right]$$
$$= -e \int \frac{d^3k}{4\pi^3} f^0(k) \frac{eV^{\text{tot}}(\vec{r})}{k_B T}$$
$$= -e^2 V^{\text{tot}}(\vec{r}) \frac{m}{k_B T}$$

So  $\frac{S_f(\vec{r})}{V^{\text{tot}}(\vec{r})} = -\frac{e^2 m}{k_B T}$  which gives

$$\epsilon(\vec{k}) = 1 - \frac{4\pi}{k^2} \frac{S_f(\vec{k})}{V^{\text{tot}}(\vec{k})} = 1 + \frac{4\pi e^2 m}{k^2 k_B T}$$

This is known as the Debye-Hückel dielectric function - it applies to a liquid or gas of charged particles obeying classical statistics (for example is  $T \gg T_F$ ). It has the same function form as the Thomas-Fermi dielectric function, but now with

$$k_0^2 = \frac{4\pi e^2 m}{k_B T}$$

So to compare Thomas - Fermi with classical Debye - Hückel

$$\frac{k_0^{TF}}{k_0^{DH}} = \left( \frac{6\pi e^2 m}{k_B T_F} \frac{k_B T}{4\pi e^2 m} \right)^{1/2} = \left( \frac{3}{2} \left( \frac{T}{T_F} \right) \right)^{1/2} \ll 1 \Rightarrow k_0^{TF} \ll k_0^{DH}$$

so Debye Hückel screening length  $\frac{1}{k_0^{DH}} \ll \frac{1}{k_0^{TF}}$  Thomas-Fermi screening length, for the same density  $n$ .

Back to Thomas - Fermi

$$k_0^2 = \frac{6\pi e^2 m}{E_F} \quad \text{using } m = \frac{k_F^3}{3\pi^2}, \quad E_F = \frac{\hbar^2 k_F^2}{2m}$$

$$\Rightarrow k_0^2 = \frac{4me^2}{\pi\hbar^2} k_F \quad \text{using Bohr radius } a_0 = \frac{\hbar^2}{me^2}$$

$$\Rightarrow k_0^2 = \frac{4}{\pi} k_F / a_0 \quad \text{using } \frac{4}{3}\pi r_s^3 = \frac{1}{n}$$

$$k_F = \left( \frac{9\pi}{4} \right)^{1/3} \frac{1}{r_s}$$

$$\Rightarrow k_0 = \sqrt{\frac{4}{\pi} \left( \frac{9\pi}{4} \right)^{1/3}} \frac{1}{\sqrt{r_s a_0}}$$

$$\frac{1.56}{\sqrt{r_s a_0}} = 1.56$$

$$\frac{1}{a_0 k_0} = \left( \frac{1}{1.56 \sqrt{r_s}} \right) \sqrt{a_0} \sim \frac{1}{\sqrt{r_s}} \quad \text{since } r_s \sim 3a_0 \text{ for most metals}$$

$$\Rightarrow \frac{1}{k_0} \sim a_0 \sim 0.5 \text{ \AA} \quad \text{screening length very small!}$$

## Thomas-Fermi dielectric function

$$\epsilon(k) = 1 + k_0^2/k^2, \quad \text{with } 1/k_0 \sim \text{\AA}$$

One consequence of this form is something you have already learned in your EM class.

If we take the limit  $k \rightarrow 0$ , then  $\epsilon \rightarrow \infty$ .

So a uniform electric field applied to a metal is completely screened out!  $E^{\text{tot}} = \frac{E}{\epsilon} \rightarrow 0$ .

In practice, provided the applied  $E$  field is slowly varying on the length scale  $1/k_0 \sim \text{\AA}$ , it is still screened out because  $\epsilon$  is so large for  $k \ll k_0$ . This is what you learned in EM

- there can be no static macroscopic electric field inside a metal.

Another extremely important consequence of the T-F dielectric function is seen if we consider the effect on a point charge  $Q$  placed in the electron gas.

