Exam 2010-03-27 Cond-Mat I

1a) Discuss Drude model

Classical model of metallic state

- Electrons as independent, classical particles
- Immobile background of metallic ions (continuum)
- Electrons scatter in random directions
- Instantaneous collisions, local thermal equilib.

Use to explain (partly) electrical conductivity, Hall effect, thermal conductivity, thermoelectric effect.

Limitation: Cannot explain low-temp. specific heat, magnetoresistance etc. that require quantum mech.

Sommerfeld theory ≈ Drude model + Fermi-Dirac distrib. and Q.M. descr. of el.

1b) Given: Relaxation time τ:

probability $\frac{dt}{\tau}$ for collision during dt.

Wanted: Probability of not colliding during time t.

$P(t)$

Solution:

$$P(0) = 1 \qquad P(t_1) \cdot P(t_2) = P(t_1 + t_2)$$

$$P(t+dt) = P(t) \cdot P(dt) = P(t) \cdot \left(1 - \frac{dt}{\tau}\right)$$

$$\Rightarrow \quad \frac{P(t+dt) - P(t)}{dt} = -\frac{P(t)}{\tau}$$

$$\frac{dP}{dt} = -\frac{1}{\tau} \cdot P \qquad \boxed{P(t) = e^{-t/\tau}}$$

Interpretation: τ is the average time between collisions for an electron

2 a) Describe difference between ε_F and μ

Solution μ is appearing in the Fermi-Dirac distribution function: $f_{FD} = \dfrac{1}{e^{(\varepsilon-\mu)/k_BT}+1}$

At any temperature, the value of μ is obtained from

μ: $N = \int_0^\infty D(\varepsilon)\cdot f_{FD}(\varepsilon)\, d\varepsilon$ where $D(\varepsilon)$ is the density of states and N is # of free el.

ε_F is defined as the highest energy occupied at $T=0$.

$$\varepsilon_F: \quad N = \int_0^\infty D(\varepsilon)\cdot f_{FD}(\varepsilon, T=0)\, d\varepsilon = \int_0^{\varepsilon_F} D(\varepsilon)\, d\varepsilon$$

i.e. $\mu(T=0) = \varepsilon_F$.

2b) Show $\mu - \varepsilon_F \propto T^2$ in free el. model. * Prefactor containing ε_F

Solution: Free el. model: $D(\varepsilon)d\varepsilon = 2\cdot\frac{V}{8\pi^3}\cdot 4\pi k^2 dk$

$$N = \int_0^\infty D(\varepsilon)\cdot f(\varepsilon)\, d\varepsilon = \left\{\text{Sommerfeld expansion}\right\} = \int_0^\mu D(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_BT)^2 \underbrace{D'(\mu)}_{\approx D'(\varepsilon_F)}$$

$$= \int_0^{\varepsilon_F} D(\varepsilon)\, d\varepsilon \qquad \approx \int_0^{\varepsilon_F} D(\varepsilon)\, d\varepsilon + D(\varepsilon_F)\cdot(\mu-\varepsilon_F)$$

$$\Rightarrow D(\varepsilon_F)\cdot(\mu-\varepsilon_F) = -\frac{\pi^2}{6}(k_BT)^2\cdot D'(\varepsilon_F)$$

$$\left.\begin{aligned} &D(\varepsilon)\,d\varepsilon = A\cdot k^2 dk \\ &\varepsilon = \tfrac{\hbar^2k^2}{2m}\ ;\ k\sim\sqrt{\varepsilon} \\ &d\varepsilon \sim k\,dk \end{aligned}\right\} \Rightarrow \left.\begin{aligned} &D(\varepsilon)\sim\sqrt{\varepsilon} \\ &D'(\varepsilon) = \frac{1}{2\varepsilon}\cdot D(\varepsilon) \end{aligned}\right\} \Rightarrow \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} = \frac{1}{2\varepsilon_F}$$

$$\Rightarrow \mu - \varepsilon_F = -\frac{\pi^2}{6}(k_BT)^2\cdot\frac{1}{2\varepsilon_F}$$

