QCMP 2021/22 — 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-directions, 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.*

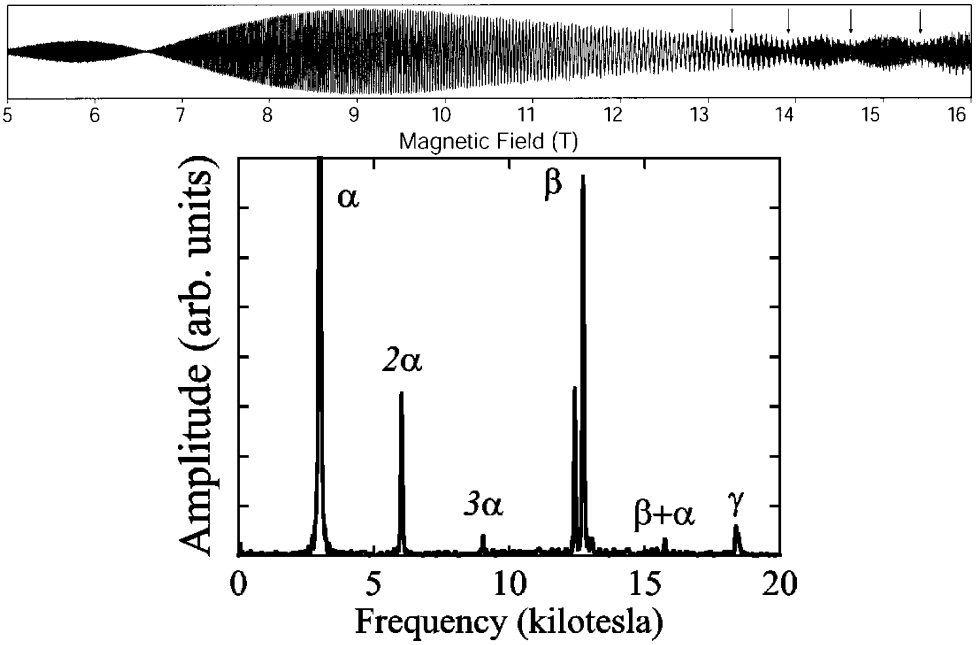

Figure 1: De-Haas–van-Alphen signal measured with $B||c$ in Sr_2RuO_4. Upper panel: experimental raw data. Lower panel: Fourier-transformed data, showing fundamental frequencies corresponding to three Fermi-surface sheets, α, β and γ [Mackenzie and Maeno, Rev. Mod. Phys. **75,** 657 (2003)].

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?

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?

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	$m_{\mathrm{e}}^*/m_{\mathrm{e}}$	E_{gap}/eV
InSb	0.015	0.23
InAs	0.026	0.43
InP	0.073	1.42

4. **Hole statistics**
   Show that $f_{\mathrm{h}}(\epsilon) = 1 - f_{\mathrm{e}}(\epsilon)$, where

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

   is the Fermi distribution function for electrons and

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

   describes the distribution function for holes.

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 $3 \times 10^{22}\,\mathrm{m}^{-3}$, and that of trivalent acceptors, N_{a}, is $10^{22}\,\mathrm{m}^{-3}$. 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 300 K is $2.4 \times 10^{19}\,\mathrm{m}^{-3}$.]

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

6. **Impurity Bands**

   InSb has a dielectric constant $\epsilon = 18$ and an effective mass for electrons $m^* = 0.015\,m_{\mathrm{e}}$. 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.