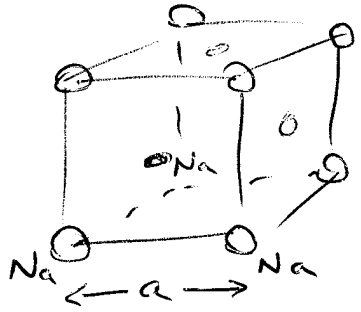
Exam 2008-06-05 | Condensed Matter Physics I

**Problem 1** Given: NaCl structure: fcc lattice with basis of two ions at $\bar{0}$ and $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

Ion radii $r_{Na}$, $r_{Cl}$ "spheres"
0.95 Å 1.81 Å

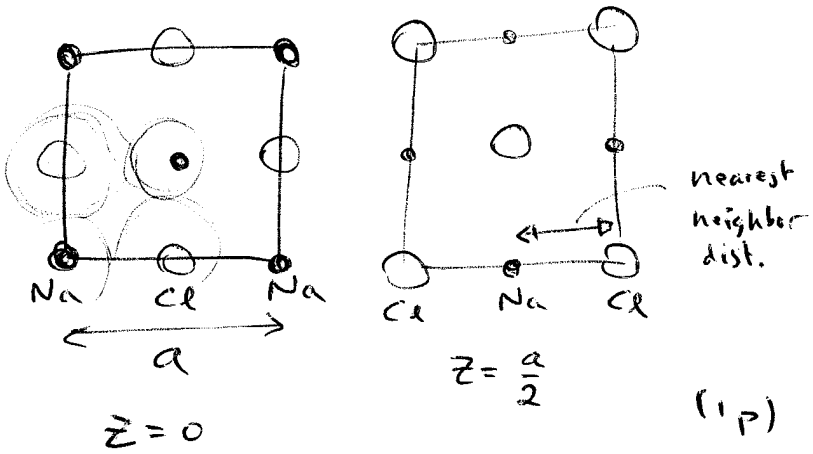
a) Wanted: Ion arrangement in (100) plane

Solution: If Na is at $\bar{0}$ and Cl at $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$
there will also be Na at $\frac{a}{2}(\hat{x}+\hat{y})$




Na on fcc lattice

The Cl ions will also fill up all edges




(1 p)

b) Verify: ⊙ Cl ions make contact only with Na ions.
⊗ Calc. a

Solution: The nearest neighbor distance Na-Cl is $\frac{a}{2}$
The nearest —"— Cl-Cl is $\sqrt{2}\cdot\frac{a}{2}$

Is $\dfrac{r_{Na}+r_{Cl}}{a/2}$ larger than $\dfrac{r_{Cl}+r_{Cl}}{\sqrt{2}\cdot\frac{a}{2}}$ ?

$$2(r_{Na}+r_{Cl}) > \sqrt{2}(r_{Cl}+r_{Cl})\ ?$$

(1.5p)

4 at/cell

$5.52 > 5.12$ (OK) $\quad a = 2\cdot(r_{Na}+r_{Cl}) = 5.52$ Å

c) $$f = \frac{4\cdot\frac{4}{3}\pi r_{Na}^3 + 4\cdot\frac{4}{3}\pi r_{Cl}^3}{a^3} = \frac{2\pi}{3}\frac{(r_{Na}^3+r_{Cl}^3)}{(r_{Na}+r_{Cl})^3} = 0.676$$

68 %

(1.5p)

# Problem 2

**Given:** Metal with $n$ valence el per volume

a) **Show:** $\varepsilon_F = \dfrac{\hbar^2 (3\pi^2 n)^{2/3}}{2m}$

**Solution:** Periodic boundary conditions give spacing of k-points by $\frac{2\pi}{L}$ $\Leftrightarrow$ volume per k-point $\left(\frac{2\pi}{L}\right)^3$

$$\varepsilon = \frac{\hbar^2 k^2}{2m}, \quad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

The Fermi sphere contains $\frac{4}{3}\pi k_F^3 \Big/ \left(\frac{2\pi}{L}\right)^3$ k-points (volume of Fermi sphere)