2c) Define

Bravais lattice: Infinite, periodic array of points that appears exactly the same from any point

$$\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3 \qquad n_i = 0, \pm 1, \pm 2 \ldots$$

($\bar{a}_1, \bar{a}_2, \bar{a}_3$: primitive vectors not all in the same plane)

Reciprocal lattice: The reciprocal lattice $\bar{G}$ of the Bravais lattice $\bar{R}$ is also a Bravais lattice:

$$\bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3 \,, \quad h, k, l = 0, \pm 1, \pm 2 \ldots$$

where $\bar{a}_i \cdot \bar{b}_j = 2\pi\delta_{ij} = \begin{cases} 2\pi & i = j \\ 0 & i \neq j \end{cases}$

(this defines $\bar{b}_j$ and thus $\bar{G}$)

3) a) Given: Monoatomic fcc lattice, Miller indices (hkl)

Wanted: Rule for diffraction

Solution: Structure factor $S_{\bar{G}} = \sum_{\substack{\text{all} \\ \text{atoms} \\ \text{in cell}}} f_j \cdot e^{i\bar{G}\cdot\bar{r}_j}$

$\bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$

Describe fcc lattice as cubic lattice + basis of 4 atoms

$\Rightarrow$ $\bar{G}$ cubic lattice with $\bar{b}_1 = \frac{2\pi}{a}\hat{x}$ etc.

Basis: $\bar{0}$, $\left(\frac{1}{2}, \frac{1}{2}, 0\right)$, $\left(\frac{1}{2}, 0, \frac{1}{2}\right)$, $\left(0, \frac{1}{2}, \frac{1}{2}\right)$

expressed in $(\bar{a}_1, \bar{a}_2, \bar{a}_3)$

$$S_{\bar{G}} = \left\{\begin{array}{c}\text{all atoms the same} \\ \Rightarrow f_j = f\end{array}\right\} = f \cdot \left(1 + e^{i\bar{G}\cdot\left(\frac{\bar{a}_1+\bar{a}_2}{2}\right)} + e^{i\bar{G}\left(\frac{\bar{a}_1+\bar{a}_3}{2}\right)} + e^{i\bar{G}\left(\frac{\bar{a}_2+\bar{a}_3}{2}\right)}\right)$$

Use $\bar{a}_i \cdot \bar{b}_j = 2\pi\delta_{ij}$

$$\Rightarrow S_{\bar{G}} = f\left(1 + e^{i\pi(h+k)} + e^{i\pi(h+l)} + e^{i\pi(k+l)}\right) \neq 0$$ for diffraction

If all $h\,k\,l$ are odd or all are even

$\Rightarrow S_{\bar{G}} = 4f$

If one or two of them are odd $\Rightarrow S_{\bar{G}} = 0$ $\left(e^{i\pi} = -1\right)$

3b) Given NaCl structure $\Longleftrightarrow$ fcc lattice with basis $\bar{0}$ and $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$ (Na, Cl)

Explain: Why same rule as above for NaCl?

Solution: The atomic form factors f_j are different for Na and Cl $\Rightarrow$ no general cancellation of further reflexes

3c) Given KCl : NaCl structure but missing reflexes

Explain why missing reflexes. Show All-even reflexes remain

Solution : The atomic form factors for K^+ and Cl^- are very similar, since they contain the same number of electrons.

We thus have both the condition that all hkl are odd or even and a condition that

$$\sum_{\substack{\text{two-atom} \\ \text{basis}}} e^{i\bar{G}\cdot r_j} \neq 0$$

$$e^{i\bar{G}\cdot\bar{0}} + e^{i\bar{G}\cdot\left(\frac{\bar{a}_1+\bar{a}_2+\bar{a}_3}{2}\right)} = 1 + e^{i\pi(h+k+l)} = \begin{cases} 2 & \text{even sum} \\ 0 & \text{odd sum} \end{cases} \quad h+k+l$$

If all hkl are odd $\Rightarrow$ odd sum $\Rightarrow$ no reflex

Thus only all hkl even remains.

