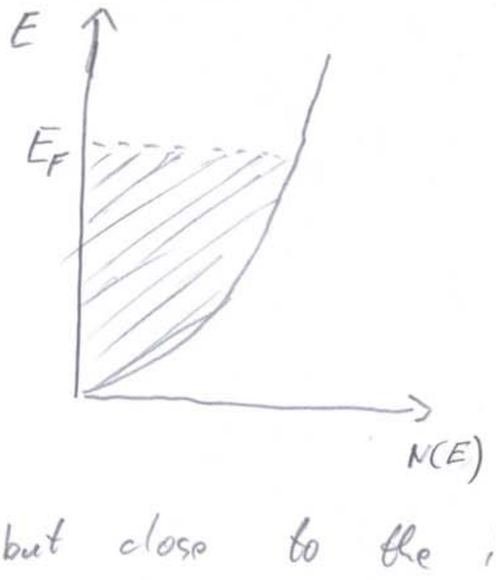
Screening

How does the electron gas react if we place a charged impurity in it?

The electrons are mobile and charged and will tend to cluster around the impurity if it is positively charged or will be repelled, if the impurity is negatively charged.

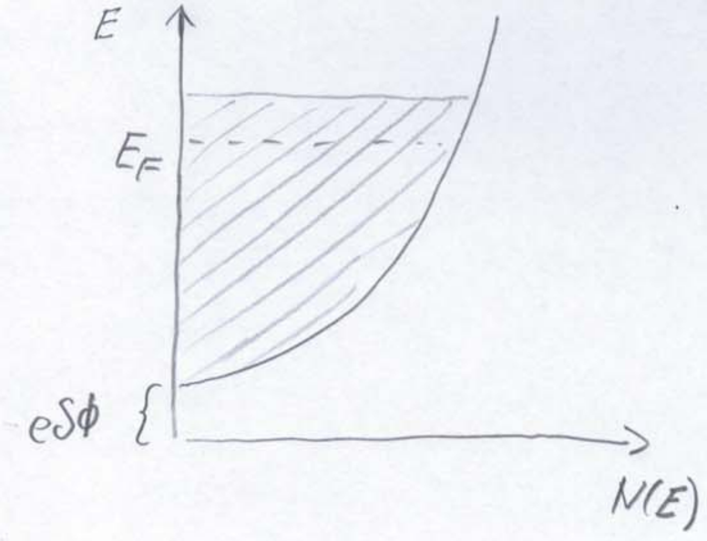
In addition, Fermi statistics leads to long-range oscillations of the electron charge density far from the impurity.

Sufficiently far away from the localized charge (impurity) we have



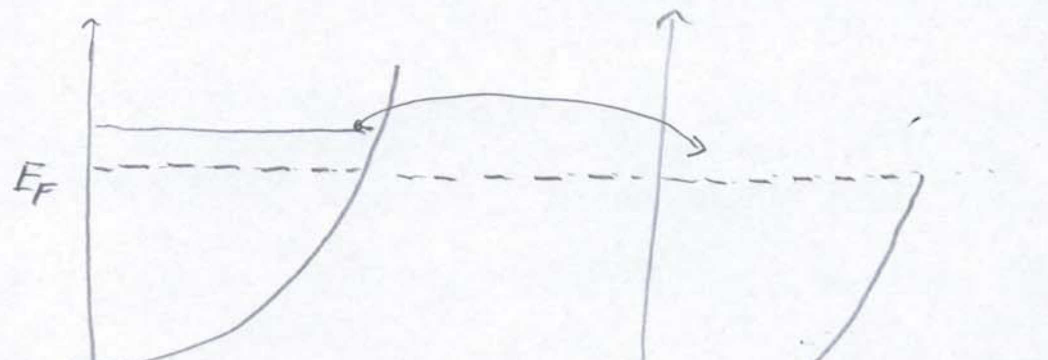
but close to the impurity, the electrons see the potential associated with the charged impurity

Therefore:



where $\delta\phi$ is the impurity potential.

