To compute $\delta\rho$ 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 $\vec{k}$ limit of $\varepsilon(\vec{k})$.

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

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

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

where $f^0(\vec{k};\mu) = \dfrac{1}{e^{(\varepsilon_k-\mu)/k_BT}+1}$ 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

$$\delta\rho(\vec{r}) = -e\int \underbrace{\frac{d^3k}{4\pi^3}}_{\text{includes factor } \times 2 \text{ for spin degeneracy}} \left[f^0(\vec{k};\ \mu + eV^{tot}(\vec{r})) - f^0(\vec{k};\mu) \right]$$

expand in small $eV^{tot} \ll \mu \simeq \varepsilon_F$

$$\delta\rho(\vec r) = -e \int \frac{d^3k}{4\pi^3} \frac{\partial f^0}{\partial \mu} eV^{tot}(\vec r)$$

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

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

~~So~~ $\cancel{\dfrac{\delta\rho(\vec k)}{V^{tot}}}$

So also $\delta\rho(\vec k) = -e^2 V^{tot}(\vec k) \dfrac{\partial n}{\partial\mu}$

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

So dielectric function is

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

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

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

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

where $1/k_0$ is called the <u>screening length</u>

Before considering the physical consequences of $\varepsilon(\vec{k})$ as above, lets first compute k_0

As $T \to 0$, $\mu \to \varepsilon_F$ the Fermi energy. Now ε_F is defined by

$$n = \int_0^{\varepsilon_F} d\varepsilon \, \underbrace{g(\varepsilon)}_{\text{density of states}} \quad \Rightarrow \quad \frac{\partial n}{\partial \varepsilon_F} = g(\varepsilon_F)$$

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

So $k_0^2 = 4\pi e^2 g(\varepsilon_F) = \frac{6\pi e^2 n}{\varepsilon_F}$

We can compare this to what one would get using classical Boltzman 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

$$f(\vec{k},\vec{r}) = \underbrace{C}_{\text{normalization constant}} e^{-(\varepsilon_k - eV^{tot}(\vec{r}))/k_B T}$$

expand for small eV^{tot}

$$f(\vec{k},\vec{r}) \simeq C e^{-\varepsilon_k/k_BT}\left[1+\frac{eV^{tot}(\vec{r})}{k_BT}\right]$$

$$= f^0(k)\left[1+\frac{eV^{tot}(\vec{r})}{k_BT}\right]$$

$$\delta\rho(\vec{r}) = -e\int\frac{d^3k}{4\pi^3}\left[f(\vec{k},\vec{r})-f^0(\vec{k})\right]$$

$$= -e\int\frac{d^3k}{4\pi^3} f^0(k)\,\frac{eV^{tot}(\vec{r})}{k_BT}$$

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

So $\dfrac{\delta\rho(\vec{k})}{V^{tot}(\vec{k})} = -\dfrac{e^2 n}{k_BT}$ which gives

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

This is known as the Debye-Huckle 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

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

So to compare Thomas - Fermi with classical Debye - Huckle

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

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

Back to Thomas - Fermi

$$k_0^2 = \frac{6\pi e^2 n}{\varepsilon_F} \qquad \text{using } n = \frac{k_F^3}{3\pi^2}, \ \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

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

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

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

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

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

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

$r_s \sim 3a_0$ for most metals

$$\Rightarrow \frac{1}{k_0} \sim a_0 \sim .5\,\text{Å}$$

sreeing length very small!

Thomas-Fermi dielectric function

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

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

If we take the limit $k \to 0$, then $\varepsilon \to \infty$. So a uniform electric field applied to a metal is completely screened out! $E^{tot} = \frac{E}{\varepsilon} \to 0$. In practice, provided the applied E field is slowly varying on the length scale $1/k_0 \sim$ Å, 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

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

$$\Rightarrow \quad V^{tot}(\vec{k}) = \frac{V(\vec{k})}{\varepsilon(\vec{k})} = \frac{4\pi Q}{k^2} \frac{1}{1 + k_0^2/k^2}$$

$$= \frac{4\pi Q}{k_0^2 + k^2}$$

whereas $V(\vec{k}) \to \infty$ as $k \to 0$, indicating a <u>long</u> ranged interaction, $V^{tot}(\vec{k}) \to$ const as $k \to \infty$, indicating a short ranged interaction.

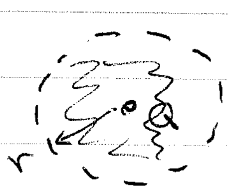
If we Fourier transform $V^{tot}(\vec{k})$ back to real space we get the interaction

$$V^{tot}(\vec{r}) = \frac{Q e^{-k_0 r}}{r}$$

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 (ie Q + induced electron charge) in a sphere of radius r centered on Q, this total charge decreases to zero as $r \to \infty$. Decay of this total charge is on length scale $1/k_0$.

Compare this to behavior in a "dielectric" (ie 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 $Q + Q_{bound} = Q/\varepsilon$, where ε is the finite "dielectric constant". A metal is like a dielectric with an infinite dielectric constant so that $Q/\varepsilon \to 0$! (any free charge in a metal must lie on its surface!). The dependence of ε on wavevector $\vec{k}$, describes how the metal screens charges on finite length scales - so $Q/\varepsilon \to 0$ is really just a statement about the $r \to \infty$, or $k \to 0$ limit of the metal.

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 $\varepsilon(k)$ ~~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.