

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 ~~charge~~ electron density as

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

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

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

charge density.

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

$$-\nabla^2 \delta V = 4\pi \delta \rho$$

Poisson's eqn for electrostatics

So the total potential is then

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

Consider this in Fourier transform space

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

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

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

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

[In your EM course you probably saw the dielectric constant ϵ , 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 $\vec{E} = -\vec{\nabla} V^{tot}$, while $\vec{D} = -\vec{\nabla} V$ the applied potential]

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

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

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

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

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

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

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

(Note: the electrons see not just the applied potential V , but also the induced potential δV . Hence, when considering the behavior of an isolated electron, it sees the total potential $V^{\text{tot}} = V + \delta V$, where δV 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 δV 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 $\vec{k}$ at position $\vec{r}$ is given by the Fermi function

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

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

where $f^0(\vec{k}; \mu) = \frac{1}{e^{(\epsilon_{\vec{k}} - \mu)/k_B T} + 1}$ 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

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

↑
includes factor
x2 for spin degeneracy

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

$$\begin{aligned}\delta p(\vec{r}) &= -e \int \frac{d^3k}{4\pi^3} \frac{\partial f^0}{\partial \mu} eV^{tot}(\vec{r}) \\ &= -e^2 V^{tot}(\vec{r}) \frac{\partial}{\partial \mu} \underbrace{\int \frac{d^3k}{4\pi^3} f^0(\vec{k})}_{\text{equilibrium density } n(\mu) \text{ as function of chemical pot } \mu.}\end{aligned}$$

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

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

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

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

So dielectric function is

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

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

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

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

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 ϵ_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, $g(\epsilon_F) = \frac{3}{2} \frac{M}{\epsilon_F}$

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

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

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

↑
normalization constant

expand for small eV^{tot}

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

$$\begin{aligned} \delta\rho(\vec{r}) &= -e \int \frac{d^3k}{4\pi^3} [f(\vec{k}, \vec{r}) - f^0(k)] \\ &= -e \int \frac{d^3k}{4\pi^3} f^0(k) \frac{eV^{\text{tot}}(\vec{r})}{k_B T} \\ &= -e^2 V^{\text{tot}}(\vec{r}) \frac{n}{k_B T} \end{aligned}$$

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

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

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

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

So to compare Thomas - Fermi with classical Debye - Hückle

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

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

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

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

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

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

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

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

$$\frac{1}{a_0 k_0} = \frac{1}{1.56} \sqrt{\frac{r_s}{a_0}}$$

$r_s \sim 3a_0$ 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! $E_{tot} = \frac{E}{\epsilon} \rightarrow 0$.

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 ϵ 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

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

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

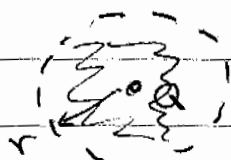
whereas $V(\vec{k}) \rightarrow \infty$ as $k \rightarrow 0$, indicating a long ranged interaction, $V^{\text{tot}}(\vec{k}) \rightarrow \text{const}$ as $k \rightarrow \infty$, indicating a short ranged interaction.

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 $Q + Q_{\text{bound}} = Q/\epsilon$, where ϵ 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 ϵ 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 $\epsilon(k)$ 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 $\epsilon(k)$.

As 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 ^{the} 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 $\epsilon(k)$ ~~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.