Coulomb interaction in metals

Before we considered single electron spectrum. In calculation of the band structure only interaction with ion lattice was taken into account. But the electron electron interaction is as strong. It is also long range. In this lecture we will do the opposite — we will consider Coulomb interaction between the electrons neglecting effects of the band structure. This is rather good approximation for Alkali metals (Li, Na, K). For these materials conduction electrons are from s-orbitals. For half filled band Fermi surface is far away from the Brillouin zone boundaries so spherical approximation works well.

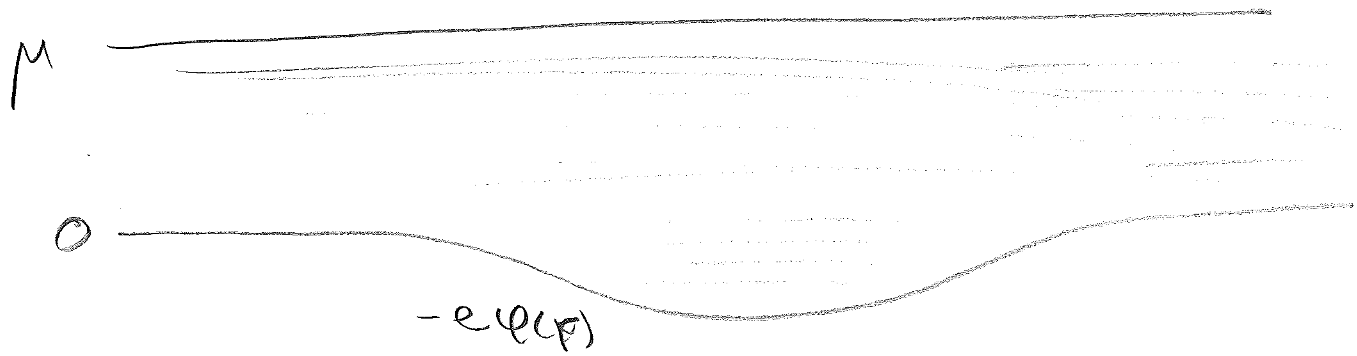
We also replace the ionic lattice by a homogeneous positively charged background. This is called the Jellium model

Screening – Thomas Fermi approximation

For slowly varying electric field we can define local chemical potential of the electron gas. This chemical potential is constant throughout the whole volume. In a region where electrostatic potential is absent

$$\mu = \varepsilon_F = \frac{\hbar^2}{2m}\left(3\pi^2 n_0\right)^{2/3},$$ where n_0 is electron density. If $\varphi(x) \neq 0$ then

$$\mu = \varepsilon_F(x) - e\varphi(x) = \text{const} = \frac{\hbar^2}{2m}\left(3\pi^2 n_0\right)^{2/3}$$



Assuming that the Fermi energy and density are everywhere related by the same formula we can rewrite

$$\mu = \varepsilon_F(n_0 + \delta n(r)) - e\varphi(r) = \varepsilon_F(n_0)$$

Or $\frac{d\mathcal{E}_F}{dn_0}\,\delta n(r) = e\varphi(r)$

with $\mathcal{E}_F \propto n_0^{2/3}$ $\quad \frac{d\mathcal{E}_F}{dn_0} = \frac{2}{3}\frac{\mathcal{E}_F}{n_0}$ and

$$\delta n(r) = \frac{3}{2} n_0 \frac{e\varphi(r)}{\mathcal{E}_F}$$

This change in density we should substitute to the Poisson equation

$$\nabla^2\varphi = -4\pi\left(-e\,\delta n(r) + \rho_{ind}(r)\right)$$

$$\nabla^2\varphi - \frac{6\pi e^2 n_0}{\mathcal{E}_F}\varphi = -4\pi\rho_{ind}$$

$$\nabla^2\varphi - \frac{\varphi}{\lambda_{TF}^2} = -4\pi\rho_{ind}$$

The Coulomb interaction is screened on the Thomas Fermi length λ_{TF}

$$\underline{\varphi = \frac{q e^{-\frac{r}{\lambda_{TF}}}}{r}}\ , \quad \lambda_{TF}^{-2} = \frac{6\pi n_0 e^2}{\mathcal{E}_F} = 4\pi e^2 N(\mathcal{E}_F)$$

