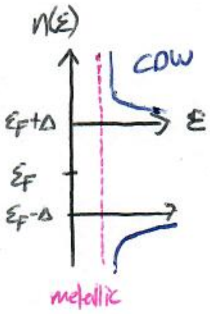
Charge Density Wave

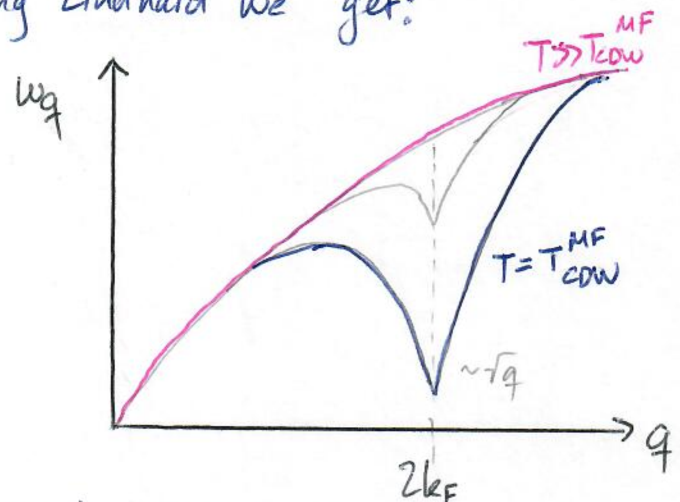
Definition: The charge density wave ground state consists of a periodic charge density modulation accompanied by a periodic lattice distortion. It develops in low-dimensional metals as a consequence of electron-phonon interaction.

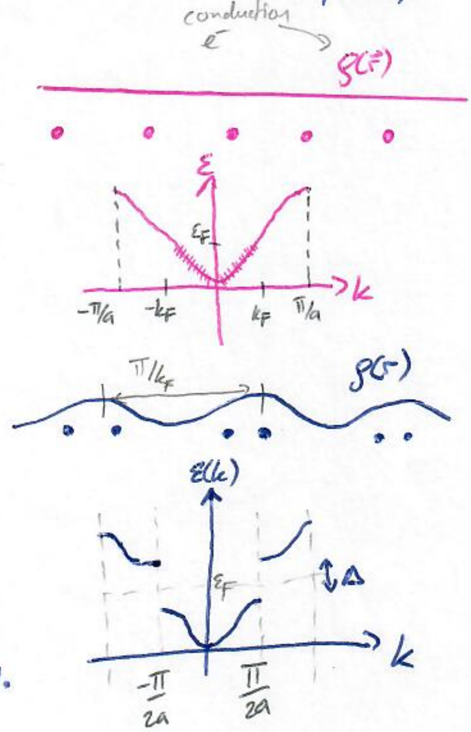
Derivation: (1-dim electron gas)

Using the Born-Oppenheimer approximation, Lattice vibration $\xrightarrow[\text{distortion}]{e^- \text{ screen lattice}}$ renormalized phonon frequency

and then using Lindhard we get:

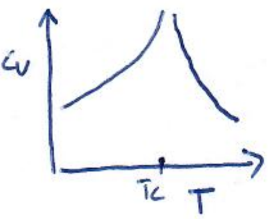


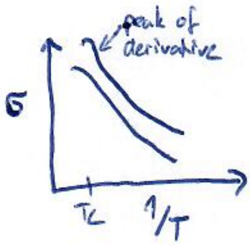


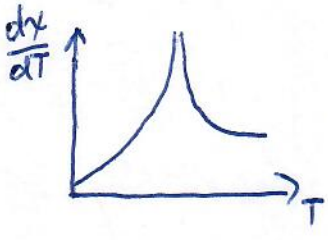


Below the phase transition, the renormalized phonon frequency is zero, indicating a "frozen-in" lattice distortion.

Experimental evidence:







- specific heat
- conductivity (dc)
- magnetic susceptibility

- lattice distortion ⇒ e^-/n diffraction or X-Ray
- Kohn anomaly
- Scanning tunnel microscopy
- photoemission for Gap

Δ has the meaning of magnitude and phase of the electrostatic energy potential

Charge density wave Overview

p.44. Grüner

In general incommensurate with period of lattice, usually occur in quasi-one-dimensional metals, but not endemic to this family.

→ density of conduction electrons spatially modulated, probed by scanning tunnel microscopy.

→ periodicity usually corresponds to nesting vector of Fermi surface

→ lattice distorted by same periodicity, measured by X-Ray, electron neutron diffraction, scanning probe techniques.

