**Examination in Condensed Matter Physics I, FK7042, 7.5 hp**
Tuesday, March 14, 2017, 08.00-13.00.

Solutions

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**Allowed help:**
- periodic table and fundamental constants (distributed)
- formula sheet (distributed)
- pocket calculator, BETA / mathematics handbook or similar

**Instructions:**
All solutions should be easy to read and have enough details to be followed. The use of nontrivial formulas from the formula sheet should be explained. *Summarize each problem* before its solution, so that the solution becomes self-explained. State any assumptions or interpretation of a problem formulation and define any introduced variables.

Good luck! / A.R.

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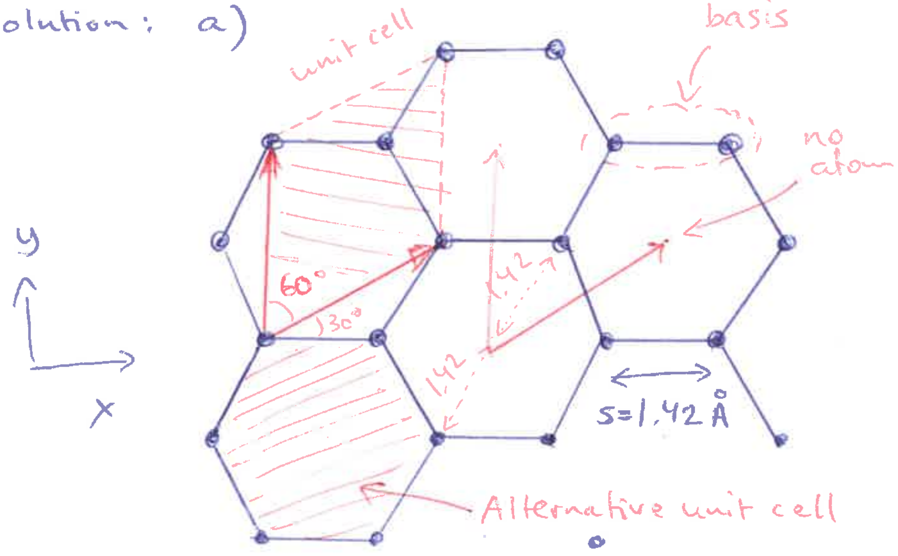
**1.** A single graphite sheet, called graphene, has a honeycomb structure with a nearest-neighbor distance of 1.42 Å.
**a)** Sketch the (2-dim) real-space structure of graphene. Find the number of atoms per cell. Indicate a unit cell, and give the length of the lattice parameters. (2p)
**b)** Draw the (2-dim) Brillouin zone of graphene. Find the area of the Brillouin zone. Hint: the reciprocal lattice of a simple hexagonal lattice is also a simple hexagonal lattice. (2p)

Solution: a)



The structure is simple hexagonal with a basis of 2 atoms

$\Rightarrow$ 2 atoms/cell.

$$\cos 30° = \frac{a/2}{s}$$

$$\Rightarrow a = 2s\cdot\cos 30° = \sqrt{3}\cdot s \approx \underline{\underline{2.46\ \text{Å}}}$$

$$\underline{V_c/c} = 6\cdot\frac{s\cdot s\cdot\sin 60°}{2} = 3s^2\sin 60° = a^2\cdot\sin 60°$$

b)

$$\text{Set}\begin{cases}\bar{a}_2 = a\hat{y}\\ \bar{a}_1 = \frac{a}{2}\hat{y} + a\sin 60°\hat{x} = a\cdot(\sin 60°\hat{x} + \cos 60°\hat{y})\\ \bar{a}_3 = c\hat{z} \quad \text{(help vector)}\end{cases}$$

Cont. 1b) Calculate reciprocal lattice

$$\bar{b}_1 = \frac{2\pi}{V_c}\,\bar{a}_2 \times \bar{a}_3 = \frac{2\pi}{V_c}\, ac\,\hat{x} = \frac{2\pi}{a\cdot\sin 60^\circ}\cdot\hat{x}$$

$$\bar{b}_2 = \frac{2\pi}{V_c}\,\bar{a}_3 \times \bar{a}_1 = \frac{2\pi}{a^2 c\sin 60^\circ}\left(\frac{ac}{2}\,\hat{x} + ac\sin 60^\circ\,\hat{y}\right) =$$