As a result, the electrons redistribute to ensure a global Fermi energy (compare this to what you learned about the chemical potential in equilibrium)



near impurity:

$-e\delta\phi(\vec{r}) \neq 0$

far away from impurity:

$-e\delta\phi(\vec{r}) = 0$

near the impurity, the electronic number density is

$$n(r) \approx \int_{-e\delta\phi(r)}^{E_F} dE\, N(E + e\delta\phi(r)) = \int_0^{E_F + e\delta\phi(r)} dE\, \underbrace{N(E)}_{\text{density of states}}$$

and we assumed $T = 0$.

In first approximation, we therefore have for the change in particle density

$$\delta n(r) = \int_0^{E_F + e\delta\phi} dE\; N(E) - \int_0^{E_F} dE\, N(E) = \int_{E_F}^{E_F + e\delta\phi} dE\, N(E)$$

and if $e\delta\phi \ll E_F$ we can estimate that

$$\delta n(r) \approx N(E_F) \cdot (e\delta\phi) = +e\delta\phi \underbrace{N_0}_{\substack{\text{density of states} \\ \text{at } E = E_F}}$$

To determine the change in electrostatic potential $\delta\phi(r)$ from the change in charge density, we use Poisson's equation:

$$\nabla^2 \delta\phi = -4\pi\,\delta\rho = 4\pi e\,\delta n = 4\pi e^2 N_0\, \delta\phi$$

In a spherical system,

$$\nabla^2 \delta\phi = r^{-2}\partial_r r^2 \partial_r \delta\phi = 4\pi e^2 N_0\, \delta\phi$$

This equation has the solution

$$\delta\phi(r) = C\,\frac{e^{-k_{TF}\cdot r}}{r}$$

where $k_{TF} = \sqrt{4\pi e^2 N_0}$ and k_{TF}^{-1} has dimensions of length. It is called <u>Thomas-Fermi screening length</u>

→ The impurity is screened exponentially fast with distance from it.

To repeat our somewhat hand waving arguments in a more rigorous fashion, we start by recalling, that the central quantity of electrodynamics, that describes the response of a material to an electric field $\vec{E}$ and is responsible for the difference between $\vec{D}$ and $\vec{E}$ field, is the dielectric constant $\varepsilon(q)$
In electrodynamics, this quantity (in general, a tensor) was introduced phenomenologically.
Here, we will try to calculate it (in some approximation) from a microscopic model

(67)

We need to distinguish external and induced charge and external and induced electostatic potential.

$\phi(\vec{q})$: Fourier transform of total potential

$\phi^{ext}(\vec{q})$: — " — external potential

$\rho^{ext}(\vec{q})$: — " — external charge density

$\rho^{ind}(\vec{q})$: — " — induced charge density

$\rho(\vec{q})$: — " — total charge density

We have:
$$\phi^{ext}(\vec{q}) = \varepsilon(\vec{q})\,\phi(\vec{q})$$

$$\left.\begin{aligned} q^2\phi^{ext}(\vec{q}) &= 4\pi\rho^{ext}(\vec{q}) \\ q^2\phi(\vec{q}) &= 4\pi\rho(\vec{q}) \end{aligned}\right\}\ \text{Poisson equations}$$

$$\rho^{ind}(\vec{q}) = \rho(\vec{q}) - \rho^{ext}(\vec{q}) = \underbrace{\chi(\vec{q})}_{\text{charge susceptibility}}\phi(\vec{q})$$

This implies
$$\phi^{ext}(\vec{q}) = \phi(\vec{q}) - \frac{4\pi}{q^2}\rho^{ind}(\vec{q}) = \phi(\vec{q}) - \frac{4\pi}{q^2}\chi(\vec{q})\phi(\vec{q})$$

or $\phi^{ext}(\vec{q}) = \left(1 - \frac{4\pi}{q^2}\chi(\vec{q})\right)\phi(\vec{q})$

$$\rightarrow \quad \boxed{\varepsilon(q) = 1 - \frac{4\pi}{q^2}\,\frac{\rho^{ind}(\vec{q})}{\phi(\vec{q})}}$$

Thomas - Fermi theory of screening

We already saw the basic idea of Thomas and Fermi
we want to calculate the induced charge density
due to an electrostatic potential $\phi(\vec{r})$. Here, $\phi(\vec{r})$
denotes the full potential including the changes
generated by the charge redistribution.

