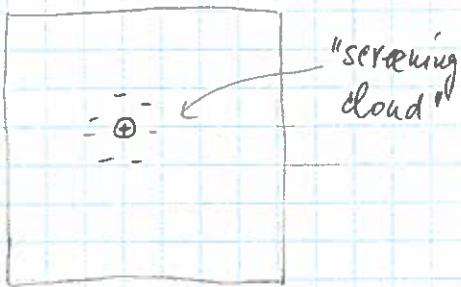


SCREENING

$$\left[\begin{array}{l} \phi^{\text{ext}}, \phi \\ \rho^{\text{ext}}, \rho, \rho^{\text{ind}} = \rho - \rho^{\text{ext}} \end{array} \right]$$



- for definition and general discussion
see A&M p. 337-9

$$\phi(\vec{q}) = \frac{1}{\epsilon(\vec{q})} \phi^{\text{ext}}(\vec{q})$$

$$\rho^{\text{ind}}(\vec{q}) = \chi(\vec{q}) \phi(\vec{q}) \quad (1)$$

$$\epsilon(\vec{q}) = 1 - \frac{4\pi}{\vec{q}^2} \chi(\vec{q})$$

$\epsilon(\vec{q})$ - dielectric function

$\chi(\vec{q})$ - dielectric susceptibility

(I) Thomas-Fermi theory of dielectric response

$$\hat{H} = \int d\vec{x} \hat{\psi}^+(\vec{x}) T(\vec{x}) \hat{\psi}(\vec{x}) \quad (\text{we neglect interactions})$$

$$T(\vec{x}) = \frac{\hbar^2 \nabla^2}{2m} - e\phi(\vec{x}) \quad (2)$$

• For $\phi(\vec{x}) = \phi_0 = \text{const}$ we can solve the problem exactly

$$H = \sum_k \left(\frac{\hbar^2 k^2}{2m} - e\phi_0 \right) c_k^+ c_k = \sum_k \epsilon_k c_k^+ c_k \quad (3)$$

• TF theory assumes that $\phi(\vec{x})$ varies slowly in space.
Therefore, in a semiclassical approximation we may write

$$\epsilon_k \rightarrow \frac{\hbar^2 k^2}{2m} - e\phi(\vec{r}) \quad (4)$$

• Calculate electron density at \vec{r} :

$$\rho(\vec{r}) = -e \langle \hat{\psi}^+(\vec{r}) \hat{\psi}(\vec{r}) \rangle = -2e \sum_{kk'} \langle \psi_e^*(\vec{r}) \psi_{e'}(\vec{r}) c_k^+ c_{k'} \rangle$$

$$\rho(\vec{r}) = -2e \sum_{kk'} \psi_{k'}^*(\vec{r}) \psi_k(\vec{r}) \underbrace{\langle c_k^+ c_{k'}^- \rangle}_{\delta_{kk'} f(\epsilon_k(\vec{r}))} \xrightarrow{\text{Fermi-Dirac distribution}}$$

$$= -2e \sum_k |\psi_k(\vec{r})|^2 f(\epsilon_k(\vec{r})) \quad (5)$$

For plane wave basis $\psi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{-ik \cdot \vec{r}}$ we have

$$\begin{aligned} \rho(\vec{r}) &= -\frac{2e}{V} \sum_k \frac{1}{e^{\beta(\epsilon_k(\vec{r})-\mu)} + 1} \quad (\beta = \frac{1}{k_B T}) \quad (6) \\ &= -e \int \frac{d^3 k}{4\pi^3} \frac{1}{e^{\beta[\hbar^2 k^2/2m - e\phi(\vec{r}) - \mu]} + 1} \\ &\equiv -n_0(\mu + e\phi(\vec{r})) \end{aligned}$$

where

$$n_0(\mu) = - \int \frac{d^3 k}{4\pi^3} \frac{1}{e^{\beta[\hbar^2 k^2/2m - \mu]} + 1} \quad (7)$$

So the induced charge density can be written as

$$\left[\rho^{\text{ind}}(\vec{r}) = -e [n_0(\mu + e\phi(\vec{r})) - n_0(\mu)] \simeq -e^2 \phi(\vec{r}) \frac{\partial n_0}{\partial \mu} \right] \quad (8)$$

assuming that $\phi(\vec{r})$ is small enough that we may neglect higher order terms.

