QCMP-2014/15 — Quantum Condensed Matter Physics

Problem sheet 3: Band structure probes, semiconductors

1. **Quantum oscillations and band structure in Sr_2RuO_4**
   A square lattice of ruthenium, Ru, atoms forms the key structural element of the layered compound Sr_2RuO_4. Three of the five Ru d-orbitals are degenerate and contribute to the band structure close to the Fermi energy: $|d_{xy}\rangle$, $|d_{xz}\rangle$ and $|d_{yz}\rangle$. The d_{xy} orbitals hybridise with those of neighbours in the x- and y- direction, the d_{xz} orbitals only hybridise with those of neighbours along the x-direction, and the d_{yz} orbitals only hybridise with those of neighbours along the y-direction. Hybridisation along the z-direction is negligible. *Four electrons per Ru are distributed equally across the three bands arising from the hybridisation of these orbitals.*

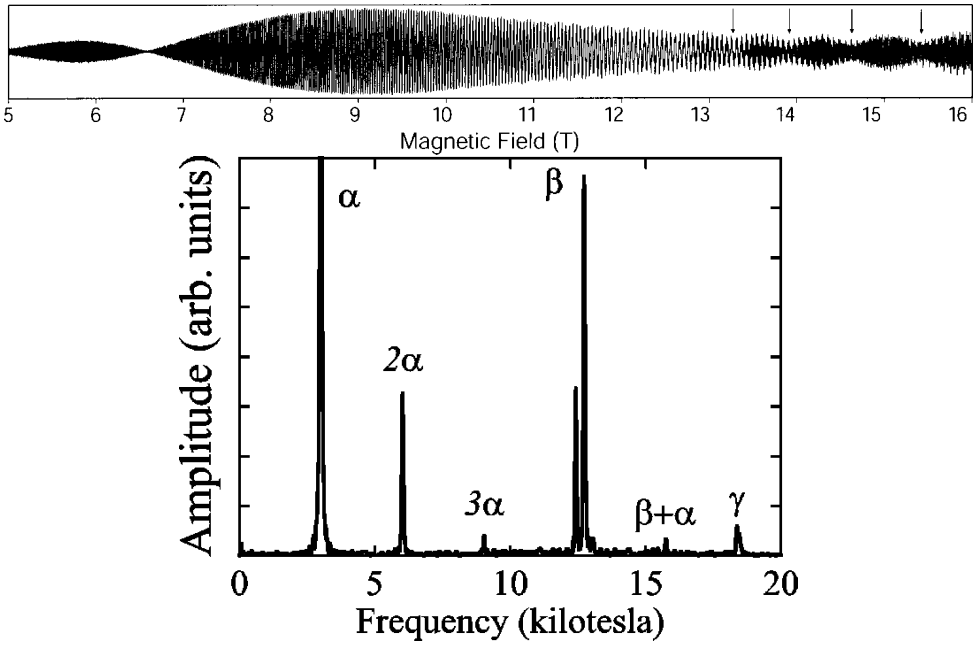


Figure 1: De Haas van Alphen signal measured with $B||c$ in Sr_2RuO_4. Upper panel: experimental raw data. Lower panel: Fourier transformed data, showing fundamental frequencies corresponding to three Fermi surface sheets, α, β and γ [Mackenzie and Maeno, Rev. Mod. Phys. **75,** 657 (2003)].

Hybridisation between the $|d_{xy}\rangle$ orbitals gives rise to the γ Fermi surface sheet, which can be approximated as a cylinder pointing along the c^*-direction with a circular cross-section in the a^*b^* plane. Use data from Fig. 1 to determine the Fermi wavevector k_F characterising this cylinder and to estimate the lattice constant a of the square Ru lattice.

Nearest neighbour hybridisation between the $|d_{xz}\rangle$ orbitals gives rise to Fermi surface sheet A, whereas hybridisation between the $|d_{yz}\rangle$ orbitals leads to Fermi surface sheet B. Sketch the three Fermi surface sheets A, B and γ and state their characteristic dimensions.

A higher order mechanism induces a small hybridisation between the $|d_{xz}\rangle$ and $|d_{yz}\rangle$ orbitals, which causes two new Fermi surface sheets, α and β to emerge from sheets A and B. Relate the dimensions of these sheets to the corresponding de Haas van Alphen frequencies in Fig. 1. Which of these sheets would you expect to be a hole sheet?