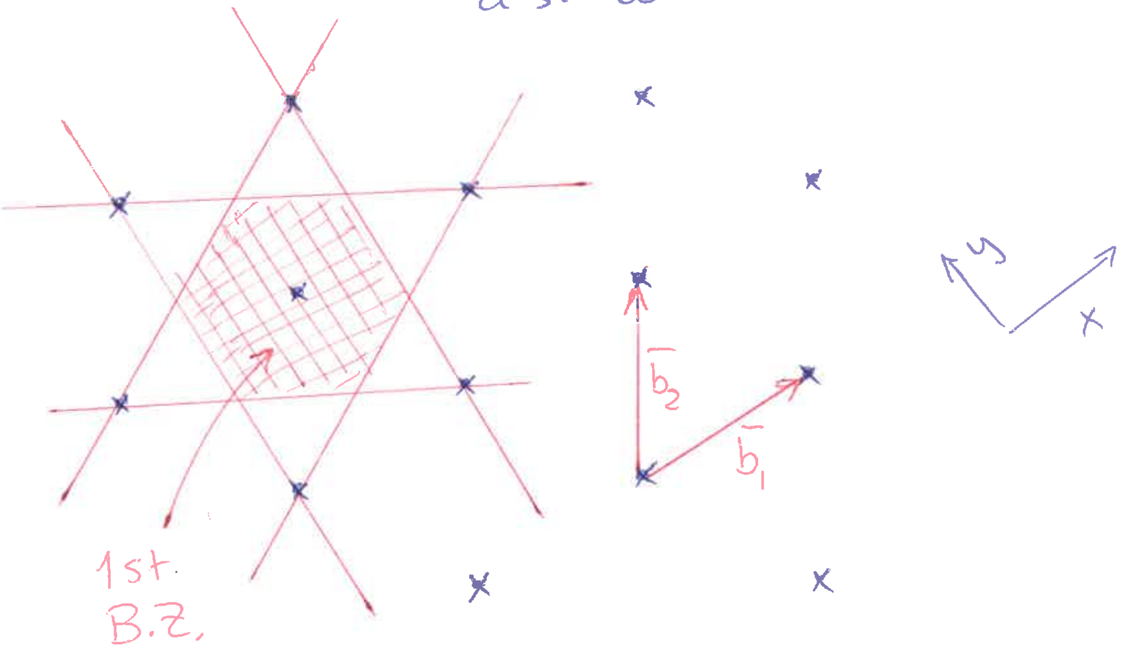
$$= \frac{2\pi}{a\sin 60^\circ}\left(\cos 60^\circ\,\hat{x} + \sin 60^\circ\,\hat{y}\right) =$$

$$= \frac{2\pi}{a\cdot\sin 60^\circ}\left(\sin 30^\circ\,\hat{x} + \cos 30^\circ\,\hat{y}\right)$$

$\Rightarrow$ Reciprocal lattice is simple hexagonal lattice rotated by 30°, with lattice parameter $b = \frac{2\pi}{a\cdot\sin 60^\circ}$

Volume of Brillouin zone (with support vector) $V_g = \frac{(2\pi)^3}{V_c} = \frac{(2\pi)^3}{a^2 c\sin 60^\circ}$

Area of Brillouin zone: $\frac{(2\pi)^2}{a^2\sin 60^\circ} = b^2\sin 60^\circ$



Check: 1st B.Z. placed on each reciprocal lattice point will fill k-space

**2.** Bloch oscillations are oscillations of electrons in periodic potentials in the presence of a constant force. They are really hard to observe in nature, due to scattering, but have been observed in semiconductor superlattices.
**a)** Assume a tight-binding form of the dispersion relation $\varepsilon(k) = A\cos ak$, where $a$ is a lattice parameter. Find an expression for the angular frequency of the Bloch oscillations in the presence of an electrical field $E$. Make suitable assumptions. (3p)
**b)** Explain how Bloch electrons move in reciprocal space in the presence of a magnetic field under otherwise similar conditions. (1p)

a) Solution : Assume that we can disregard scattering.