4) Given: Al: fcc with lattice param. $a = 4.05$ Å

a) Wanted: Expression for the k-volume of 1:st B.Z.

Solution: The Brillouin zone is the Wigner-Seitz cell of the reciprocal lattice, which is a primitive cell, containing one lattice point.

The primitive cell volumes are related by $V_g = \frac{(2\pi)^3}{V_c}$

Since fcc contains 4 lattice points/cell

$$\Rightarrow \quad V_g = \frac{(2\pi)^3}{\left(\frac{a^3}{4}\right)} = \frac{32\pi^3}{a^3}$$

b) Describe Debye model and find volume of Debye sphere for Al.

Solution: Basic assumptions:

* Linear relation $\omega = v_s \cdot |\bar{K}|$ ($\bar{K}$: K-vector of lattice vibrations; v_s: sound velocity)

* Cut-off frequency ω_D such that

$$3N = \int_0^{\omega_D} D(\omega)\, d\omega$$

(3: pol. dir.; N: # atoms; $D(\omega)$: phonon density of states)

With $D(\omega)\, d\omega = 3 \cdot \left(\frac{L}{2\pi}\right)^3 \cdot 4\pi K^2 dK$

and $\frac{N}{L^3} = \frac{N_{cell}}{V_{cell}} = \frac{4}{a^3}$

$$\Rightarrow \quad 3 \cdot \left(\frac{4}{a^3}\right) = \int_0^{K_D} 3 \cdot \frac{1}{(2\pi)^3} \cdot 4\pi K^2 dK = \frac{K_D^3}{2\pi^2}$$

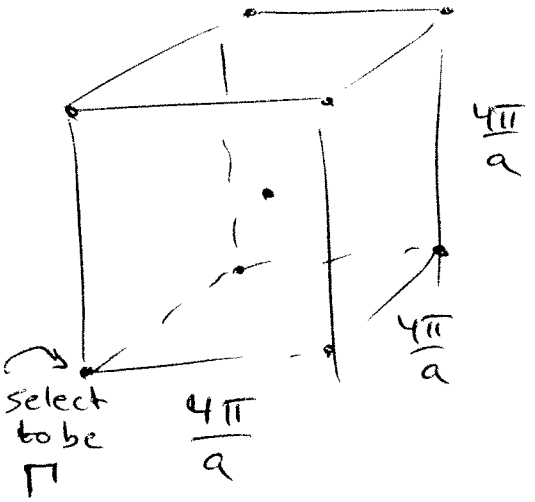
$$\Rightarrow K_D^3 = \frac{24\pi^2}{a^3} \; ; \quad \frac{4}{3}\pi K_D^3 = \frac{32\pi^3}{a^3} = \text{volume of Debye sphere}$$

4c) Compare Debye sphere radius $\left(\frac{(24\pi^2)^{1/3}}{a}\right.$ from b$\left.\right)$ with distance from center Γ of B.Z. to zone boundary in [100] and [111] dir. for Al.

$\hookrightarrow \left(\frac{3}{\pi}\right)^{1/3} \cdot \frac{2\pi}{a}$

Solution: The Brillouin zone is obtained as the Wigner-Seitz cell constructed in the reciprocal lattice.

The reciprocal lattice of fcc is a bcc lattice with lattice param. $\frac{4\pi}{a}$



The Wigner-Seitz cell is constructed by bisecting nearest-neighbor distances with perpendicular planes.

⊛ In the [100] direction K-max will thus be

$$K_{max}^{[100]} = \frac{1}{2}\cdot\left(\frac{4\pi}{a}\right) = \frac{2\pi}{a} \;;\; \frac{2\pi}{(24\pi^2)^{1/3}} \approx 1.015 = \left(\frac{\pi}{3}\right)^{1/3}$$

i.e. Debye sphere a bit smaller than B.Z. in [100] dir.