Eq. (8) combined with (1) implies

$$\left[\begin{aligned} \chi(\vec{q}) &= -e^2 \frac{\partial n_0}{\partial \mu} \quad (\text{indep. of } \vec{q}) \\ \varepsilon(\vec{q}) &= 1 + \frac{4\pi e}{q^2} \frac{\partial n_0}{\partial \mu} \end{aligned} \right] \quad (9)$$

main result of the TF theory of screening.

Eq. (9) is often given as

$$\epsilon(\vec{q}) = 1 + \frac{k_{TF}^2}{q^2}, \quad \rightarrow k_{TF}^2 = 4\pi e^2 \frac{\partial n_0}{\partial \mu} \quad (10)$$

"Thomas-Fermi momentum"

To illustrate the significance of k_{TF} consider the screened potential of a point charge:

$$\phi^{ext}(\vec{r}) = \frac{Q}{r} \rightarrow \phi^{ext}(\vec{q}) = \frac{4\pi Q}{q^2} \quad (11)$$

$$\phi(\vec{q}) = \frac{1}{\epsilon(\vec{q})} \phi^{ext}(\vec{q}) = \frac{4\pi Q}{q^2 + k_{TF}^2} \quad (12)$$

In real space this becomes

$$\phi(\vec{r}) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}} \frac{4\pi Q}{q^2 + k_{TF}^2} = \frac{Q}{r} e^{-k_{TF}r} \quad (13)$$

This is known as "screened Coulomb" or "Yukawa" potential.

The potential rapidly vanishes at distances $r > k_{TF}^{-1} = \lambda_{TF}$ with λ_{TF} the "screening length".

• Estimate $\lambda_{TF} = 1/k_{TF}$ in a metal:

$$\frac{\partial n_0}{\partial \mu} = - \int \frac{d^3k}{4\pi^3} \frac{1}{\epsilon(\epsilon_k - \mu)} \left[\frac{1}{e^{(E_k - \mu)/k_B T} + 1} \right] \xrightarrow{T \rightarrow 0} \int \frac{d^3k}{4\pi^3} \delta(\epsilon_k - \mu) = g(\mu) = \frac{m k_F}{t^3 \pi^2}, \quad (14)$$

(Density of states at the Fermi level in 3D)

$$\rightarrow \frac{k_{TF}^2}{k_F^2} = \frac{4}{\pi} \frac{m e^2}{t^3 k_F} = \frac{4}{\pi} \frac{1}{\epsilon_F a_0} = \left(\frac{16}{3\pi^2} \right)^{3/2} t_S$$

$$k_{TF} = 0.815 k_F \sqrt{t_S} \quad (15)$$

$$\lambda_{TF} = k_{TF}^{-1} = \frac{\sqrt{t_S}}{2.95} \text{ Å}$$

• In a metal Coulomb interaction is screened at VERY SHORT distance comparable to ionic lattice spacing.

(II) Lindhard Theory

- Assume that $\phi(\vec{r})$ is small and can be treated as a perturbation:

$$H = \underbrace{\frac{\hbar^2}{2m} \nabla^2}_{H_0} - e \underbrace{\phi(\vec{r})}_{H_1} \quad (15)$$

- Calculate the charge density using Eq. (5). Need to find the correction to $\psi_e(\vec{r})$ due to perturbation:

$$\psi_e(\vec{r}) = \psi_e^0(\vec{r}) + \sum_{k'} \frac{\langle \psi_{k'}^0 | -e\phi(\vec{r}) | \psi_k^0 \rangle}{\epsilon_k^0 - \epsilon_{k'}^0} \psi_{k'}^0(\vec{r}) + \dots \quad (16)$$

$$\psi_k^0(\vec{r}) = \frac{1}{V} e^{i\vec{k} \cdot \vec{r}}, \quad \epsilon_k^0 = \frac{\hbar^2 k^2}{2m}$$

$$\rightarrow \langle \psi_{k'}^0 | -e\phi(\vec{r}) | \psi_k^0 \rangle = -\frac{e}{V} \int d\vec{r} e^{-i\vec{k}' \cdot \vec{r}} \phi(\vec{r}) e^{i\vec{k} \cdot \vec{r}} = -\frac{e}{V} \phi(\vec{k} - \vec{k}') \quad (17)$$

$$\psi_k(\vec{r}) \approx \psi_k^0(\vec{r}) - \frac{e}{V} \sum_{k'} \frac{\phi(\vec{k} - \vec{k}')}{\epsilon_k^0 - \epsilon_{k'}^0} \psi_{k'}^0(\vec{r}) \quad (18)$$