Here q is the charge we insert, $\rho_{ind}(r) = q\delta^3(r)$

Substituting parameters and introducing the Bohr radius $a_0 = \frac{\hbar^2}{me^2} = 0{,}53\,\mathring{A}$ we obtain

$$\lambda_{TF}^2 = \frac{1}{4}\left(\frac{\pi}{3}\right)^{1/3} \frac{a_0}{n_0^{1/3}}$$

or $\lambda_{TF} \simeq \frac{r_0}{2}\left(\frac{a_0}{r_0}\right)^{1/2}$, where $r_0 = n_0^{-1/3}$ – inter electron distance. $\lambda_{TF} \simeq 0{,}55\,\mathring{A}$ for Cu

Coulomb interaction is screened at the distances comparable to interelectron distances!

Note that for classical electron gas replacing $\delta n(r) = n_0 \exp\left(-\frac{U(r)}{T}\right) - n_0 =$

$$= \frac{n_0 e \varphi(r)}{T}$$ and we

obtain Debye - Hückel screening with

$$\lambda_D^2 = \frac{T}{4\pi e^2 n_0}$$

Plasma frequency

The long wave dielectric response $\varepsilon(\omega, 0)$ of an electron gas can be obtained from the equation of motion of a free electron in an electric field

$$m\frac{d^2x}{dt^2} = -eE \quad \Rightarrow \quad x = \frac{eE}{m\omega^2}$$

The dipole moment of one electron is

$$-ex = -\frac{e^2E}{m\omega^2},$$

and the polarization

$$P = -nex = -\frac{ne^2}{m\omega^2}E$$

n is the electron concentration

Since $D = E + 4\pi P = \varepsilon E$ we obtain

$$\varepsilon = 1 - \frac{4\pi ne^2}{m\omega^2} = 1 - \frac{\omega_p^2}{\omega^2}$$

with plasma frequency $\omega_p^2 = \frac{4\pi ne^2}{m}$

The electromagnetic wave equation is

$$\nabla^2 E = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\varepsilon E = -\frac{\omega^2}{c^2}\varepsilon(\omega) E$$

Since $\varepsilon = 1 - \frac{\omega_p^2}{\omega^2}$

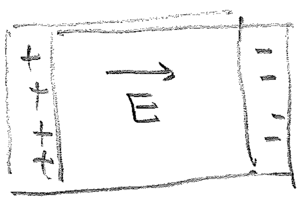
for $\omega < \omega_p$ $\quad \varepsilon < 0$

and we have decaying inside the sample solution $E \propto e^{-\frac{x}{\lambda}}$ solution $\Rightarrow$ wave is absorbed by the sample

for $\omega > \omega_p$ ($\sim$ 6–8 eV - ultraviolet)

$\varepsilon > 0$ and material is transparent for the wave.

At $\omega = \omega_p$ – <u>plasma resonance</u>



$$m\ddot{x} = -eE = -4\pi e^2 n x$$

Good discussion of it is at the very beginning of Ashkroft & Mermin textbook.

Linear response and the Lindhard function

Both screening and plasma oscillation can be described through the dielectric function $\varepsilon(q,\omega)$. Thomas Fermi screening corresponds to behavior $\varepsilon(q,0) = 1 + \frac{K_{TF}^2}{q^2}$,

Plasma mode $\varepsilon(0,\omega) = 1 - \frac{\omega_p^2}{\omega^2}$.