Each point can take two states (spin ↑ ↓)

$$\text{Eq: } N = 2 \cdot \frac{\frac{4}{3}\pi k_F^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{1}{3\pi^2} k_F^3 \cdot V$$

$$n = \frac{N}{V} \Rightarrow k_F = (3\pi^2 n)^{1/3}$$

$$\Rightarrow \varepsilon_F = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} \qquad (1.5\text{p})$$

b) **Given:** $T_F = 8.16 \cdot 10^4$ K for Cu

**Wanted:** Lattice parameter of Cu

**Solution:** Cu is fcc. Assume 1 val el/atom

$\Rightarrow$ 4 val el per $a^3$ $\quad n = \dfrac{4}{a^3}$

$$\varepsilon_F = k_B T_F \qquad \text{Eq: } k_B T_F = \frac{\hbar^2}{2m} \left(3\pi^2 \frac{4}{a^3}\right)^{2/3}$$

$$\Rightarrow a = \left( (3\pi^2 \cdot 4)^{2/3} \cdot \frac{\hbar^2}{2m k_B T_F} \right)^{1/2} \Rightarrow a = (3\pi^2 \cdot 4)^{1/3} \cdot \frac{\hbar}{(2m k_B T_F)^{1/2}} = 3.62\ \text{Å}$$

$\hbar = 1.055 \cdot 10^{-34}$ J·s
$k_B = 1.38 \cdot 10^{-23}$ J/K
$m_e = 9.11 \cdot 10^{-31}$ kg

Answer: Cu has $a = 3.62$ Å (compare given table value!) (1.5p)

problem 2c)

Given: $C_{v,el} = \gamma T$

Lorenz number $L = \frac{\pi^2 k_B^2}{3e^2}$

Wiedemann-Franz law

Wanted: Express $\gamma$ in terms of $\varepsilon_F$

Solution: Wiedemann-Franz law: $\frac{K}{\sigma T} = L$

Therm. cond. $K = \frac{1}{3} C_{v,el} \cdot l \cdot v_F$

Electr. cond. $\sigma = \frac{n e^2 \tau}{m}$

$n$ = free el. conc., $\tau$ = relaxation time; $l = v_F \cdot \tau$ mean free path

$$L = \frac{K}{\sigma T} = \frac{\frac{1}{3} C_v l v_F}{\frac{n e^2 \tau}{m} \cdot T} = \frac{1}{3} \cdot \frac{m v_F^2}{2} \cdot \frac{1}{n e^2} \cdot \frac{1}{T} \cdot C_v$$

$$\Rightarrow \quad C_v = \frac{3}{2} \cdot L e^2 n \cdot T \cdot \left(\frac{m v_F^2}{2}\right)^{-1}$$

$$C_v = \frac{\pi^2 k_B^2}{2} \cdot n \cdot T \cdot \frac{1}{\varepsilon_F} = \frac{\pi^2}{2} \cdot n k_B \cdot \left(\frac{k_B T}{\varepsilon_F}\right)$$

$$\Rightarrow \quad \boxed{\gamma = \frac{\pi^2}{2} \cdot n k_B \cdot \frac{k_B}{\varepsilon_F}}$$

(1p)

## Problem 3

Given: a) Show that $v_g = \frac{(2\pi)^3}{v_c}$

($v_g$: reciprocal lattice cell volume; $v_c$: real lattice cell volume)

Solution: $v_c = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)$ $\quad \bar{a}_i$ = lattice param.

$v_g = \bar{b}_1 \cdot (\bar{b}_2 \times \bar{b}_3)$ $\quad \bar{b}_i$ = rec. lattice param.

Use $\bar{b}_3 = 2\pi \frac{\bar{a}_1 \times \bar{a}_2}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)} = 2\pi \frac{\bar{a}_1 \times \bar{a}_2}{v_c}$

$$v_g = \bar{b}_1 \cdot \left( \bar{b}_2 \times \left( 2\pi \frac{\bar{a}_1 \times \bar{a}_2}{v_c} \right) \right) = \frac{2\pi}{v_c} \bar{b}_1 \cdot \left( \bar{b}_2 \times (\bar{a}_1 \times \bar{a}_2) \right) =$$

$$= \frac{2\pi}{v_c} \bar{b}_1 \cdot \left\{ (\bar{b}_2 \cdot \bar{a}_2)\bar{a}_1 - (\bar{b}_2 \cdot \bar{a}_1)\bar{a}_2 \right\} =$$

using $\bar{B} \times (\bar{C} \times \bar{D}) = (\bar{B} \cdot \bar{D})\bar{C} - (\bar{B} \cdot \bar{C})\bar{D}$

$$= \left\{ \bar{b}_i \cdot \bar{a}_j = 2\pi \delta_{ij} \right\} = \frac{2\pi}{v_c} \bar{b}_1 \cdot \left\{ 2\pi \bar{a}_1 - 0 \right\} =$$

$$= \frac{(2\pi)^3}{v_c}$$

(1.5 p)