→ anomalies in phonon dispersion, energy might go to zero at phase transition

→ $\nu(\varepsilon_F)$ reduced in CDW phase.

Nesting alone does not lead to CDW at $T>0$. See graph

Electron-lattice interactions

→ Born oppenheimer approximation

phonon → ionic density modulation $\xrightarrow{\text{Lindhard}}$ periodic charge density

$\xrightarrow[\text{on ions}]{\text{acts back}}$ change in phonon frequency

Renormalization of phonon frequencies

Electronic problem

$$\vec{u}_j = \underset{\text{amplitude of mode}}{\vec{u}}\, e^{i\vec{q}\cdot\vec{R}_j} + c.c. \qquad \text{(static lattice distortion)}$$

$\vec{R}_j$: position at rest

$-\omega_q t = 0$ (ω_q: phonon frequency)

$$\vec{F}_{ext} = \underbrace{\omega_q^2 M}_{=:k}\vec{u} \qquad \text{(static spatially modulated external force)}$$

$$=: k\vec{u} \qquad , k \,\hat{=}\, \text{elastic susceptibility}$$

Lattice problem

$$E_{lat} = N M \omega_q^2 |u|^2$$

$$\phi(\vec{r}) = -i(\vec{q}\cdot\vec{u})\, U_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} + c.c.$$

$U_{\vec{q}}$: F.T. of single ion potential

$$\Rightarrow \qquad \rho_{el} = \underbrace{-i(\vec{q}\cdot\vec{u})\, U_{\vec{q}}}_{\phi}\, \chi(\vec{q})$$

$$E_{tot} = E_{lat} + E_{el} = MN|u|^2\left[\omega_{\vec{q}}^2 + (\vec{q}\cdot\hat{u})^2 \frac{V}{N}|U_{\vec{q}}|^2 \chi(\vec{q})/M\right] \qquad \text{] important}$$

$$\Omega_{\vec{q}}^2 = \omega_{\vec{q}}^2\left[1 + 2\lambda_{\vec{q}} \frac{\chi(\vec{q})}{e^2 \nu(\varepsilon_F)}\right] \qquad \text{(renormalized phonon frequency)}$$

$\lambda_{\vec{q}}$: electron-phonon coupling constant

$\lambda_{\vec{q}} \sim \vec{q}\cdot\hat{u}$
$\Rightarrow$ longitudinal phonons

$\chi < 0$!
$\Rightarrow \Omega < \omega$

electrons screen lattice distortion, making it softer. May help CDW-formation?

p. 57 Grüner
p. 156 Ziman

Kohn anomaly

$\chi(q) \Rightarrow$ renormalization of phonon frequencies strong, where $q \hat{=}$ nesting vector.

Dips in phonon dispersion curves are called Kohn anomalies.
Typically T-dependent, see Fermi-Dirac distribution.

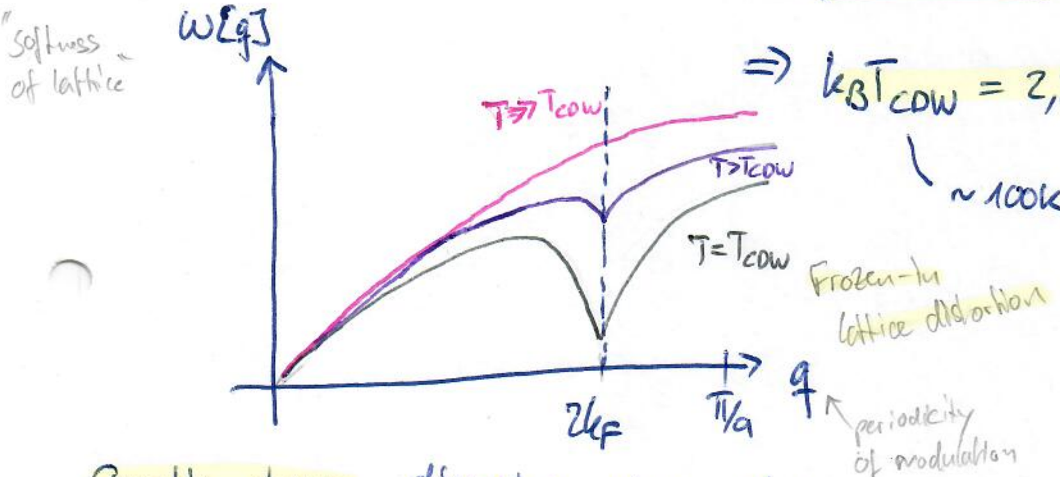
Example: one dimensional Fermi liquid

$$\chi(q=2k_F) = -\frac{e^2 \nu(\varepsilon_F)}{2} \log\left(\frac{2{,}28\,\varepsilon_F}{k_B T}\right) \qquad \text{important}$$