⊛ In the [111] direction:

$$K_{max}^{[111]} = \frac{1}{4}\cdot\sqrt{3}\cdot\frac{4\pi}{a} = \frac{\sqrt{3}\pi}{a} \;;\; \frac{\sqrt{3}\pi}{(24\pi^2)^{1/3}} \approx 0.88$$

i.e. $K_{max}^{[111]} < K_D$

5) a) Given : Color of gemstones

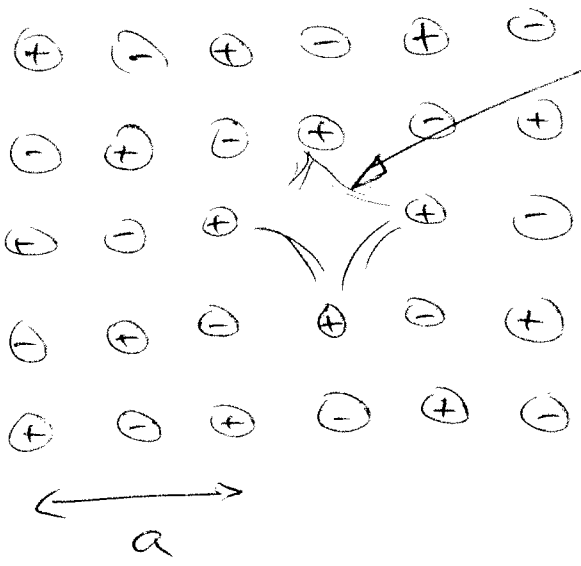
Often due to incomplete 3d shells of metal ions.

Sometimes no metal ions

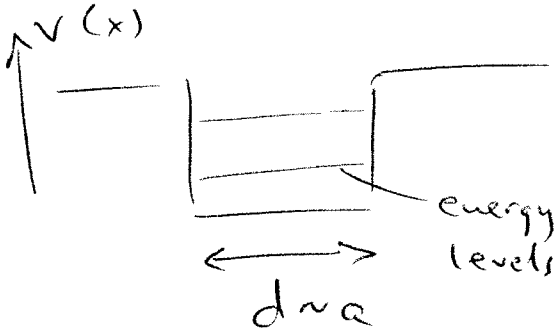
Wanted : Explanation for colors of crystals and gemstones even without metal ions with 3d orbital

Solution : Such colors arise from color centers, which are created by vacancies in ionic crystals or charged ions in otherwise charge-neutral crystals.

Color can, for instance, arise due to γ-irradiation



Color center works as a potential well for electron, that may be bound



$$\mathcal{E} = \frac{\hbar^2 k^2}{2m} = h\nu = \frac{hc}{\lambda}$$

$$\Rightarrow \lambda \sim \frac{1}{k^2} = \left\{ k = n \cdot \frac{2\pi}{d} \right\} \sim d^2$$

The localized states arise in the energy gap

$\Longrightarrow$ optically active in transparent crystal.

5b) Discuss heat conduction in non-metals

× thermal conductivity low, high temp.

× Why diffusion-like?

Solution: Heat conduction in non-metals due to phonons.

Thermal conductivity $K = \frac{1}{3} C_v \ell v$

C_v: heat capacity; ℓ: phonon mean free path; v: phonon velocity = sound velocity v_s

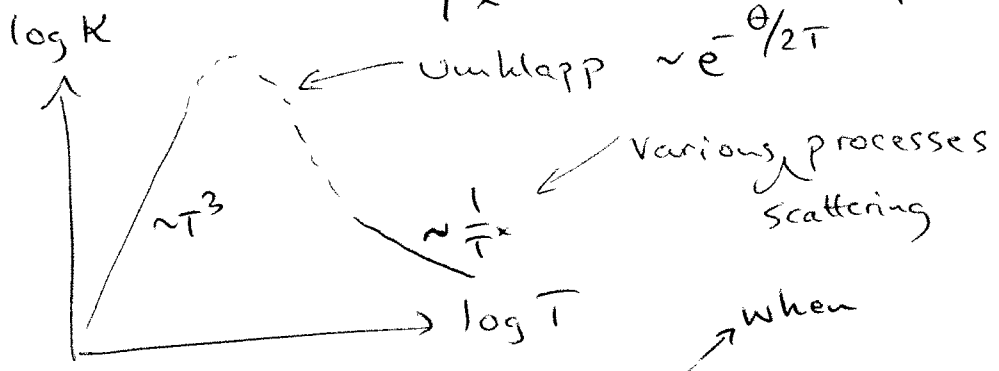
Low temp: $C_v \sim T^3$ (Debye)