Now we are going to derive general expression for $\varepsilon(q,\omega)$

Consider position dependent weak external potential $V(r,t) = V(q,\omega)\, e^{i\vec{q}\vec{r} - i\omega t} e^{\eta t}$

where $\eta \to 0_+$ describes switching on the potential

Hamiltonian has the form

$$H = H_0 + H_V = \sum \varepsilon_k c^+_k c_k + \sum_r V(r)\, c^+(r)\, c(r)$$

or in Fourier space

$$H = \sum \varepsilon_k c_k^+ c_k + \sum_k V(q,\omega)\, c^+_{k+q} c_k$$

The density operator in momentum space is

$$\rho_{k,q} = c_k^+ c_{k+q}$$

In linear response equation of motion for $\rho_{k,q}(t)$ is

$$i\hbar \frac{d}{dt}\rho_{k,q} = [\rho_{k,q}, H] = [\rho_{k,q}, (H_0 + H_v)] =$$

$$= (\varepsilon_{k+q} - \varepsilon_k)\rho_{k,q} + (c_k^+ c_k - c_{k+q}^+ c_{k+q}) V(q,\omega) e^{-i\omega t + \eta t}$$

To get it we commute ρ_{kq} with H

e.g. $$[\rho_{k,q}, H_0] = c_k^+ c_{k+q} \sum_{k'} \varepsilon_{k'} c_{k'}^+ c_{k'} -$$

$$- \left(\sum_{k'} c_{k'}^+ c_{k'}\right) c_k^+ c_{k+q}$$

For $k' \neq k, k+q$ Because of the anticommutation rules for $c_k c_{k'}^+ + c_k^+ c_{k'} = \delta_{kk'}$

we can interchange 2 times each c_{k+q} and c_k^+ with $c_{k'}^+$ and c_k and cancel the second term

For $k' = k$

$$C_k^+ C_{k+q}\, \varepsilon_k C_k^+ C_k = \varepsilon_k\, C_k^+ C_k^+ C_k C_{k+q} =$$

$$= \underline{-\varepsilon_k C_k^+ C_{k+q}} + \varepsilon_k C_k^+ C_k C_k^+ C_{k+q}$$

And analogously term with $k' = k+q$ will give $\varepsilon_{k+q}\, C_k^+ C_{k+q} = \varepsilon_{k+q}\, \rho_{k,q}$

Taking thermal average $\langle A \rangle = \dfrac{\mathrm{Tr}\left(A e^{-\beta H}\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)}$ of equation of motion and assuming the same time dependence $\langle \rho_{k,q}(t)\rangle \propto e^{-i\omega t + \eta t}$ we obtain

$$(\hbar\omega + i\hbar\eta)\langle \rho_{k,q}\rangle = (\varepsilon_{k+q} - \varepsilon_k)\langle \rho_{k,q}\rangle +$$

$$+ (n_k - n_{k+q})\, V(q,\omega) ,$$

with $n_k = C_k^+ C_k$

Solving it we arrive at

$$\delta n_{ind}(q,\omega) = \frac{1}{\Omega} \sum_k \langle \rho_{k,q}\rangle =$$

$$= \frac{1}{\Omega} \sum_k \frac{n_{k+q} - n_k}{\varepsilon_{k+q} - \varepsilon_k - \hbar\omega - i\hbar\eta}\, V_{q,\omega} = \chi_0(q,\omega)\, V(q,\omega)$$

Where $\chi_0(q,\omega) = \frac{1}{\Omega} \sum \frac{n_{k+q} - n_k}{\varepsilon_{k+q} - \varepsilon_k - \hbar\omega - i\hbar\eta}$

is called the Lindhard function.