With a constant electrical field $\bar{E}$, we can write

$$\bar{F} = -e\bar{E} = \hbar \frac{d\bar{k}}{dt}$$

This gives $k(t) = k(0) - \frac{eEt}{\hbar}$

group velocity $v(k) = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial k} = \left\{ \text{use } \varepsilon(k) = A\cos ak \right\} = -\frac{1}{\hbar} Aa\sin ak$

$\Rightarrow$ Semiclassical electron position

$$x(t) = \int_0^t v(k(t'))\,dt' = x(0) - \frac{Aa}{\hbar} \cdot \frac{1}{\left(\frac{eE}{\hbar}\right)} \cos\left(a\frac{eE}{\hbar}t\right)$$

$\Longrightarrow$ oscillation angular freq. $\underline{\underline{\omega = \frac{aeE}{\hbar}}}$

b) The motion is perpendicular to $\bar{B}$, following the Fermi surface/constant energy surface

**3. a)** Explain the following concepts related to lattice vibrations: Phonon, normal mode, Umklapp process. (1.5p)
**b)** Find an expression for the lattice zero-point vibration energy expressed in $nk_B$ and $\theta_D$, where $n$ is the atomic density and $\theta_D$ is the Debye temperature. Make suitable assumptions. (2.5p)

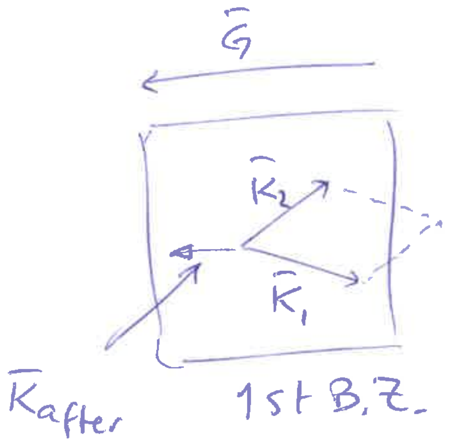
a) Phonon : Energy quantum of elastic wave

Properties : $\begin{cases} \text{frequency } \omega \text{, energy } \hbar\omega \\ \text{wave vector, } |K| = \frac{2\pi}{\lambda} \\ \text{polarization direction: } 1L, 2T \end{cases}$

Normal mode : Lattice vibration characterized by the phonon properties above, but each mode having $n$ phonons and total energy $(n+\frac{1}{2})\hbar\omega$

Umklapp process : Phonon collision where

$$\bar{K}_{after} = \bar{K}_1 + \bar{K}_2 + \bar{G}, \quad \bar{G} \neq 0$$



3b) Wanted: Lattice zero-point vibration energy (in $\overset{}{n}k_B, \Theta_D$) $\hookrightarrow N/V$

Solution: Each normal mode has energy $(n_{ph}+\frac{1}{2})\hbar\omega(K)$

At zero temperature, only the zero-point vibration remains, $n_{ph}=0$

This gives $u_0 = \frac{1}{V}\sum\limits_{\substack{\text{all}\\ \text{normal}\\ \text{modes}\\ K,s}} \frac{1}{2}\hbar\omega(K,s)$ ; $u_0 = \frac{U_{tot}}{V}$

Assume: Debye model, $\omega = v_s \cdot K$, $K_D$ to preserve $N_{total}$

$$\Rightarrow \quad u_0 = \underbrace{\sum_s}_{3\text{ pol, dir.}} \cdot \frac{1}{V}\int_0^{K_D} \frac{1}{2}\hbar v_s K \cdot D(K)\,dK$$

where $D(K)\,dK = 4\pi K^2 dK \cdot \frac{1}{\left(\frac{2\pi}{L}\right)^3}$ is density of states (K-points)

$$\Rightarrow \quad u_0 = 3\cdot\frac{1}{2}\cdot\frac{4\pi}{(2\pi)^3}\cdot\hbar v_s\int_0^{K_D} K^3\,dK = \frac{3\hbar v_s}{4\pi^2}\cdot\frac{K_D^4}{4}$$

with $K_D = (6\pi^2 n)^{1/3}$, we have $u_0 = \frac{3\hbar v_s}{16\pi^2}\cdot 6\pi^2 n \cdot K_D =$

$$= \frac{9}{8}\hbar v_s K_D \cdot n = \frac{9}{8}\hbar\omega_D \cdot n = \frac{9}{8}k_B\Theta_D \cdot n =$$

$$= \underline{\underline{\frac{9}{8} n k_B \cdot \Theta_D}}$$

(approximately $\frac{1}{3}$ of $u_{tot}$ at $T \sim \Theta_D$)