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3c) (After b):

Wanted: $\lambda$ where no diffraction peaks

Solution: $\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2+k^2+l^2)$

for $h^2+k^2+l^2 = 2$ (first reflex) for bcc

when is $\sin^2\theta = 1$ ?

$$\Rightarrow \lambda^2 = \frac{4a^2}{2} = 2a^2 \; ; \quad \boxed{\lambda = \sqrt{2}\, a}$$

$\lambda_{max} = 4.06 \text{ Å}$

(0.5 p)

3b) Given: X-ray (iron powder)

First diffraction peak at $2\theta = 44.60°$

Wanted: Maximum number of diffraction peaks + locations

Solution: Fe is bcc with $a = 2.87$ Å from periodic table

For bcc: structure factor $S_G = \sum e^{i\bar{G}\cdot\bar{r}_j}$

with $\bar{r}_j = \left\{ \bar{0} \text{ and } \underbrace{\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})}_{\frac{1}{2}(\bar{a}_1+\bar{a}_2+\bar{a}_3)} \right\}$

$$S_G = 1 + e^{i\bar{G}\cdot\frac{1}{2}(\bar{a}_1+\bar{a}_2+\bar{a}_3)} =$$

$$= 1 + e^{i\pi(h+k+l)}$$

$\therefore$ Reflex when $h+k+l = \text{even}$

$\left( \bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3 \right)$

Bragg law in quadratic form: $\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2+k^2+l^2)$

First reflex: $h+k+l = 2$ giving $h^2+k^2+l^2 = 2$

ex: $h=k=1$, $l=0$

$\theta = 22.30°$ gives then $\lambda = 1.540$ Å (use to calc.)

| $h+k+l$ | $(h\ k\ l)$ | $h^2+k^2+l^2$ | $\sin^2\theta$ | $\theta$ | |
|---|---|---|---|---|---|
| 2 | 1 1 0 | 2 | 0.144 | 22.30° | 6 reflections |
| 2 | 2 0 0 | 4 | 0.288 | 32.45° | |
| 4 | 2 1 1 | 6 | 0.432 | 41.09° | |
| 4 | 2 2 0 | 8 | 0.576 | 49.36° | |
| 4 | 3 1 0 | 10 | 0.720 | 58.04° | |
| 6 | 2 2 2 | 12 | 0.864 | 68.34° | |
| 6 | 3 2 1 | 14 | 1.008 | | not possible (>1) |

(2p)

**Problem 4 |** **Given:** Monoatomic, one-dim. crystal, N at.

Intern. energy $U = \int_0^{\omega_{max}} \frac{\hbar\omega}{\exp(\frac{\hbar\omega}{k_B T}) - 1} \cdot \frac{2N\, d\omega}{\pi\sqrt{\omega_{max}^2 - \omega^2}}$

a) Show this

**Solution:** A one-dim. model for lattice vibrations has

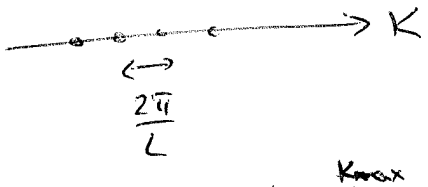
$$\omega = \underbrace{\sqrt{\frac{4C}{M}}}_{= \omega_{max}} \cdot \left|\sin\frac{Ka}{2}\right| \qquad \text{(see lectures + labs)}$$

energy

$$U = \sum_K \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

sum over K-points

Bose-Einstein distr. funct.




$$\sum_K \longrightarrow \frac{L}{2\pi}\int_{-K_{max}}^{K_{max}} dK$$

$$U = \frac{L}{2\pi} \cdot \int_0^{K_{max}} 2 \cdot \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}\, dK$$

↑ pos. and neg. K

Convert to integral over $\omega$: $\frac{d\omega}{dK} = \frac{a}{2} \cdot \omega_{max} \cdot \cos\frac{Ka}{2}$

$$\sin^2 + \cos^2 = 1 \Rightarrow \cos = \sqrt{1 - \sin^2}$$

$$\Rightarrow \frac{d\omega}{dK} = \frac{a}{2}\omega_{max} \cdot \sqrt{1 - \left(\frac{\omega}{\omega_{max}}\right)^2} =$$

$$= \frac{a}{2}\sqrt{\omega_{max}^2 - \omega^2}$$

With $L = N \cdot a$:

$$U = \frac{N \cdot a}{2\pi} \int_0^{\omega_{max}} 2 \cdot \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} \cdot \frac{d\omega}{\left(\frac{d\omega}{dK}\right)}$$