$$\Omega^2_{2k_F} = \omega^2_{2k_F}\left[1 - \underbrace{\lambda_{2k_F} \log\left(\frac{2{,}28\,\varepsilon_F}{k_B T}\right)}\right]$$

$$\Rightarrow k_B T_{CDW} = 2{,}28\,\varepsilon_F\, e^{-\frac{1}{\lambda_{2k_F}}}$$

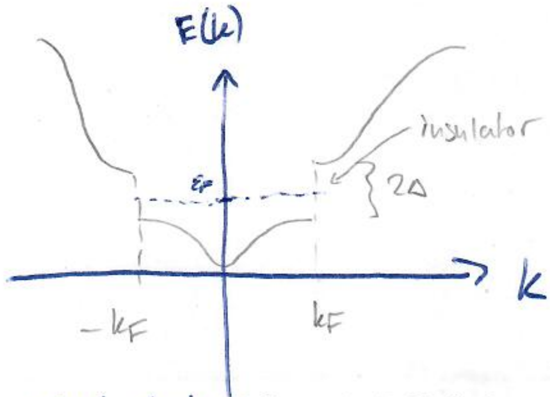
$\sim 100K$



Acoustic phonon dispersion relation of a one-dimensional metal. MF approx

$\frac{1}{\omega_{q}^2} \sim \chi$

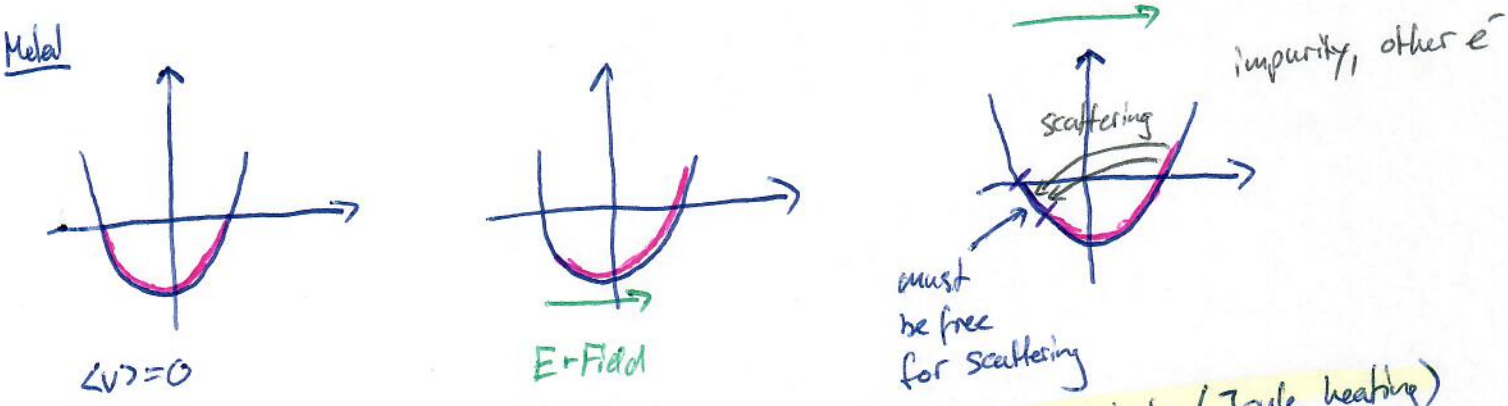
zero frequency $\Rightarrow$ divergent elastic susceptibility $\underset{\text{to}}{\overset{\text{points}}{\leadsto}}$ second order phase transition