**4.** The following three expressions can be found in the formula collection:

$$g_c(\varepsilon) = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(\varepsilon - \varepsilon_c)^{1/2}$$

$$n_c(T) = \int_{\varepsilon_c}^{\infty} \frac{1}{e^{(\varepsilon-\mu)/k_BT}+1} g_c(\varepsilon)d\varepsilon$$

$$N_c(T) \approx \frac{1}{4}\left(\frac{2m_e k_B T}{\pi\hbar^2}\right)^{3/2}$$

Explain what they describe and and under what conditions/assumptions they apply. Also explain variables etc. in the expressions. (4p)

Solution: (see exam 2015-03-19)

- $g_c(\varepsilon)$ is the density of states for the conduction band in a semiconductor. The energy $\varepsilon$ is measured relative to the conduction band edge $\varepsilon_c$.

  $m_e$ is the effective electron mass, including the effect of the number of conduction band edges.

  Assumptions: Parabolic bands, spherical energy surfaces.

- $n_c(T)$ is the electron concentration for the conduction band. $\mu$ is the chemical potential (Fermi level).

  $f_{FD} = \frac{1}{e^{(\varepsilon-\mu)/k_BT}+1}$ is the probability that a certain state is occupied.

- If $|\varepsilon-\mu| \gg k_BT$, the $n_c(T)$ expression can be simplified to

$$n_c(T) = e^{-(\varepsilon_c-\mu)/k_BT} \cdot \underbrace{\int_0^{\infty} e^{-(\varepsilon-\varepsilon_c)/k_BT} \cdot g_c(\varepsilon)\, d(\varepsilon-\varepsilon_c)}_{}$$

This integral of $x = \varepsilon - \varepsilon_c$ is a function of $T$, $N_c(T)$

**5. a)** The paramagnetic susceptibility $\chi$ of rare-earth ions at high temperature is proportional to the square of the effective Bohr magneton number $p$ and inversely proportional to temperature. The ions $Ce^{3+}$, $Gd^{3+}$, and $Dy^{3+}$ have the electron configurations $4f^1 5s^2 p^6$, $4f^7 5s^2 p^6$, and $4f^9 5s^2 p^6$. Which one of these ions has the highest effective Bohr magneton number? (1.5p)

**b)** Pauli paramagnetism is a type of paramagnetism that is related to conduction electrons. Discuss the physics behind this type of paramagnetism. (2p)

**c)** Explain briefly the concept of diamagnetism. (0.5p)

Solution a) $$\chi = \frac{g^2 J(J+1)}{3} \frac{\mu_0 \mu_B^2 n}{k_B T} \propto p^2/T$$

$$\longrightarrow \quad p = g\sqrt{J(J+1)}$$

We want co calculate $p$ for the 3 given configurations.

With $$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$ we have

$Ce^{3+}: 4f^1[\;]$ $\boxed{\uparrow}\boxed{\phantom{\uparrow}}\boxed{\phantom{\uparrow}}\boxed{\phantom{\uparrow}}\boxed{\phantom{\uparrow}}\boxed{\phantom{\uparrow}}\boxed{\phantom{\uparrow}}$

$m_\ell$: 3 2 1 0 -1 -2 -3

$\left.\begin{matrix} S = \frac{1}{2} \\ L = 3 \end{matrix}\right\} J = \frac{5}{2} = |L - S|$

$\nearrow$ less than half-filled shell

$g = \frac{6}{7}$, $\underline{p = 2.54}$

$L = \sum m_\ell$

$Gd^{3+}: 4f^7[\;]$ $\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$

$m_\ell$: 3 2 1 0 -1 -2 -3

$\left.\begin{matrix} S = \frac{7}{2} \\ L = 0 \end{matrix}\right\} J = \frac{7}{2}$

$g = 2$, $\underline{p = 7.94}$

$Dy^{3+}: 4f^9[\;]$ $\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$

3 2 1 0 -1 -2 -3

$\left.\begin{matrix} S = \frac{5}{2} \\ L = 5 \end{matrix}\right\} J = \frac{15}{2} = |L + S|$