Solution:

1) Outline origin of Onsager relation:

* Bohr Sommerfeld $\oint \underline{p}\, d\underline{r} = 2\pi\hbar\left(n+\frac{1}{2}\right)$

In high field: $\underline{p} = m\underline{v} + q\underline{A}$

$m\dot{\underline{v}} = q(\dot{\underline{r}} \times \underline{B}) \Rightarrow m\underline{v} = q(\underline{r}\times\underline{B})(+v_0)$

$\Rightarrow \oint \underline{p}\, d\underline{r} = 2\pi\hbar\left(n+\frac{1}{2}\right) = \oint q(\underline{r}\times\underline{B})\cdot d\underline{r} + q\oint \underline{A}\, d\underline{r} =$

$= -q\underline{B} \cdot \int \underline{r}\, d\underline{r} + q\cdot\Phi = -q\Phi = -qA_r\cdot B$

$\int \underline{r}\, d\underline{r}$: 2 · area; $q = -|e|$; area of orbit in real space

$\Rightarrow$ quantization of orbit area in real space

$$A_r = \frac{1}{B}\cdot\frac{\hbar}{e}\left(n+\frac{1}{2}\right) \qquad (1)$$

* $\underline{k}$-orbits $\hat{=}$ r-orbits: $\hbar\dot{\underline{k}} = q(\underline{v}\times\underline{B})$

$\dot{\underline{r}} = \underline{v}$

$\Rightarrow q(\dot{\underline{r}}\times\underline{B}) = q(\underline{v}\times\underline{B}) = \hbar\dot{\underline{k}}$

$\Rightarrow$ projection of $\underline{r}$ into plane $\perp \underline{B}$ follows $\underline{k}$

$$\Delta\underline{r}_\perp \times \underline{B} = \frac{\hbar}{q}\underline{k}$$

$\Rightarrow$ real space area relates to k-space area:

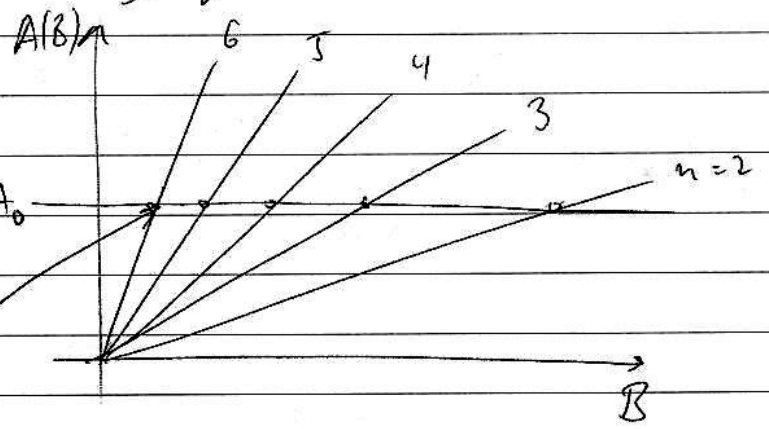
$$\boxed{A_r \cdot B^2 = \left(\frac{\hbar}{q}\right)^2 A_k}$$

$q = -|e|$

⇒ From (1), get

$$A_k(B) = B \cdot \frac{e \cdot 2\pi}{\hbar} \left(n + \frac{1}{2}\right)$$

For Fermi surface cross-section A_0, observe oscillations in density of states at E_F, whenever $A_k(B) = A_0$



Crossing points are at $\frac{2\pi e}{\hbar}\left(n+\frac{1}{2}\right) B_n = A_0$

$$\frac{1}{B_n} = \frac{2\pi e}{\hbar}\left(n+\frac{1}{2}\right) \cdot \frac{1}{A_0}$$

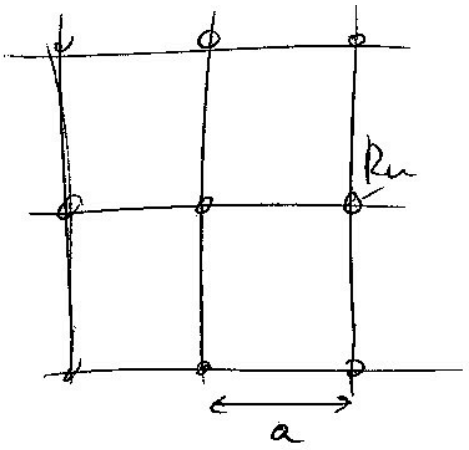
$$\frac{1}{B_{n+1}} - \frac{1}{B_n} = \frac{2\pi e}{\hbar} A_0^{-1}$$

$$\Rightarrow A_0 = \frac{2\pi e}{\hbar} \frac{1}{\Delta(1/B)}$$

* Only the oscillations connected to <u>extremal</u> orbits can be observed, the others smear out.