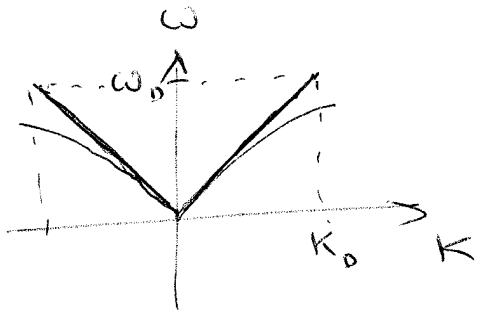
$$U = \int_0^{\omega_{max}} \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} \frac{2N\, d\omega}{\pi\sqrt{\omega_{max}^2 - \omega^2}}$$

(2.5?)

4b) Describe Debye model

Solution The Debye model is a model for the dispersion-relation between phonon frequency $\omega$ and wave vector $K$.

It states: ⊛ linear relation $\omega = v_s \cdot |K|$ ($v_s$: sound velocity)




⊛ Cut-off frequency $\omega_D$ such that the total number of states is obtained by $\int_0^{\omega_D} D(\omega)\,d\omega$ ($D(\omega)$: phonon density of states)

Find an expression for $\omega_D$ for a one-dimensional system

Solution $D(\omega)d\omega = D(K)dK$ or $D(\omega)d\omega = 2\,D(K)dK$ (for pos. K)

For 1D: $D(K)dK = 1 \cdot \left(\frac{L}{2\pi}\right) \cdot dK$

1 ← pol. dir.; $\frac{L}{2\pi}$ ← K-length per K-point is $\frac{2\pi}{L}$ ⇒ number of K-points per K-length = $\frac{L}{2\pi}$

A motion of N atoms/ions is described by N normal modes (1 pol. dir.)

$$\Rightarrow \text{Eq: } N = \int_0^{K_D = \omega_D/v_s} 2 \cdot \left(\frac{L}{2\pi}\right) dK = \frac{L}{\pi} \cdot K_D = \frac{L}{\pi}\frac{\omega_D}{v_s}$$

$$\Rightarrow \omega_D = \pi \cdot v_s \cdot \frac{N}{L} = \frac{\pi v_s}{a} \qquad (1.5\text{p})$$

($\frac{N}{L} = \frac{1}{a}$ ← $L = N \cdot a$, $a$ = lattice param.)

Note: $\frac{\omega_D}{\omega_{max}(\text{probl.a})} = \left\{ v_s = \left.\frac{d\omega}{dk}\right|_{k\to 0} \right\} = \frac{\pi v_s / a}{2 v_s / 1} = \frac{\pi}{2}$

## Problem 5

a) Given: Rare-earth ions $\chi \propto \frac{p^2}{T}$ ($p$: effective Bohr magneton number; $\chi$: paramagn. susceptibility)

$Ce^{3+}: 4f^1 5s^2 p^6$
$Gd^{3+}: 4f^7 5s^2 p^6$
$Dy^{3+}: 4f^9 5s^2 p^6$

One has $p \approx 8.0$

Wanted: Which one?

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

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

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

Hund's rules:
1) Maximize $S = \Sigma s$
2) Maximize $L = \Sigma \ell$
3) $J = |L-S|$ less than half-filled
   $J = |L+S|$ more — " —

$Ce^{3+}$: $4f^1$: ↑ | | | | | | | (3 2 1 0 −1 −2 −3 ℓ) $S = \frac{1}{2}$, $L = 3$ $\Rightarrow J = \frac{5}{2}$

$Gd^{3+}$: $4f^7$: ↑ ↑ ↑ ↑ ↑ ↑ ↑ $\Rightarrow g = \frac{6}{7}$, $p = 2.54$

$S = \frac{7}{2}$, $L = 0$, $J = \frac{7}{2}$ $\Rightarrow g = 2$

$p = 7.94$

$Dy^{3+}$: $4f^9$: ↓ ↓ ↑ ↑ ↑ ↑ ↑

$S = \frac{5}{2}$, $L = 5$, $J = \frac{15}{2}$ $\Rightarrow g = 4/3$

$p = 10.65$

Answer: $Gd^{3+}$

(1.58)