→ selfconsistency problem

We will consider the effect of the electron - electron
interaction on the electrostatic potential only on
the level of the Hartree approximation.

At the single particle level, we have

$$-\frac{\hbar^2}{2m}\nabla^2 \psi_i(\vec{r}) - e\,\phi(\vec{r})\,\psi_i(\vec{r}) = \varepsilon_i \psi_i(\vec{r})$$

We will have to assume that $\phi(\vec{r})$ is a spatially
slowly changing potential so that we can think of the
system as being composed of subsystems, such that
$\phi(\vec{r})$ is constant for each subsystem.
But these subsystems should be big enough so that we can
use the results and relations from
equilibrium statistical mechanics.

→ in each subsystem we have a free electron gas with slightly different, constant potential and thus changing average particle number

→ local Fermi distribution

$$n(\vec{r}) = \int \frac{d^3k}{4\pi^3} \frac{1}{\exp[\beta(\frac{\hbar^2k^2}{2m} - e\phi(\vec{r}) - \mu)] + 1}$$

or $n(\vec{r}) = n_0(\mu + e\phi(\vec{r}))$ and we have

$$\rho^{ind}(\vec{r}) = -e\left(n_0(\mu + e\phi(\vec{r})) - n_0(\mu)\right)$$

The charge susceptibility $\chi(\vec{q})$ was defined through

$$\rho^{ind}(\vec{q}) = \chi(\vec{q})\,\phi(\vec{q})$$

so that we have for a weak potential ($e\phi \ll \mu$):

$$\chi(\vec{q}) = -e^2 \frac{\partial n_0}{\partial \mu}$$

and we obtain for the static dielectric constant in Thomas-Fermi approximation

$$\varepsilon(q) = 1 + \frac{4e^2}{q^2} \frac{\partial n_0}{\partial \mu} = 1 + \frac{k_{TF}^2}{q^2}$$

where the Thomas-Fermi wavenumber k_{TF} is

$$k_{TF}^2 = 4\pi e^2 \frac{\partial n_0}{\partial \mu}$$

Let us consider the screening of a point charge:

$$\phi^{ext}(r) = \frac{Q}{r} \rightsquigarrow \phi^{ext}(\vec{q}) = \frac{4\pi Q}{q^2}$$

we then have

$$\phi(\vec{q}) = \frac{1}{\varepsilon(\vec{q})}\,\phi^{ext}(\vec{q}) = \frac{4\pi Q}{q^2 + k_{TF}^2}$$

and Fourier transforming this expression, we have

$$\phi(\vec{r}) = \frac{Q}{r}\, e^{-k_{TF} r}$$

(we already did this Fourier transform when calculating the Fourier transform of the Coulomb potential)

$\rightsquigarrow$ at short distances the potential appears as an ordinary Coulomb potential but for large distances, the potential vanishes exponentially

$\frac{1}{k_{TF}}$ is the characteristic length scale for this change in behavior

The weakest point in our treatment is the use of the equilibrium distribution function.
One way to improve the treatment is to treat the linearized potential in perturbation theory.

Lindhard theory of screening

In lowest order perturbation theory, we have for a perturbation $H_1 = -e\phi(\vec{r})$

$$|\psi_k\rangle = |\psi_k^0\rangle + \sum_{k\neq k'} \frac{|\psi_{k'}^0\rangle\langle\psi_{k'}^0|H_1|\psi_k^0\rangle}{\varepsilon_k - \varepsilon_{k'}}$$

For the homogeneous electron gas, $|\psi_k^0\rangle$ are plane waves and we therefore have

$$\langle\psi_{k'}^0|H_1|\psi_k^0\rangle = -\frac{e}{V}\int d^3r\, e^{i(\vec{k}-\vec{k}')\vec{r}}\phi(\vec{r}) = -e\,\phi(\vec{q})$$

where $\vec{q} = \vec{k} - \vec{k}'$.