(2)

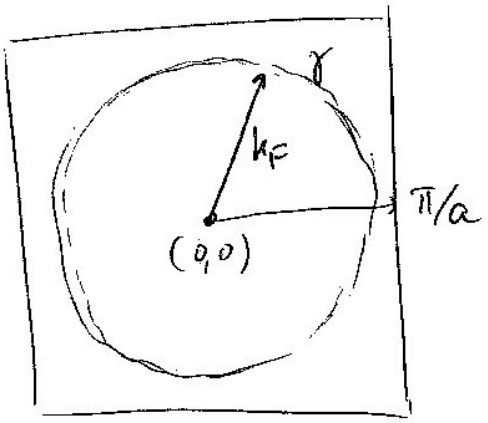
Ru lattice



$|d_{xy}\rangle \rightarrow \gamma$ surface

$4/3$ e^- inside γ.

In k space:



γ = cylindrical

$$2 \cdot \pi k_F^2 \cdot \frac{a^2}{(2\pi)^2} = 4/3$$

↑ spin degeneracy

$$\Rightarrow \pi k_F^2 = A_k = \frac{2}{3} \cdot \frac{(2\pi)^2}{a^2}$$

(γ takes up $\frac{2}{3}$ of B.Z.)

Figure gives $\frac{1}{\Delta(1/B)} \sim 18 \cdot 10^3\ T$

$$\Rightarrow A_k = \frac{2\pi e}{\hbar} \frac{1}{\Delta(1/B)} \simeq 1.72 \frac{1}{\text{Å}^2} = \frac{2}{3} \frac{(2\pi)^2}{a^2}$$

$$\Rightarrow \underline{a \approx 3.91\ \text{Å}}.$$

(Note: actual value is 3.862 Å)