5b) Given: Exchange field $B_E = \mu_0 \lambda M$

Derive: An expression for the Curie temperature in the mean-field approximation

Solution:

Start with magnetization for free spin paramagn:

$$M = \frac{\mu_B N}{V} \tanh\left(\frac{\mu_B B}{k_B T}\right)$$

If $B = B_E$ (no applied field):

$$M = \frac{\mu_B N}{V} \tanh\left(\frac{\mu_0 \mu_B \lambda M}{k_B T}\right)$$

set $m = \frac{M \cdot V}{N \mu_B} \Longrightarrow m = \tanh\left(\frac{\mu_0 \mu_B^2 \lambda}{V \cdot k_B T} \cdot m\right)$

set $t = \frac{V \cdot k_B T}{\mu_0 \mu_B^2 \lambda N} \Rightarrow \boxed{m = \tanh\left(\frac{m}{t}\right)}$

this equation has nontrivial ($m \neq 0$) solution for $t < 1$

i.e. $t = 1 \Leftrightarrow$ critical temp $T_c$ (compare formula sheet)

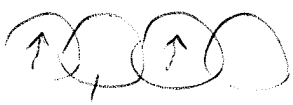
$$T_c = \frac{\mu_0 \mu_B^2 \lambda N}{V k_B} = \frac{\mu_0 \mu_B^2 \lambda n}{k_B} \qquad (1.5\text{p})$$

5c) Describe: Interactions of magn. ions

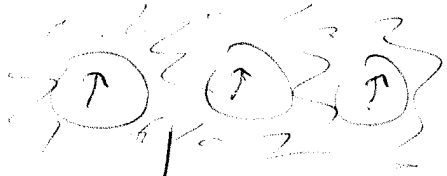
Solution The main source is electrostatic electron-electron interaction

Direct exchange:

Superexchange:




Indirect exchange:



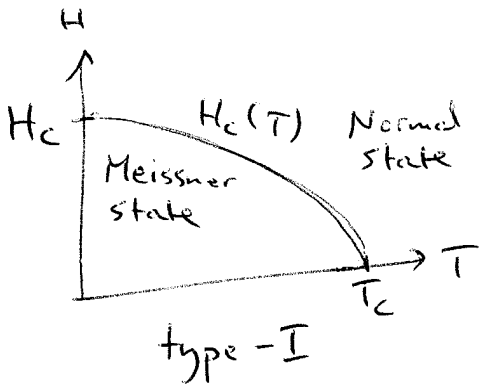

(1p)

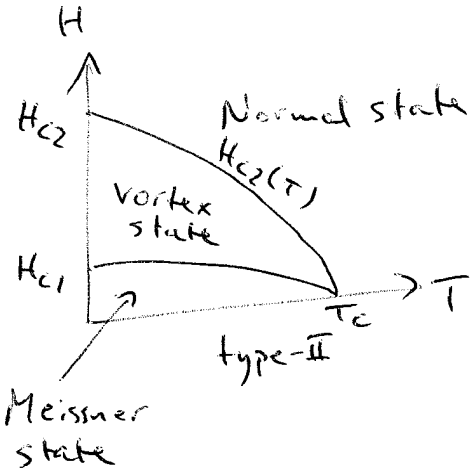
Problem 6

a) Describe ⊗ H-T phase diagram of type-I and type-II supercond.

⊗ What vortices are and why they appear

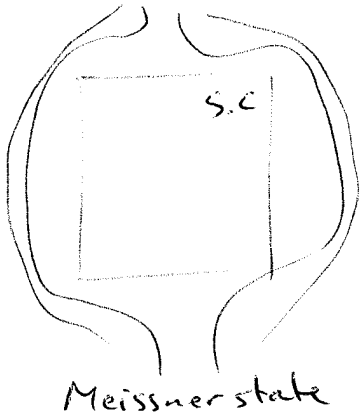
Solution

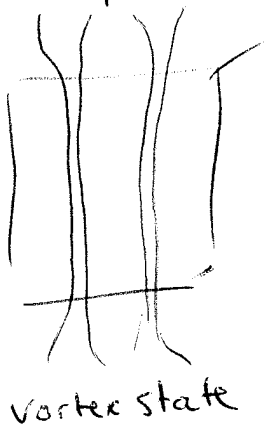



The vortex is a singularity in the shape of a line threading the superconductor. The center of the vortex is normal and is surrounded by a "vortex" of supercurrent circulating it.

They appear in type-II superconductors to lower the energy needed to sustain the magnetic pressure.