ℓ long, increases with decreasing temp. until it reaches sample size → const.

$\Rightarrow K \sim T^3$

High temp.: $(T >> \Theta_D)$: $C_v \sim$ const.

$\ell \sim \frac{1}{T^x} \Rightarrow K \sim \frac{1}{T^x}$



Heat conduction diffusion-like since high-K phonons are involved. $\Rightarrow$ Umklapp processes $\Rightarrow$ change of group velocity.

Compare propagation of sound that occur at low-K $\Longleftrightarrow$ n-process where $\bar{K}_{total}$ remains unchanged.

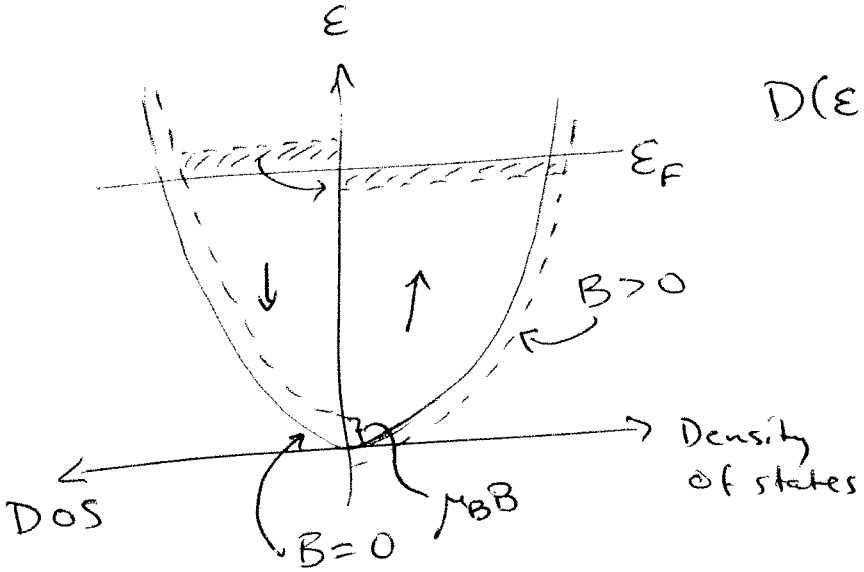
6a) Given: Pauli paramagnetism – itinerant electrons

Wanted: Susceptibility of Pauli paramagnet.

Solution: $\chi = \frac{\partial M}{\partial H} \approx \frac{M}{H} = \frac{\mu_0 M}{B_a}$

$M = \mu_B [n(\uparrow) - n(\downarrow)]$

$n(\uparrow)$, $n(\downarrow)$ → number of free electrons with spin up / down.



$D(\varepsilon) \sim \sqrt{\varepsilon}$

In applied field the electrons with spin along the field will lower their energy.

⟹ some electrons will flip their spin to maintain ε_F.