$\delta n = \chi_0 V$ is valid for any potential

If $V = e\varphi$ is scalar potential then δn gives modulation of the charge density that brings additional Coulomb potential from the Poisson Eq.

$$\nabla^2 \varphi_\delta(r,t) = -4\pi e\, \delta n(r,t)$$

$$\varphi_\delta(q,\omega) = \frac{4\pi e}{q^2} \delta n(q,\omega)$$

Adding it selfconsistently (so called Random Phase Approximation RPA)

$$\varphi = \varphi_a(q,\omega) + \frac{4\pi e}{q^2} \delta n(q,\omega)$$

with $\delta n(q,\omega) = \chi_0(q,\omega)\, e\, \varphi(q,\omega)$

Then $\varphi(q,\omega) = \dfrac{\varphi_a(q,\omega)}{\varepsilon(q,\omega)}$

with dielectric function $\varepsilon(q,\omega) = 1 - \frac{4\pi e^2}{q^2} \chi_0(q,\omega)$

Now we will analise different limits

for static case we can expand

$$n_{k+q} = n_k + \frac{\partial n}{\partial \varepsilon_k} \vec{q} \cdot \nabla_k \varepsilon_k ,$$

Since n_k is Fermi function and at $T=0$

$$\frac{\partial n}{\partial \varepsilon_k} = -\delta(\varepsilon_k - \varepsilon_F)$$ then using $\varepsilon_{k+q} = \varepsilon_k + \vec{q} \cdot \nabla_k \varepsilon_k$

$$\chi_0(q,\omega) = -\frac{1}{\Omega} \sum_k \delta(\varepsilon_k - \varepsilon_F) = -\frac{1}{\pi^2} \frac{k_F^2}{\hbar v_F} = -\frac{3 n_0}{2 \varepsilon_F}$$

Thus $\varepsilon(q,0) = 1 + \frac{k_{TF}^2}{q^2}$ with $k_{TF}^2 = \frac{6\pi e^2 n_0}{\varepsilon_F}$

and we rederived the Thomas Fermi screening.

To get plasma mode we expand both numerator and denominator in the Lindhard function

$$\chi_0(q,\omega) = -2 \int \frac{d^3k}{(2\pi)^3} \frac{\vec{q} \cdot \vec{v}_F \, \delta(\varepsilon_k - \varepsilon_F)}{q \cdot v_F - \omega - i\eta}$$

near the Fermi surface $\vec{v}_F = \nabla_k \varepsilon_k = v_F \frac{\vec{k}}{|k|}$

Then $\chi_0(q,\omega) = \frac{2}{(2\pi)^2} \int_{-1}^{+1} d\cos\theta \, \frac{k_F^2}{\hbar v_F} \left[\frac{q v_F \cos\theta}{\omega + i\eta} + \right.$

$$\left. + \left(\frac{q v_F \cos\theta}{\omega + i\eta} \right)^2 + \frac{(q v_F)^3 \cos^3\theta}{(\omega + i\eta)^3} + \ldots \right] =$$

$$= \frac{k_F^2 \, q^2}{3\pi^2 m (\omega + i\eta)^2} \left(1 + \frac{3}{5} \frac{v_F^2 q^2}{(\omega + i\eta)^2} \right) =$$

$$= \frac{n_0 q^2}{m(\omega + i\eta)^2} \left(1 + \frac{3}{5} \frac{v_F^2 q^2}{(\omega + i\eta)^2} \right)$$

And $\lim_{q \to 0} \varepsilon(q,\omega) = 1 - \frac{\omega_p^2}{\omega^2}$

with $\omega_p^2 = \frac{4\pi e^2 n_0}{m}$

Friedel oscillations

The static dielectric function can be calculated exactly for free electron gas (Problem set)

$$\varepsilon(q,\omega) = \frac{4e^2 m K_F}{\pi q^2}\left[\frac{1}{2} + \frac{4K_F^2 - q^2}{8K_F q} \ln\left|\frac{2K_F+q}{2K_F-q}\right|\right]$$

At $q = \pm 2K_F$ there is a logarithmic singularity. This is a consequence of the sharpness of the Fermi surface.