③ Tight binding for $|d_{xz}\rangle$ gives

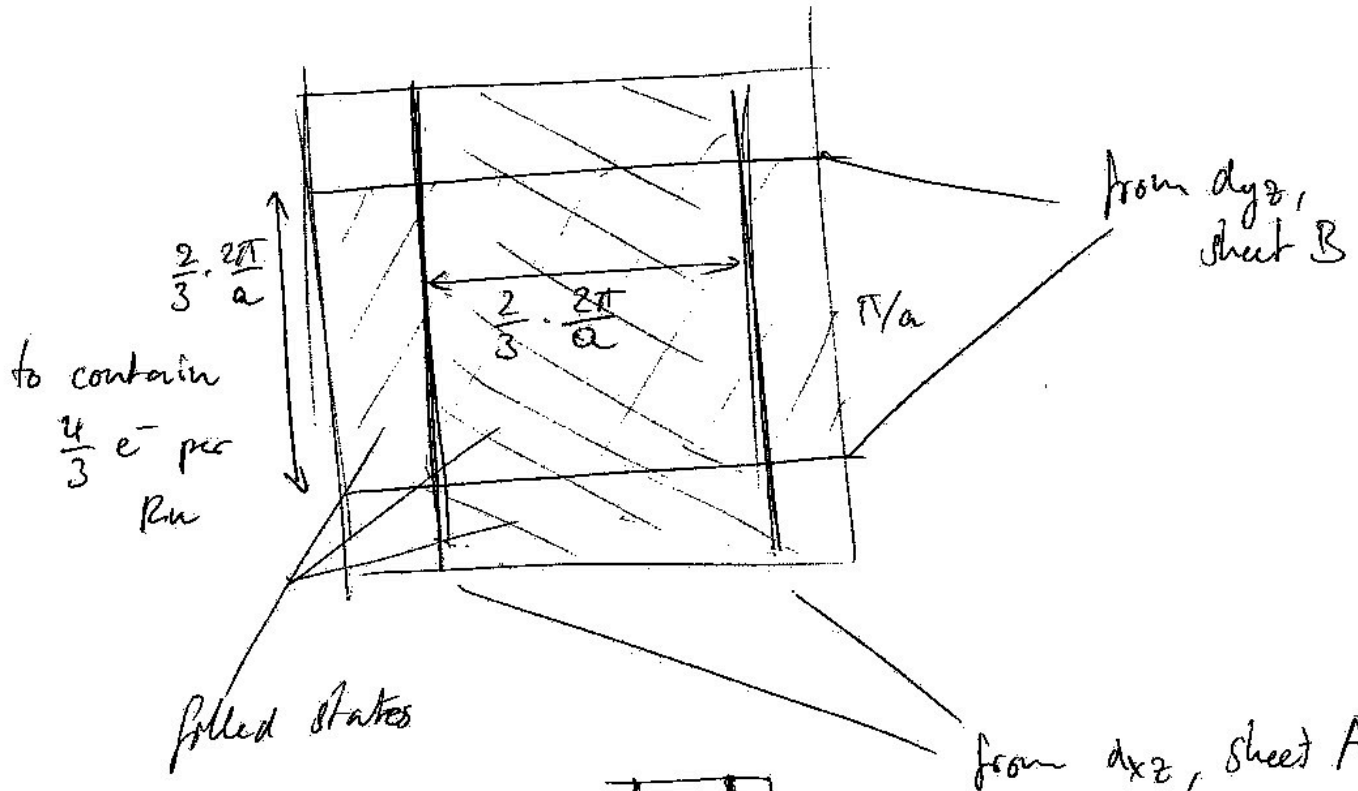
$$|k\rangle = \sum e^{i\underline{k}\cdot\underline{r}_n} |d_{xz}^n\rangle$$

$$\langle d_{xz}|\hat{H}|k\rangle = E_0 + t_x \cos k_x a = E_k^{(x)}$$

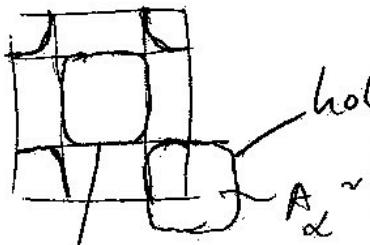
for $|d_{yz}\rangle$ get

$$E_k^{(y)} = E_0 + t_y \cos k_y a$$

These correspond to plane FS sheets:



④ Hybridising these gives



$A_\alpha \sim \left(\frac{1}{3}\frac{2\pi}{a}\right)^2 \rightarrow \frac{1}{6} F_g \sim 3kT$

$A_\beta \sim \left(\frac{2}{3}\frac{2\pi}{a}\right)^2 \rightarrow \frac{2}{3} F_g \sim 12kT$

↑ 18kT

↖ corresponds to exp.

2. **De Haas-van Alphen period of potassium**
   Calculate the period $\Delta(1/B)$ expected for potassium within the free electron model.

   What is the area in real space of the extremal orbit, for $B = 1$ T?

   Solution:

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Potassium: bcc, $a = 5.23\,\text{Å}$. bcc: 2 atoms/conv. unit cell

$$k_F^3 = 3\pi^2 \frac{N}{V} = 3\pi^2 \cdot \frac{2}{(5.23)^3\,\text{Å}^3}$$

$$k_F = \frac{3.89}{5.23}\,\text{Å}^{-1} = 0.745\,\text{Å}^{-1} \qquad \text{(typical metallic } k_F\text{)}$$

$$\pi k_F^2 = A_k = 1.74\,\text{Å}^{-2}$$

Onsager: $\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar} \frac{1}{A_k} = 9.57 \cdot 10^{15} \left(\frac{10^{-20}\,\text{kg}^2}{\text{Å}^2}\right) \frac{\text{Å}^2}{1.74} \frac{1}{\text{kg}^2}$

$$= \underline{5.5 \cdot 10^5 \frac{1}{T}}$$

Frequency $F = 18200\,\text{T} = \underline{18.2\,\text{kT}}$

Real space area $A_r = \left(\frac{\hbar}{eB}\right)^2 A_k = 4.3 \cdot 10^{-31} \frac{\text{m}^4}{\text{m}^4} \cdot 10^{40}\,\text{Å}^4\, A_k =$

$$= 4.3 \cdot 10^9 \left(\frac{A_k}{\text{Å}^{-2}}\right) \text{Å}^2 = \underline{7.5 \cdot 10^9\,\text{Å}^2}$$