CDW-state $\Rightarrow$ ideally insulator

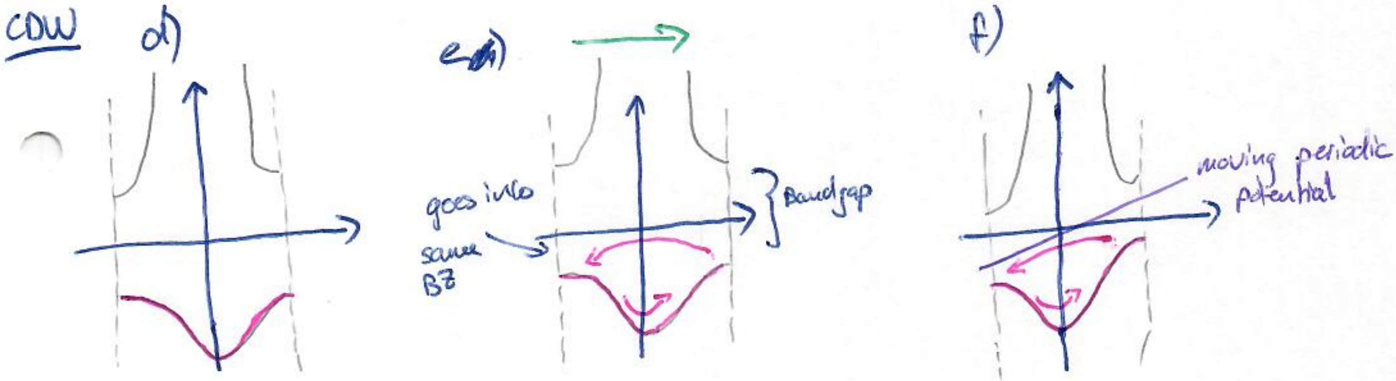
... CDW state T=0 Fig 3.5 Grüner

Current in a normal metal and in a sliding CDW



$\langle v \rangle = 0$ $\langle v \rangle > 0$

⇒ release of heat (Joule heating)



CDW ⇒ insulator

$\langle v \rangle = 0$

Zone structure prevents from current

sliding of CDW

$\langle v \rangle \neq 0$

Sliding as ~~a~~ a whole ⇒ transfer to reference ~~w~~ frame

⇒ same as in d) $\xRightarrow[\text{lab frame}]{\text{back in}}$ increase in velocity, + linear function

↖ slope of dispersion curve

⇒ average velocity is v

⇝ no Joule heating!, but dissipation due to collisions with impurities

⇝ energy ~~heat~~ released as phonons ⇒ stop of CDW sliding.

⇒ pinned to impurities ⇒ insulator for E not too strong.

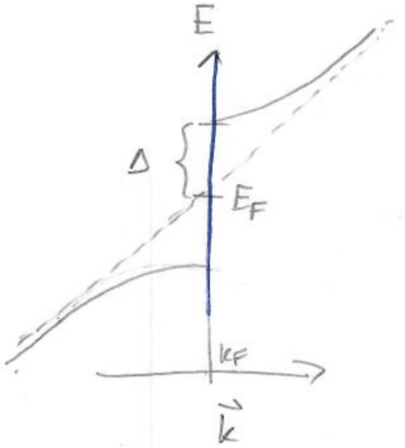
CDW: Order parameter

ionic displacement $\sim 10^{-3} - 10^{-2}\ a$

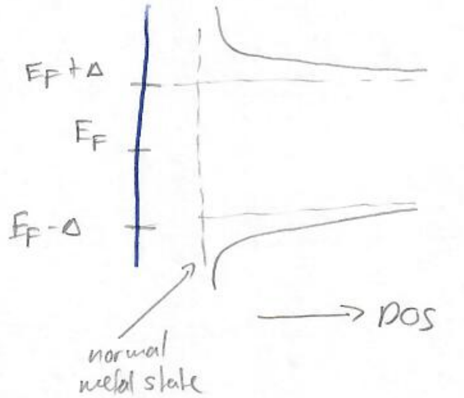
OP: complex amplitude of the electric potential produced by the lattice distortion

$$\Delta = i(\vec{q}\cdot\hat{u})\, U_{\vec{q}}\, u = |\Delta| e^{i\phi}$$

CDW: Band gap



Dispersion near k_F with lattice modulation $2k_F$



corresponding DOS

Estimating Δ

breaks translational symmetry modulo the CDW period, SO(2)

Opening the gap $\Rightarrow$ lowered the energy of the Fermi Sea.

Calculation

$\Rightarrow$ One-dimensional metallic state is unstable against the formation of a CDW.

measured by optical spectroscopy, dc conductivity $\longrightarrow$ $|\Delta| = 8\varepsilon_F \exp\left(-\frac{1}{\lambda_{2k_F}}\right) \sim 10\text{-}100\,K$

Experiments: $\frac{2\Delta}{k_B T_{CDW}} \simeq 7{,}0$