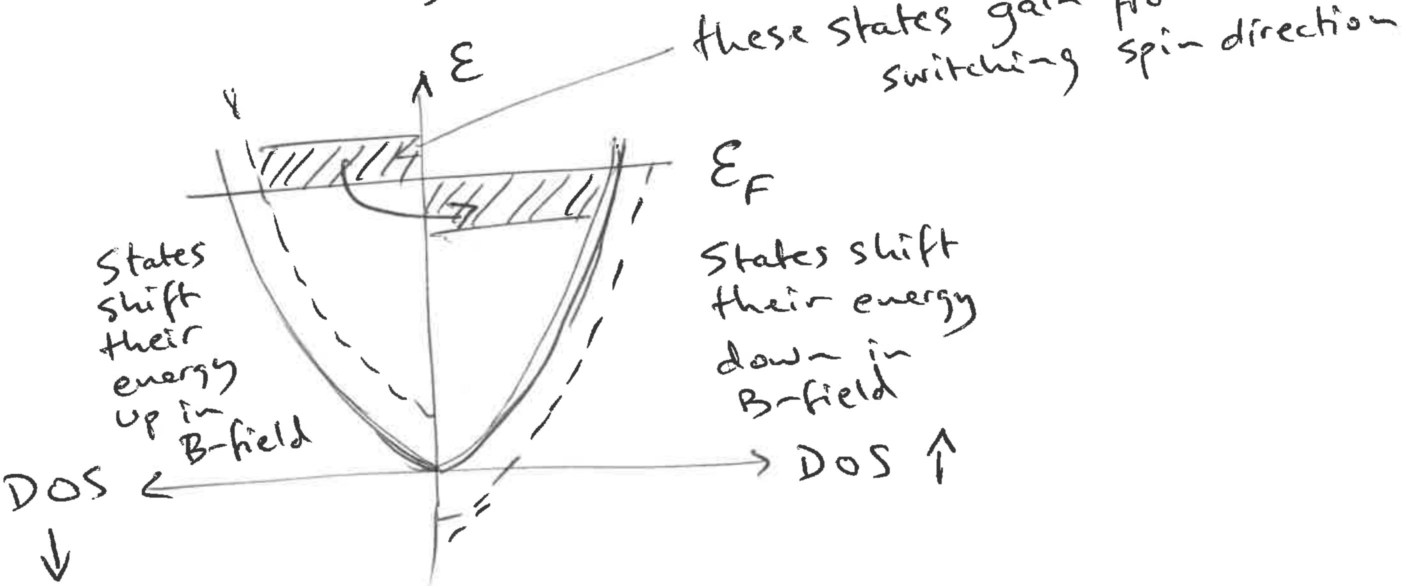
$\nearrow$ more than half-filled shell

$g = \frac{4}{3}$, $\underline{p = 10.65}$

Answer: $Dy^{3+}$ has the highest effective Bohr magneton number, assuming that the Hund's rules can be applied.

5b) Wanted: Discuss Pauli paramagnetism

In applied magnetic field, the electrons in the conduction band (partially filled bands), i.e, the free electrons may change their spin direction to lower their energy. Not all of them will, since the Pauli principle would force the electrons to assume higher energy states.



The energy shift in B-field is $\pm\mu_B B$

Magnetization $M = \mu_B (n_\uparrow - n_\downarrow) =$

$$\approx \mu_B \cdot \left(\tfrac{1}{2} D(\mathcal{E}_F) \cdot \mu_B B \times 2\right)$$

↳ states changing from ↑↓

$$M \approx \mu_B^2 B \cdot D(\mathcal{E}_F) = \mu_0 \mu_B^2 H D(\mathcal{E}_F)$$

$$\chi = \mu_0 \mu_B^2 D(\mathcal{E}_F)$$

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5c) Diamagnetism: Susceptibility $\chi < 0$

Typically a small contribution from all electrons classically seen as precessing with a Larmor freq. $\omega = \frac{eB}{2m}$

6. **a)** We would like to study vacancies in a material. Discuss an experiment that could be used to estimate the activation energy for forming vacancies. Explain introduced concepts and the experimental execution in enough detail to understand if the proposed experiment could solve the problem. (2p)
**b)** Discuss thermal conductivity for metals at low temperature, including the temperature dependence. Explain why so called oxygen-free high thermal conductivity (OFHC) copper has much higher thermal conductivity than stainless steel. (2p)

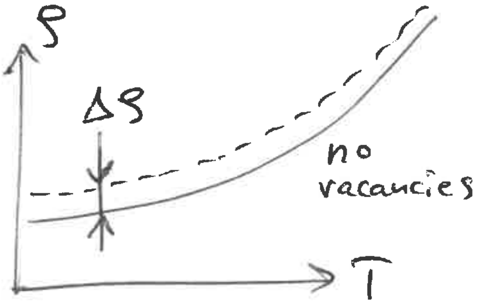
a) Solution : Vacancies are thermally activated, with an equilibrium concentration

