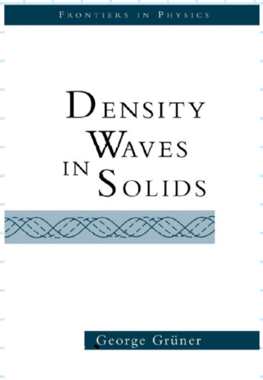
Charge Screening in Metals + Charge Density Waves

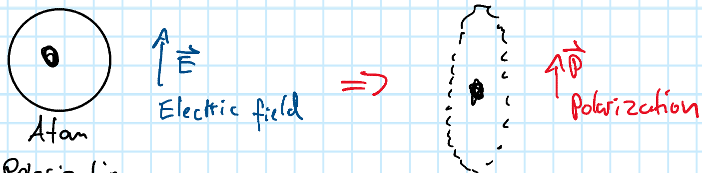
Friday, 10. December 2021 09:54

- Electron transport
  Boltzmann
- Scattering
- Magnetotransport
- Photoemission
- Phase transitions
  + Landau theory
- Charge screening + CDW
- Magnetism



Literature
- Gross + Marx 11.7
- Grüner - Density Waves in Solids

① Generalized Susceptibility



Polarization

$\vec{P} = \varepsilon_0 \chi \vec{E}$ $\Rightarrow$ $\vec{P}(\vec{r},t) \Rightarrow \vec{P}(\vec{q},\omega) \propto \chi(\vec{q},\omega)\cdot\vec{E}$

↳ Susceptibility : rank 2 tensor $\hat{=}$ Response of the system to $\vec{E}$

Displacement field:

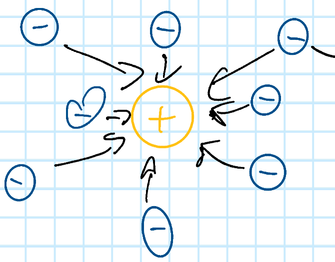
$\vec{D} = \varepsilon_0 \vec{E} + \vec{P} = \varepsilon_0 \cdot \varepsilon \cdot \vec{E}$ $\Rightarrow$ $\vec{D}(\vec{q},\omega) = \varepsilon_0 \cdot \varepsilon(\vec{q},\omega)\cdot\vec{E}$

↳ Dielectric function

- For instance, in electromagnetism: $q=0$ $\hat{=}$ homogeneous electric field
  $(\lambda \gg a)$ $\varepsilon(\omega) = 1 + \chi(\omega)$

② Charge Screening of a test charge

- Consider a single static $(\omega = 0)$ charge in a free e^- gas



e^- will screen that charge

related via Poisson:

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ϕ^{ext} : Potential } of $\oplus$ $\longrightarrow$ $-\nabla^2 \phi^{ext}(\vec{r}) = \frac{\rho^{ext}(\vec{r})}{\varepsilon_0}$ $(\hat{=} \vec{D})$

ρ^{ext} : charge density

$\Rightarrow \rho^{tot}(\vec{r}) = \rho^{ext}(\vec{r}) + \rho^{ind}(\vec{r})$

$\Rightarrow$ and of course again $-\nabla^2 \phi^{tot}(\vec{r}) = \frac{\rho^{tot}(\vec{r})}{\varepsilon_0}$ $(\hat{=} \vec{E})$

$$\phi^{tot}(\vec{r}) = \phi^{ext}(\vec{r}) + \phi^{ind}(\vec{r})$$

- Same relation holds for the definition of the dielectric function

$$\phi^{ext}(\vec{q}) = \varepsilon(\vec{q}) \cdot \phi^{tot}(\vec{q})$$

$\hookrightarrow$ assumed to be a scalar

$$\rho^{ind}(\vec{q}) \approx \chi(\vec{q}) \cdot \phi^{tot}(\vec{q})$$

linear response theory
$\hat{=}$ weak test charge
(this is an assumption)

- After same calculation...

$$\boxed{\varepsilon(\vec{q}) = 1 - \frac{1}{\varepsilon_0 q^2} \chi(\vec{q}) = 1 - \frac{1}{\varepsilon_0 q^2} \frac{\rho^{ind}(\vec{q})}{\phi^{tot}(\vec{q})}}$$

How to calculate $\chi(\vec{q})$:

① Thomas - Fermi - Screening

-> Semiclassical treatment $q \ll k_F$

-> Slow variation of the perturbing potential $\phi^{tot}(\vec{r})$

$$E(\vec{r}, \vec{k}) = \frac{\hbar^2 k^2}{2m^*} - e\,\phi^{tot}(\vec{r})$$

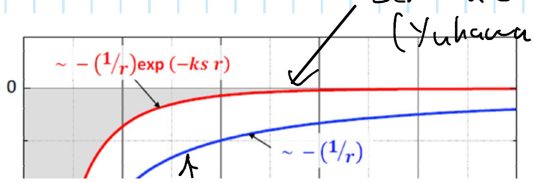
$\vdots$

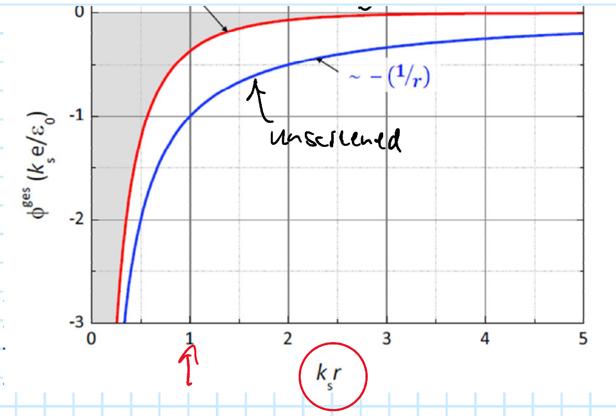
$$\Rightarrow \varepsilon(\vec{q}) = 1 + \frac{k_s^2}{q^2} \qquad k_s = \sqrt{\frac{e^2}{\varepsilon_0} \cdot \frac{D(E_F)}{V}}$$ – Density of States

$\frac{1}{k_s}$: Thomas-Fermi Screening length

$$\chi(\vec{q}) = -e^2 \frac{D(E_F)}{V}$$

Example: Screened Coulomb Potential
e.g. Zn atom in copper ?
screened ( )
(Yukawa Potential)





② Lindhard - Method

→ ρ^{ind} and ϕ^{tot} are only connected in linear order

→ Perturbation theory possible

- Assume an unperturbed wave function (free e^-)

$$\psi_0(\vec{r}) = \frac{1}{L^3} \cdot \exp\left(\vec{k}\cdot\vec{r} + \frac{\vec{E}(k)\cdot t}{\hbar}\right) : |\vec{k}\rangle \qquad E(\vec{k}) = \frac{\hbar^2 \cdot k^2}{2m}$$

- now under a perturbing potential $\phi^{tot}(\vec{r},t) = \phi_0^{tot} \cdot e^{i\vec{q}\cdot\vec{r} \cancel{-i\omega t}}$ static potential

$$\Rightarrow \psi_k(\vec{r}) = |\vec{k}\rangle + c_{k+q} \cdot |\vec{k}+\vec{q}\rangle$$

$$c_{k+q} = \frac{\langle \vec{k}+\vec{q} \,|\, \phi^{tot} \,|\, \vec{k}\rangle}{E(\vec{k}+\vec{q}) - E(\vec{k})}$$

⇒ gives charge density

$$\rho^{ind}(\vec{r}) = e \sum_k \left(|\psi_k(\vec{r})|^2 - 1 \right)$$

$$\approx e \sum_k \left(\frac{1}{E(\vec{k}+\vec{q}) - E(\vec{k})} + \frac{1}{E(\vec{k}-\vec{q}) - E(\vec{k})} \right) \cdot \phi_0^{tot}$$

add Fermi functions

$$= e \sum_k \left(\frac{f_0(\vec{k}) - f_0(\vec{k}+\vec{q})}{E(\vec{k}+\vec{q}) - E(\vec{k})} \right) \cdot \phi_0^{tot}$$

↳ now, we need to make this self-consistent with via the Poisson Eq.

$$-\nabla^2 \phi^{ind}(\vec{r}) = \frac{e\,\rho^{ind}(\vec{r})}{\varepsilon_0} \quad \text{and} \quad \phi^{tot} = \phi^{ext} + \phi^{ind}$$

⋮

Result: $\phi_0^{tot} = \dfrac{\phi_0^{ext}}{\varepsilon(\vec{q})}$

with $$\varepsilon(\vec{q}) = 1 + \underbrace{\frac{e^2}{q^2 \cdot \varepsilon_0} \cdot \sum_k \frac{f_0(\vec{k}+\vec{q}) - f_0(\vec{k})}{E(\vec{k}+\vec{q}) - E(\vec{k})}}_{\text{Charge susceptibility } \chi(\vec{q})}$$

Charge susceptibility $\chi(\vec{q})$

„Lindhard responce function"

- above we derived the equations just for one Fourier component, but since everything is linearly approximated, we can write

$$\phi^{tot}(\vec{r}) = \int \frac{\phi_{ext}(\vec{q})}{\varepsilon(\vec{q})} \cdot e^{i\vec{q}\cdot\vec{r}}\, d^3q$$

Lindhard approximation