The "applied" potential ~~of the~~ from the point charge is just the bare Coulomb potential

$$V(\vec{r}) = \frac{Q}{r}$$

The Fourier transform of the Coulomb potential is

$$V(\vec{k}) = \frac{4\pi Q}{k^2}$$

$$\begin{aligned}\Rightarrow V^{\text{tot}}(\vec{k}) &= \frac{V(\vec{k})}{\epsilon(\vec{k})} = \frac{4\pi Q}{k^2} \frac{1}{1 + k_0^2/k^2} \\ &= \frac{4\pi Q}{k_0^2 + k^2}\end{aligned}$$

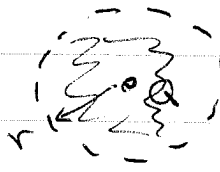
whereas  $V(\vec{k}) \rightarrow \infty$  as  $k \rightarrow 0$ , indicating a long ranged interaction,  $V^{\text{tot}}(\vec{k}) \rightarrow \text{const}$  as  $k \rightarrow 0$ , indicating a short ranged interaction.

If we Fourier transform  $V^{\text{tot}}(\vec{k})$  back to real space we get the interaction

$$V^{\text{tot}}(\vec{r}) = \frac{Qe^{-k_0 r}}{r} \quad \text{called the "Yukawa potential" or the "screened Coulomb potential"}$$

The effect of the dielectric function due to the free electrons is to "screen" the long range Coulomb-potential so it looks short ranged with an interaction length  $= 1/k_0$ . On length scales  $r \gg 1/k_0$ , the effect of the charge  $Q$  is entirely negligible. We say that the electrons have screened out the charge  $Q$ .

Physically, what is going on is as follows:



electrons get attracted to charge  $Q$  and so the average electron density about  $Q$  increases above average. This cloud of electron charge at  $Q$  "screens" the charge  $Q$ . If one computes the total charge (i.e.  $Q$  + induced electron charge) in a sphere of radius  $r$  centered on  $Q$ , this total charge decreases to zero as  $r \rightarrow \infty$ . Decay of this total charge is on length scale  $1/k_0$ .

Compare this to behavior in a "dielectric" (i.e. an insulator) from EM class. If you put a point charge  $Q$  in a dielectric, it polarizes the material creating bound charges at  $Q$  so that the total charge at  $Q$  becomes  $Q^{tot} = Q + Q_{bound} = Q/\epsilon$ , where  $\epsilon$  is the finite "dielectric constant". A metal is like a dielectric with an infinite dielectric constant so that  $Q/\epsilon \rightarrow 0$ ! (any free charge in a metal must lie on its surface!). The dependence of  $\epsilon$  on wavevector  $k$ , describes how the metal screens charges on finite length scales - so  $Q/\epsilon \rightarrow 0$  is really just a statement about the  $r \rightarrow \infty$ , or  $k \rightarrow 0$  limit, of the metal.



This behavior due to  $\epsilon(k)$  explains why it is not necessarily such a bad approximation that we have ignored electron-ion interactions and electron-electron interactions. Instead of these being strong long ranged Coulomb interactions, the screening by  $\epsilon(\vec{k})$  converts them into very short ranged interactions - interaction range is  $1/k_0 \sim \text{\AA}$ .

When we later consider the effect of the periodic potential of the ions on the electrons, we will see that in many cases we can describe its effect as a weak perturbation on plane wave electron eigenstates. That the electron-ion interaction can be treated as a weak perturbation is due to the screening of the ion potential by  $\epsilon(\vec{k})$ .

When we think about the electron-electron interaction between a given pair of electrons, we can similarly think of this as being screened by all the other electrons. Hence it too is short ranged and not as important as one might naively have expected. There is one complication that arises when one thinks

about the screening of <sup>the</sup> electron-electron interaction, since all electrons are identical, we cannot really distinguish between a given pair of interacting electrons and the other electrons that are screening this interaction. But despite this complication, the idea that  $\epsilon(\vec{k})$  ~~screen~~ screens the e-e interaction and makes it short ranged, remains essentially correct. See Ashcroft + Mermin Chpt 17 or Kittel chpt 14 for further discussion.

But another serious problem with the Thomas-Fermi model is that it gives a screening length  $\lambda_{TF} \sim \text{\AA}$ , but it is based on the assumption that the fields vary slowly. We have no reason to trust its conclusions down to such small atomic scales.

To get a better approximation that holds at larger  $\vec{k}$  than the T-F model, we now turn to the Lindhard calculation for the dielectric function  $\epsilon(\vec{k})$ .