$\Rightarrow$ circumference $= 2\pi\sqrt{\frac{A_r}{\pi}} = 3.1 \cdot 10^5\,\text{Å} = 31\,\mu\text{m}$

A mean free path of the order of 30 μm would be required to observe dHvA oscillations in potassium at 1 T

3. **Band gaps and effective masses**
Using the one-dimensional nearly-free electron result for the energy levels at the Brillouin zone boundary $k = \pi/a$

$$E^{\pm}(\mathbf{k}) = \frac{1}{2}\frac{\hbar^2}{2m}(k^2 + (k - 2\pi/a)^2) \pm \frac{1}{2}\sqrt{\left[\frac{\hbar^2}{2m}\left(k^2 - (k - 2\pi/a)^2\right)\right]^2 + 4\,|U_0|^2} \qquad (1)$$

calculate the effective masses of electrons and hole states in terms of the band gap.

Is the data in the table below approximately consistent with your result?

Crystal	m_e^*	E_{gap}/eV
InSb	0.015	0.23
InAs	0.026	0.43
InP	0.073	1.42

Solution:

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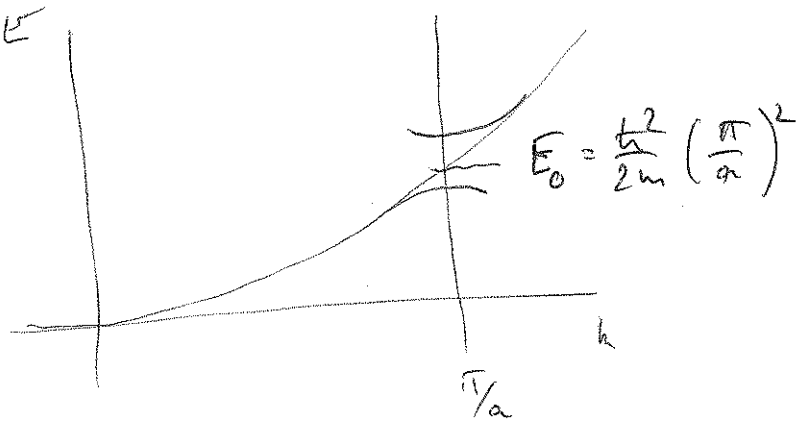
$$\left.\frac{\partial^2 E}{\partial k^2}\right|_{k=\frac{\pi}{a}} = ?$$



Near $\frac{\pi}{a}$, $k = \frac{\pi}{a} + \delta k$ ($k_0 = \frac{\pi}{a}$)

$$E_k = \frac{1}{2}\frac{\hbar^2}{2m}\left((k_0+\delta k)^2 + (k_0+\delta k-2k_0)^2\right) \pm$$

$$\pm \frac{1}{2}\frac{\hbar^2}{2m}\left[\left[(k_0+\delta k)^2-(k_0+\delta k-2k_0)^2\right]^2 + 4\frac{U_0^2}{(\hbar^2/2m)^2}\right]^{1/2} =$$

$$= \frac{\hbar^2}{2m}\left[k_0^2+\delta k^2 \pm \frac{U_0}{\hbar^2/2m}\left(1+\left(\frac{\hbar^2}{2m}\right)^2 \times \frac{1}{2} \times \frac{1}{U_0^2} \times 4k_0^2\delta k^2\right)\right]$$

(Taylor exp. of $\sqrt{1+x}$)

$$= E_0 \pm \left(U_0 + \hbar^2 \frac{2E_0}{U_0}\frac{\hbar^2}{2m}\delta k^2\right) + \frac{\hbar^2}{2m}\delta k^2$$

$$\Rightarrow \frac{1}{m^*} = \frac{1}{m} \pm \frac{1}{m} \times \frac{2E_0}{U_0} \sim \frac{1}{m}\frac{2E_0}{U_0} \sim \frac{1}{m}\frac{4E_0}{E_g}$$