$$M = \mu_B (n_\uparrow - n_\downarrow) = \mu_B \int_{-\infty}^{\infty} \left[f_{FD}(\varepsilon) \cdot \frac{1}{2} D(\varepsilon + \mu_B B) - f_{FD}(\varepsilon) \cdot \frac{1}{2} D(\varepsilon - \mu_B B) \right] d\varepsilon =$$

$$= \mu_B \int_{-\infty}^{\infty} f_{FD} \cdot \frac{1}{2} \cdot \left\{ D(\varepsilon) + \mu_B B \cdot D'(\varepsilon) - \left(D(\varepsilon) - \mu_B B \cdot D'(\varepsilon) \right) \right\} d\varepsilon =$$

$$= \mu_B^2 B \cdot \int_{-\infty}^{\infty} f_{FD}(\varepsilon)\, D'(\varepsilon)\, d\varepsilon = \left\{ \text{partial integration} \right\} =$$

$$= \mu_B^2 B \cdot \left[\underbrace{\int_{-\infty}^{\infty} f(\varepsilon) \cdot D(\varepsilon) d\varepsilon}_{=0} - \int_{-\infty}^{\infty} f'(\varepsilon)\, D(\varepsilon)\, d\varepsilon \right] =$$

($\to$ delta-spike at ε_F)

$$= \mu_B^2 B \cdot D(\varepsilon_F) \underbrace{\left(-\int_{-\infty}^{\infty} f'(\varepsilon)\, d\varepsilon \right)}_{=+1} = \mu_B^2 B \cdot D(\varepsilon_F)$$

$$\chi = \mu_0 \mu_B^2 D(\varepsilon_F)$$

6b) Given : Superconductivity

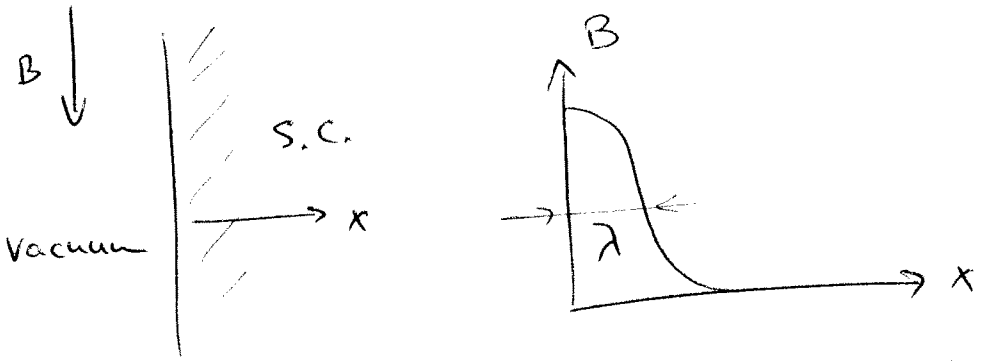
Two length scales : Coherence length ξ

Penetration depth λ

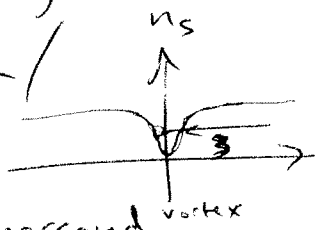
Explain their roles

* Why response to magnetic fields different for $\lambda < \xi$ and $\lambda > \xi$?

Solution : The penetration depth describes the extent of field & screening currents into the supercond.



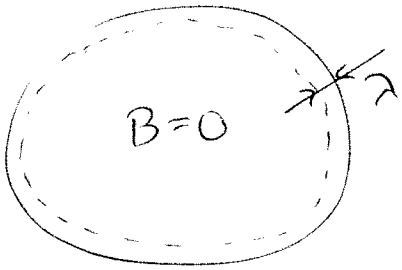
The coherence length describes over which length the superconducting condensate may change / range of interaction.



$\xi \Rightarrow$ size of core of vortex, where supercond. is destroyed

Type - I :

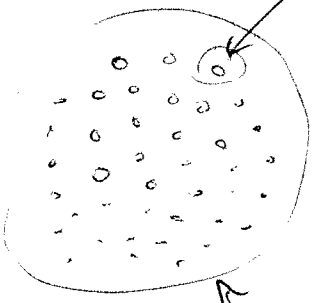
$\lambda \lesssim \xi$



Meissner state

Type - II

$\lambda \gtrsim \xi$



around each vortex : magnetic field of area $\pi \lambda^2$

core of size $\pi \xi^2$

Vortex state at high fields

Field can penetrate without completely destroying superconductivity