For the particle density at position $\vec{r}$ we find

$$n(\vec{r}) = \underset{\text{spin}}{2} \sum_{\vec{k}} f_{\vec{k}} |\psi_k(\vec{r})|^2$$

as $k' = \vec{k} - \vec{q} \rightsquigarrow \varepsilon_k - \varepsilon_{k'} = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2(k-q)^2}{2m} = \hbar^2\left(\frac{\vec{k}\cdot\vec{q}}{m} - \frac{q^2}{2m}\right)$

and since we only keep terms linear in ϕ:

$$\langle\psi|\psi\rangle \doteq \langle\psi_0|\psi_0\rangle + \langle\psi_0|\psi_1\rangle + \langle\psi_1|\psi_0\rangle$$

$$n(r) = 2\sum_k f_k |\psi_k^0(\vec{r})|^2 + 2\frac{e}{V}\sum_{k,q} f_k\, \phi(q)\, \frac{e^{i\vec{k}\vec{r}}e^{-i(\vec{k}-\vec{q})\vec{r}} + e^{-i\vec{k}\vec{r}}e^{i(\vec{k}-\vec{q})\cdot\vec{r}}}{\hbar^2\left(\frac{\vec{k}\cdot\vec{q}}{m} - \frac{q^2}{2m}\right)}$$

(72)

The charge density in absence of the external potential is $2\sum_k f_k |\psi_k^0(\vec{r})|^2$

so that the induced charge density is

$$\rho^{ind}(\vec{r}) = \frac{2e^2}{V}\sum_{\vec{q}} e^{i\vec{q}\vec{r}} \sum_{\vec{k}} f_k \left(\frac{1}{\hbar^2\left(\frac{\vec{k}\vec{q}}{m} - \frac{q^2}{2m}\right)} - \frac{1}{\hbar^2\left(\frac{\vec{k}\vec{q}}{m} + \frac{q^2}{2m}\right)} \right) \phi(\vec{q})$$

as $\phi(r)$ is real and we assume $\phi(\vec{r}) = \phi(-\vec{r})$

$$\rightarrow \rho^{ind}(\vec{r}) = \frac{2e^2}{V}\sum_{q} e^{i\vec{q}\vec{r}} \phi(\vec{q}) \sum_{k} \frac{f_{k+\frac{q}{2}} - f_{k-\frac{q}{2}}}{\hbar^2 \vec{k}\vec{q}/m}$$

and therefore

$$\rho^{ind}(\vec{q}) = \frac{2e^2}{V}\sum_{k} \frac{f_{k+q/2} - f_{k-q/2}}{\hbar^2 \vec{k}\cdot\vec{q}/m} \phi(q)$$

so that

$$\chi(q) = \frac{2e}{V}\sum_{k} \frac{f_{k+\frac{q}{2}} - f_{k-q/2}}{\hbar^2 \vec{k}\cdot\vec{q}/m}$$

$$= e^2 \int \frac{d^3k}{4\pi^3} \frac{f_{k+\frac{q}{2}} - f_{k-\frac{q}{2}}}{\hbar^2 \vec{k}\cdot\vec{q}/m}$$

This is the static Lindhard susceptibility

(73)

For small q, we can expand the Fermi functions as

$$f_{k\pm q/2} = \frac{1}{\exp\left[\beta\left(\frac{\hbar^2(k\pm q/2)^2}{2m}-\mu\right)\right]+1}$$

$$= f_k \mp \frac{\hbar^2 \vec{k}\cdot\vec{q}}{2m}\frac{\partial f_k}{\partial \mu}$$

In this limit, $\chi(q)$ becomes q-independent and is equal to the Thomas-Fermi approximation.
This reflects the assumption entering Thomas-Fermi that the potential is only weakly q-dependent.

Within the Lindhard approximation we have

$$\varepsilon(\vec{q}) = 1 - \frac{4\pi}{q^2}\chi(\vec{q}) = 1 - \frac{e^2 m}{\hbar^2\pi^2 q^2}\int d^3k\,\frac{f_{k+q/2}-f_{k-q/2}}{kq}$$

Evidently, $\varepsilon(\vec{q}) = \varepsilon(-\vec{q})$ and therefore

$$\varepsilon(\vec{q}) = 1 + \frac{4e^2 m}{\pi^2\hbar^2 q^2}\int d^3k\,\frac{f(\varepsilon_k)}{q^2+2kq}$$

by making the substitutions $k \to k \pm \frac{q}{2}$ in the integrals

74

Rewriting the integral in terms of spherical coordinates:

$$\varepsilon(\vec{q}) = 1 + \frac{4e^2 m}{\pi^2 \hbar^2 q^2} 2\pi \int_0^{k_F} dk\, k^2 \int_{-1}^{+1} \frac{du}{q^2 + 2kqu}$$

where we assumed $T=0$.