- Substitute this in Eq. (5) and retain terms to first order in $\phi(\vec{r})$:

$$\rho(\vec{r}) = -e \left[\underbrace{\sum_k f_k |\psi_k^0|^2}_{\rho_0(\vec{r})} - \underbrace{\frac{e}{V} \sum_k \left(f_k \psi_k^0 * \sum_{k'} \frac{\psi_{k'}^0}{\epsilon_k^0 - \epsilon_{k'}^0} \phi(\vec{k} - \vec{k}') + c.c. \right)}_{\rho^{\text{ind}}(\vec{r})} \right] \quad (19)$$

$$f_k = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1} \quad - \text{F.D. distribution}$$

- Evaluate the k, k' sums by using a substitution

$$(\vec{k}, \vec{k}') \rightarrow (\vec{K} + \frac{1}{2}\vec{q}), (\vec{K} - \frac{1}{2}\vec{q})$$

$$g^{\text{ind}}(\vec{q}) = -\frac{e^2}{V} \sum_{K,q} e^{i\vec{F}\cdot\vec{q}} \frac{f_{K+\frac{1}{2}q} - f_{K-\frac{1}{2}q}}{\varepsilon_{K+\frac{1}{2}q}^0 - \varepsilon_{K-\frac{1}{2}q}^0} \phi(\vec{q}) + \text{c.c.}$$

$$= -\frac{e^2}{V} \sum_q e^{i\vec{F}\cdot\vec{q}} \left(\sum_K \frac{f_{K+q} - f_{K-q}}{\varepsilon_{K+q}^0 - \varepsilon_{K-q}^0} \right) \phi(\vec{q})$$
(20)

We may thus conclude that $g^{\text{ind}}(\vec{q}) = \chi(\vec{q}) \phi(\vec{q})$

with

$$\boxed{\chi(\vec{q}) = -\frac{e^2}{V} \sum_K \frac{f_{K+\frac{1}{2}q} - f_{K-\frac{1}{2}q}}{\varepsilon_{K+\frac{1}{2}q}^0 - \varepsilon_{K-\frac{1}{2}q}^0}} \quad \left| \begin{array}{l} \text{Lindhard dielectric function} \\ \text{function} \end{array} \right. \quad (21)$$

- At low T and small q the numerator is small unless $|K| \approx k_F$. We can therefore expand

$$f_{K\pm\frac{1}{2}q} \approx f_K \pm \frac{\hbar^2}{2} \frac{\vec{k}\cdot\vec{q}}{m} \frac{\partial f_K}{\partial \mu} + O(q^2) \quad (22)$$

This gives

$$\chi(\vec{q}) \approx -\frac{e^2}{V} \sum_K \frac{\partial f_K}{\partial \mu} \quad \leftarrow \text{the TF result!}$$

- At $T=0$ the K -integral can be evaluated,

$$\chi(\vec{q}) = -e^2 \left(\frac{m k_F}{\pi^2 \hbar^3} \right) \left[\frac{1}{2} + \frac{1-x}{4x^2} \ln \left| \frac{1+x}{1-x} \right| \right], \quad x = \frac{q}{2k_F} \quad (23)$$

- Because the dielectric function $\varepsilon(\vec{q}) = 1 - \frac{4\pi}{q^2} \chi(\vec{q})$ is non-analytic at $q=2k_F$ ($x \rightarrow 1$) it is possible to show that the screened potential of a point charge contains a term

$$\phi(\vec{r}) \sim \frac{1}{r^3} \cos 2k_F r \quad (r \gg \xi_F) \quad (24)$$

This is known as "Friedel" or "RKKY" oscillations, observable in experiment, e.g. scanning tunneling microscopy.