Each vortex carries a flux quantum

$$\phi_0 = \frac{h}{2e}$$

(1p)

6b) Given: Simple cubic, divalent metal

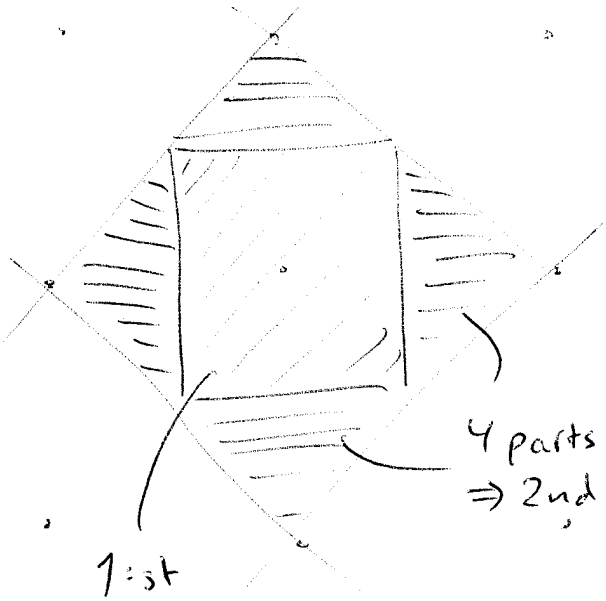
Three cases: free el, weak potential, semiconductor
(I) (II) (III)

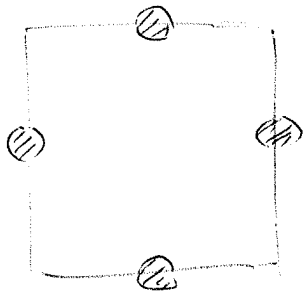
Illustrate: Change of Fermisurface going I → II → III

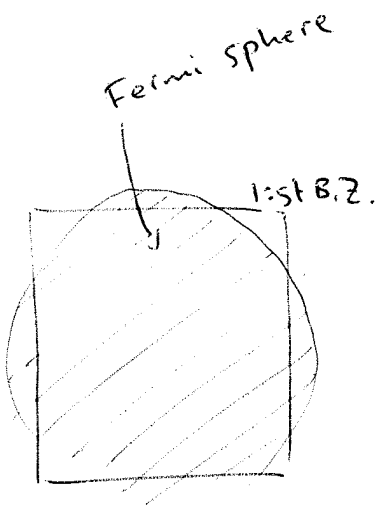
Indicate: 1st and 2nd Brillouin zone (B.Z.), hole pockets, electron pockets

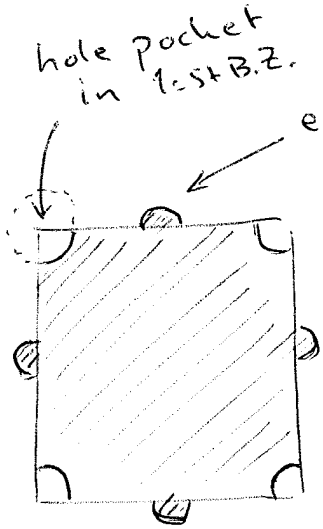
Solution: Divalent metal ⟺ Fermi "sphere" has same volume as 1:st B.Z.

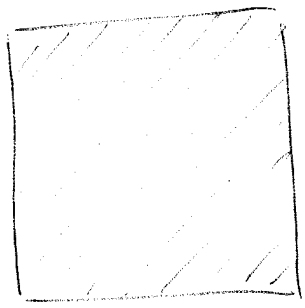
In 2D: same area of Fermi sphere and 1:st B.Z.



free el.

Weak potential

Semicond.:
1:st B.Z. filled
Gap at zone bound.
⇒ no states in 2:nd B.Z.

(1.5p)

6c) Discuss what measurements of ⊗ Hall effect
⊗ Electrical resistivity
⊗ Optical absorption
Can tell about a semiconductor

Solution

Hall effect

Gives information about majority charge carriers

$n \gg p$ : $R_H = -\frac{1}{ne}$

$p \gg n$ : $R_H = +\frac{1}{pe}$

Electrical resistivity

Measurement as a function of temperature gives information about doping (see fig 28.2 in A.M)

For intrinsic semiconductors, $\sigma \sim e^{-E_g/2k_BT}$ so that the energy gap may be obtained.

Optical absorption

Measurements give information about, for instance, band gap and if the gap is direct or indirect.