After performing the integrals, we finally have

$$\varepsilon(q) = 1 + \frac{m k_F e^2}{\pi \hbar^2 q^2} F\left(\frac{q}{2k_F}\right)$$ where the

Lindhard function

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

was already introduced in our discussion of the Hartree-Fock approximation.

In the limit $\frac{q}{2k_F} \ll 1$ we recover the Thomas-Fermi result.

$$\varepsilon(q) \to 1 + \frac{4 m k_F e^2}{\pi \hbar^2 q^2} = 1 + \frac{k_{TF}^2}{q^2}$$

For $q \to 0$, the dielectric constant diverges.

A long-wavelength potential will be completely screened as $\frac{V_q}{\varepsilon(q)} \to 0$

(75)

For large x, we have

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

$$= 2 + \frac{1-x^2}{x} \ln\left|\frac{1+\frac{1}{x}}{1-\frac{1}{x}}\right| \quad \text{and using that}$$

$$\ln\left(1+\frac{1}{x}\right) \sim \frac{1}{x} - \frac{1}{2x^2} \quad \text{and} \quad \ln\left(1-\frac{1}{x}\right) \sim -\frac{1}{x} - \frac{1}{2x^2}$$

so that

$$F(x \to \infty) \sim \frac{2x^2}{x^2} + \frac{1-x^2}{x} \cdot \frac{2}{x} \sim \frac{2}{x^2}$$

and the susceptibility vanishes as $\frac{1}{q^2}$. The deviation of the electric constant $\varepsilon(q)$ behave as

$$\sim \frac{1}{q^4}$$

$\rightsquigarrow$ short-wave-length potentials with $q \gg 2k_F$ are only screened weakly.

For $q \approx 2k_F$, one finds

$$\varepsilon(q) \approx 1 + \left(\frac{k_{TF}}{2k_F}\right)^2 \left[\frac{1}{2} + \frac{1}{2}\left(1 - \frac{q}{2k_F}\right) \ln \frac{2}{\left|1 - \frac{q}{2k_F}\right|}\right]$$

$\rightarrow$ "$2k_F$ singularity

(76)

What is the screened Coulomb potential of a point charge within the Lindhard approximation?

$$\varepsilon(q) = 1 + \frac{k_{TF}^2}{q^2} F\left(\frac{q}{2k_F}\right)$$

and $\phi(\vec{q}) = \frac{1}{\varepsilon(\vec{q})} \phi^{ext}(\vec{q})$

and therefore

$$\phi(r) = \int \frac{d^3q}{(2\pi)^3} \phi(q) e^{i\vec{q}\cdot\vec{r}} = \int \frac{d^3q}{(2\pi)^3} \frac{4\pi Q}{q^2+g^2(q)} e^{i\vec{q}\cdot\vec{r}}$$

where $g^2(q) = K_{TF}^2 F\left(\frac{q}{2k_F}\right)$

$$\rightsquigarrow \phi(r) = \frac{1}{(2\pi)^2} \int_0^\infty dq\, q^2 \phi(q) \int_{-1}^{+1} du\, e^{iqru} = \frac{1}{r} \frac{1}{2\pi^2} \int_0^\infty dq\, q\, \phi(q) \sin(qr)$$

$$= \frac{Q}{r} \frac{2}{\pi} \int_0^\infty dq \frac{q \sin(qr)}{q^2+g^2(q)}$$

$$\rightsquigarrow \underline{\phi(r) = C\,Q \frac{\cos(2k_F r)}{r^3}} \quad \text{with } C = \left(\frac{K_{TF}}{4k_F \varepsilon(2k_F)}\right)^2$$

Instead of the short-ranged Yukawa potential of the Thomas Fermi approximation, we now find a long-ranged, oscillating potential that falls off $\sim \frac{1}{r^3}$ for r large. The oscillations are called <u>Friedel oscillations</u>