(For $U_0 \ll E_0$; $E_g = 2U_0$)

$$\Rightarrow \boxed{\frac{m^*}{m} \simeq E_g/4E_0}$$

data: E_0 ~ same for ∀

$m^* \propto E_{gap}$ ✓

4. **Hole statistics**
   Show that $f_h(\epsilon) = 1 - f_e(\epsilon)$, where

$$f_e(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}$$

   is the Fermi distribution function for electrons and

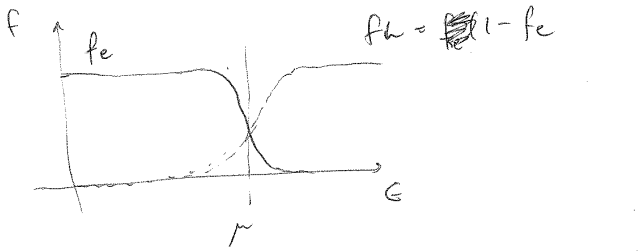
$$f_h(\epsilon) = \frac{1}{e^{\beta(\mu-\epsilon)} + 1}$$

   describes the distribution function for holes.

$f_e(\epsilon) = \left(e^{\beta(\epsilon-\mu)} + 1\right)^{-1}$

$f_h(\epsilon) = \left(e^{\beta(\mu-\epsilon)} + 1\right)^{-1}$

$1 - f_e(\epsilon) = \dfrac{1 + e^{\beta(\epsilon-\mu)} - 1}{1 + e^{\beta(\epsilon-\mu)}} = \dfrac{1}{e^{\beta(\mu-\epsilon)} + 1} = f_h$ ✓



5. **Ge**
   Give a brief explanation of the concepts of *drift velocity*, *electron mobility*, and *effective mass*, as used in solid state physics.

   A sample of Ge is doped so that the concentration of pentavalent donor impurities, N_d is $3 \times 10^{22}\, m^{-3}$, and that of trivalent acceptors, N_a, is $10^{22}\, m^{-3}$. Estimate the concentration of electrons in the conduction band and holes in the valence band at 300 K.

   [The intrinsic carrier density of Ge at 300K is $2.4 \times 10^{19} m^{-3}$.]

   Sketch a graph of the conductivity as a function of temperature you would expect to measure for this sample of Ge.

   Solution:

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Sheet 3 (4)

Drift velocity = v_g averaged over { occupied states or region in real space

$$\left(\frac{\partial}{\partial t} + \tau^{-1}\right) \underline{v} = -\frac{e}{m}\left(\underline{E} + \underline{v} \times \underline{B}\right)$$

For $\underline{B} = 0$, steady state: $\frac{\partial}{\partial t} = 0$

$$v = -\underbrace{\frac{e\tau}{m}}_{\text{mobility}} E$$

mobility = ratio $|v|/|E|$

Effective mass $\frac{\partial v_g}{\partial(\hbar k)} = \frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}$

defined near band edges (max. or min.).