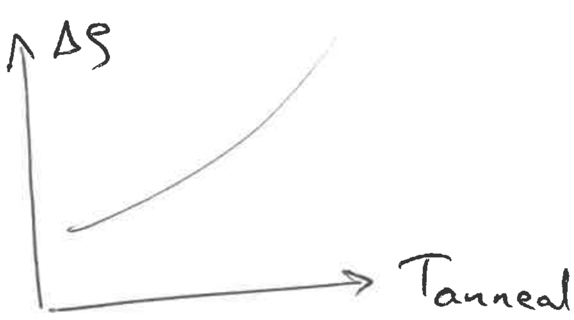
$n_v = N_0 e^{-U_0/k_B T}$ where $U_0$ is the activation energy

At low temperatures, the concentration is no longer in equilibrium, but remains unchanged.

$\Rightarrow$ Quick cooling ("quenching") freezes the $n_v(T_{anneal})$ ↗ temperature before quenching.

Since vacancies cause scattering, studying the electrical resistivity gives a tool to probe $n_v$. $\Delta\rho \propto n_v$





plotting $\ln(\Delta\rho)$ as a function of $\frac{1}{T_{anneal}}$ will give a graph with linear slope $-\frac{U_0}{k_B}$

# 6b) Thermal conductivity for metals at low T

The thermal conductivity $\kappa$ has two contributions electrons and phonons: $\kappa = \kappa_{el} + \kappa_{ph}$

Each contribution can be written $\kappa = C_v \cdot l \cdot v$

Electrons:
- $C_{el} \sim \gamma \cdot T$
- $l$ depends on scattering
- $v \sim v_F$ Fermi velocity

Phonons:
- $C_{ph} \sim T^3$, very low at low T.
- $l$ depends on scattering, sample size
- $v \sim v_s$ sound velocity

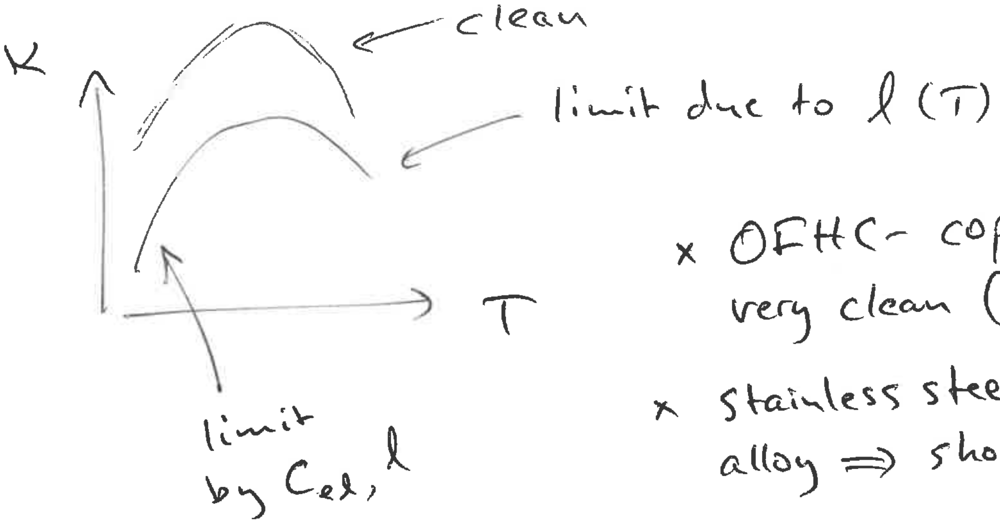
For metals @ low T: electron contribution dominates.

Compare also Wiedemann-Franz law: $\frac{\kappa}{\sigma T} = L = \frac{\pi^2}{3} \cdot \left(\frac{k_B}{e}\right)^2$

$\hookrightarrow \sigma = \frac{ne^2\tau}{m} \sim l$

$l$ decreases with temperature

$\Longrightarrow$ maximum in $\kappa$



× OFHC- copper is very clean (low scattering)

× Stainless steel is an alloy $\Rightarrow$ short mean freepath

$\Longrightarrow \kappa_{OFHC} \gg \kappa_{steel}$