Consider the induced charge at the origin

$$e n_a(r) = e n_{a0}\,\delta(r), \qquad n_{a0}(q) = n_{a0}$$

$$\delta n(r) = \int \frac{d^3q}{(2\pi)^3}\left[\frac{1}{\varepsilon(q)} - 1\right] n_{a0}(q)\, e^{i\vec{q}\vec{r}}$$

$$= -\frac{n_{a0}}{r}\int_0^\infty g(q)\sin qr\, dq$$

with $g(q) = \dfrac{q}{2\pi^2}\,\dfrac{\varepsilon(q)-1}{\varepsilon(q)}$

Integrating twice by parts we obtain

$$\delta n(r) = \frac{n_{a0}}{r^3}\int_0^\infty g''(q)\sin qr\, dq$$

Logarithmic term in $\varepsilon(q)$ gives singular behavior of $g''(q)$ close to $q = 2k_F$

$$g'(q) \simeq A \ln|q - 2k_F|$$

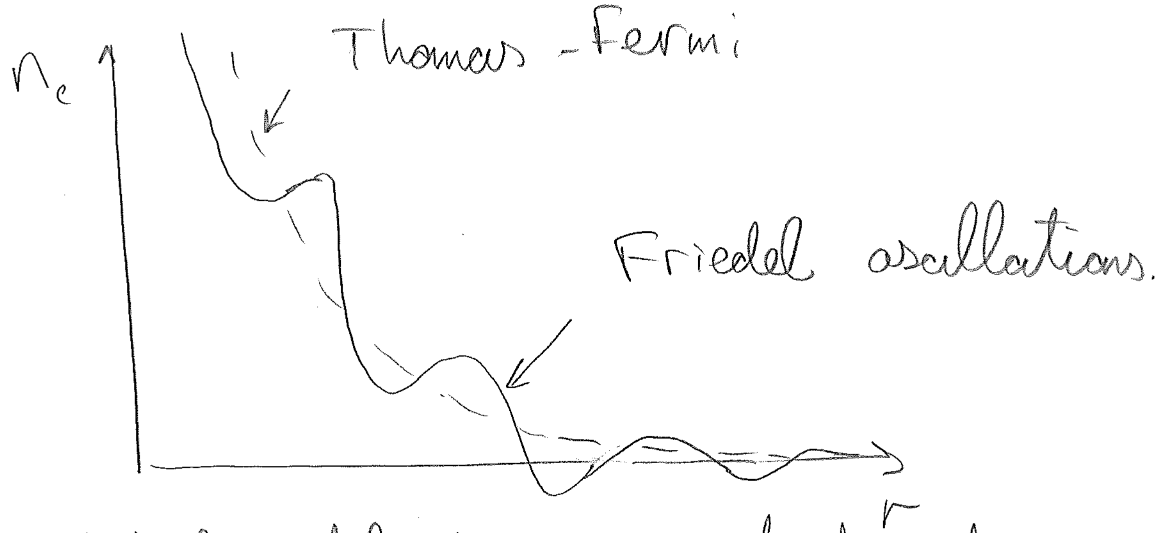
$$g''(q) \simeq \frac{A}{q - 2k_F}$$

For $k_F r >> 1$

$$\delta n(r) = \frac{n_{a0}}{r^3} \int g''(q) \sin((q - 2k_F + 2k_F)r)\, dq =$$

$$= \frac{A n_{a0}}{r^3} \int_{2k_F - \Lambda}^{2k_F + \Lambda} \frac{\sin[(q-2k_F)r] \cos 2k_F r + \cos[(q-2k_F)r] \sin 2k_F r}{q - 2k_F}\, dq$$

$$\to \pi A n_{a0} \frac{\cos 2k_F r}{r^3}$$



Note that the total charge is not changed.

$$\delta Q = e\delta n = e \int \delta n(r)\, d^3 r = \lim_{q \to 0} \left(\frac{1}{\varepsilon(q)} - 1 \right) n_a(q) = -e n_{a0}$$

since $\varepsilon(q) \to \frac{1}{q^2}$ for $q \to 0$.