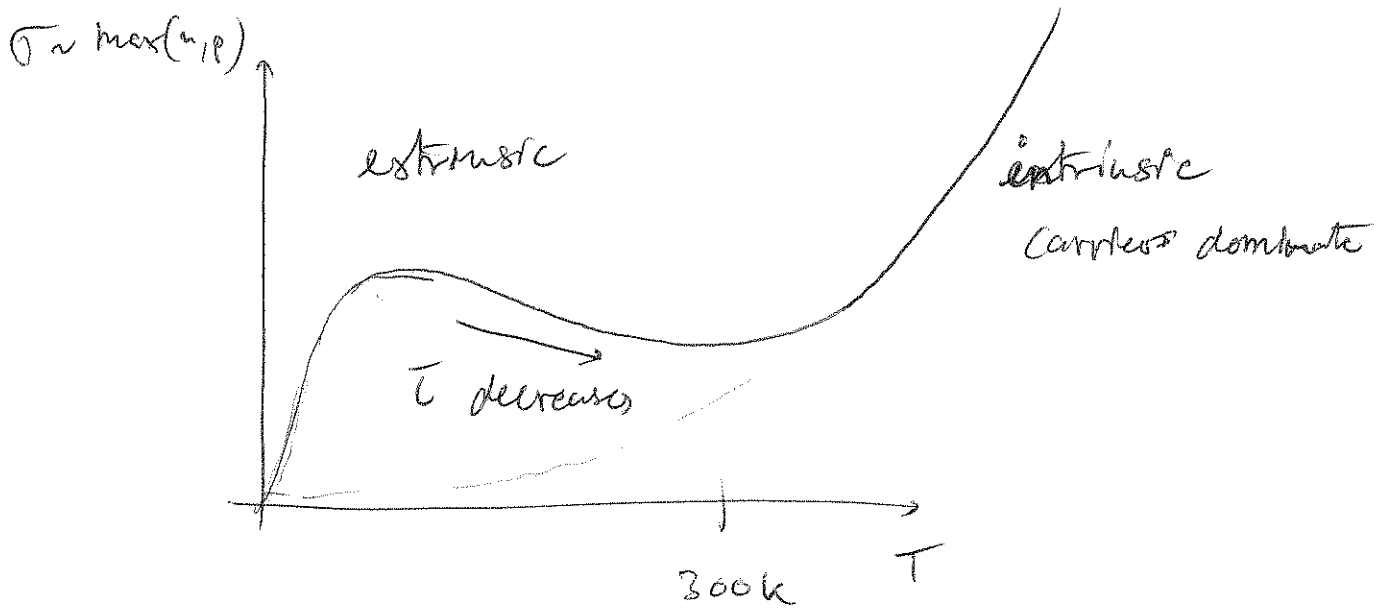
Doped Ge: donors fully ionized at 300K, acceptors likewise, $N_d \gg n_i$, $N_a \gg n_i$

$\Rightarrow$ extrinsic regime, $n = N_d - N_a = \underline{2 \cdot 10^{22} \frac{1}{m^3}}$.

$$n \cdot p = n_i p_i = (1/2)^2 \cdot \left(2.4 \cdot 10^{19} \frac{1}{m^3}\right)^2 = (N_d - N_a) \cdot p$$

$$\Rightarrow p = \frac{(2.4 \cdot 10^{19})^2}{8 \cdot 10^{22}} \frac{1}{m^3} = 0.73\, 10^{16} \frac{1}{m^3}.$$

Sheet 3, 4 ctd.


σ ~ max(n/p)
extrinsic
intrinsic
carriers dominate
T decreases
300k
T

6. **Impurity Bands**

InSb has a dielectric constant $\epsilon = 18$ and an effective mass for electrons $m^* = 0.015m$. Calculate the ionisation energy of a hydrogenic donor orbit.

At what density of donors do you expect to see the effects of overlaps between the orbits of adjacent impurities?

At low densities, donor levels are isolated, and if the temperature is so low that the probability of ionisation is very small, the system will be an insulator. But at higher density, the donor levels overlap to form an impurity band that can support metallic conduction.

Solution:

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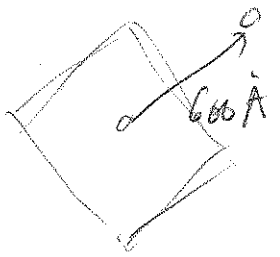
(5.2) hSb $\quad \epsilon = 18, \quad \frac{m^*}{m} = 0.015$

$$r_0 = a_B \cdot \frac{1}{\epsilon} \cdot \frac{m}{m^*}$$

$$E_0 = Ryd \cdot \frac{1}{\epsilon^2} \cdot \frac{m^*}{m_0} \approx 13.6\,eV \cdot \frac{1}{18^2} \cdot 0.015 = 6.3 \cdot 10^{-4}\,eV$$

$$= 0.63\,meV$$

$$r_0 = 0.5\,\text{Å} \cdot \frac{18}{1\text{Å}} \cdot \frac{1}{0.015} = 600\,\text{Å} = \text{extent of orbital}$$



$$\frac{N}{V} \sim \frac{1}{(600\text{Å})^3} = 5 \cdot 10^{-3} \cdot 10^{-6} \cdot 10^{30} \frac{1}{m^3}$$

$$= 5 \cdot 10^{21} \frac{1}{m^3}.$$

$\Rightarrow$ Impurity band forms when distance between donors becomes comparable to r_0. This happens at a donor density of the order of $5 \cdot 10^{21} \frac{1}{m^3}$.

Note: Starred questions are challenge problems; they will do you good, but they go beyond the minimum requirements of the course.