

NATURAL SCIENCES TRIPOS Part II

Friday 27 May 2016 1.30 pm to 3.30 pm

PHYSICS (7)

PHYSICAL SCIENCES: HALF SUBJECT PHYSICS (7)

QUANTUM CONDENSED MATTER PHYSICS

*Candidates offering this paper should attempt a total of **three** questions. The questions to be attempted are **1, 2** and **one** other question.*

*The approximate number of marks allocated to each question or part of a question is indicated in the right margin. This paper contains **five** sides, and is accompanied by a handbook giving values of constants and containing mathematical formulae which you may quote without proof.*

STATIONERY REQUIREMENTS

2 × 20 Page Answer Book
Rough workpad
Yellow master coversheet

SPECIAL REQUIREMENTS

Mathematical Formulae handbook
Approved calculator allowed

You may not start to read the questions
printed on the subsequent pages of this
question paper until instructed that you
may do so by the Invigilator.

QUANTUM CONDENSED MATTER PHYSICS

1 Attempt **all** parts of this question. Answers should be concise and relevant formulae may be assumed without proof.

(a) Sketch the behaviour of the lattice heat capacity $C_m(T)$ in the Debye approximation, indicating the asymptotic forms in the low temperature and high temperature limits. Given the speed of sound in silver, $v \simeq 3600 \text{ m s}^{-1}$, and the number of atoms per unit volume, $n \simeq 5.9 \times 10^{28} \text{ m}^{-3}$, estimate the Debye temperature θ_D . [4]

(b) Sketch the square of the absolute value of the frequency dependent Drude conductivity $\sigma(\omega)$ as a function of ω , in a metal with scattering rate τ^{-1} . Compute the value of the frequency where $|\sigma(\omega)|^2$ drops to one half of its maximum for a metal with plasma frequency $\omega_p = 5.6 \times 10^{15} \text{ s}^{-1}$ and DC conductivity $\sigma_0 \simeq 9.9 \times 10^6 \Omega^{-1} \text{ m}^{-1}$. [4]

(c) A semiconductor at 350 K and chemical potential 0.9 eV lower than the bottom of the conduction band has electron carrier density $n = 2.3 \times 10^{16} \text{ cm}^{-3}$. A crossover from intrinsic to extrinsic behaviour is observed at 280 K. Obtain the extrinsic electron carrier density n_{ext} of the semiconductor. [4]

(a) The sketch of the heat capacity should highlight the $(T/\theta_D)^3$ behaviour at low temperatures and the saturation at a constant value $3R$ (in $\text{J mol}^{-1} \text{ K}^{-1}$). Here θ_D is the Debye temperature and R is the ideal gas constant. [2]

Bonus mark: the crossover from the low temperature to the high temperature behaviour occurs at the Debye temperature θ_D .

From the lecture notes on the Debye approximation, we know that $k_D^3 = 6\pi^2 N/V$, $\omega_D = vk_D$ and $k_B\theta_D = \hbar\omega_D$. Therefore:

$$\theta_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar vk_D}{k_B} = \frac{\hbar v \sqrt{6\pi^2 n}}{k_B} \simeq 420 \text{ K}. \quad [2]$$

(b) From the lecture notes, recall that the Drude result for the frequency dependent electrical conductivity is

$$\sigma(\omega) = \frac{ne^2\tau}{m(1 - i\omega\tau)},$$

and therefore

$$|\sigma(\omega)|^2 = \frac{n^2 e^4 \tau^2}{m^2 (1 + \omega^2 \tau^2)}.$$

The sketch of this function should look like a bell-shaped curve with a finite maximum at $\omega = 0$ and a power-law decaying tail at large values of ω^2 . [2]

The HWHM is given by the value of ω where $|\sigma(\omega)|^2/|\sigma(0)|^2 = 1/2$, namely $1 + \omega^2 \tau^2 = 2$, which gives $\omega = 1/\tau$. From the expression for the plasma frequency $\omega_p^2 = ne^2/(\epsilon_0 m)$ and for the DC conductivity $\sigma_0 = ne^2\tau/m$, we obtain [2]

$$\sigma_0 = \omega_p^2 \epsilon_0 \tau \quad \text{and} \quad \omega_{\text{HWHM}} = \frac{1}{\tau} = \frac{\omega_p^2 \epsilon_0}{\sigma_0} = 2.8 \times 10^{13} \text{ s}^{-1}.$$

(c) In an intrinsic semiconductor, the electron carrier density is controlled by the concentration of electrons thermally excited above the gap:

$$n(T) \simeq A T^{3/2} e^{-\frac{E_c - \mu}{k_B T}},$$

where A is a proportionality constant and $E_c - \mu$ is the difference between the bottom of the conduction band and the chemical potential. [2]

Note: in the above, one mark will be deducted if the term $T^{3/2}$ is omitted.

The question provides all the parameters needed to obtain the constant A :

$$A = n(T) T^{-3/2} e^{\frac{E_c - \mu}{k_B T}} = 3.1 \times 10^{25} \text{ K}^{-3/2} \text{ cm}^{-3}$$

At 280 K, the semiconductor crosses over from intrinsic to extrinsic behaviour, which means that the extrinsic carrier density is equal to $n(T = 280 \text{ K})$, namely [2]

$$n_{\text{ext}} = A T^{3/2} e^{-\frac{E_c - \mu}{k_B T}} = 9.5 \times 10^{12} \text{ cm}^{-3}.$$

Note: if the factor $T^{3/2}$ had been omitted, one would have obtained $A = 2.0 \times 10^{29} \text{ cm}^{-3}$ and $n_{\text{ext}} = 1.3 \times 10^{13} \text{ cm}^{-3}$.

2 *Attempt this question. Credit will be given for well-structured and clear explanations, including appropriate diagrams and formulae. Detailed mathematical derivations are not required.*

Write brief notes on **two** of the following:

[13]

- (a) the junction field effect transistor and pinch-off;
- (b) direct exchange magnetic interaction;
- (c) quantum oscillations.

(a) You can vary the current through a doped semiconductor by changing the size of the conducting channel with the following set up:

- place metallic current contacts on opposite ends of an n-doped semiconductor (source, drain)
- add p-doped gate contacts in between source and drain, on the sides of the semiconductor.

Some sketches as on slide 150 of the lectures are expected [3]

Depletion zones surround the p-n junctions. Biasing the gates changes the width of the depletion zones. This changes the width of the remaining current-carrying channel in between the gates. [2]

At high drain-source voltages, depleted zones widen and eventually pinch off the conducting channel, resulting in the saturation of the drain-source current for high drain-source voltages. [1.5]

Bonus mark: this is the basis for operating the device as an amplifier.

(b) Direct exchange is one of the types of magnetic interactions between localised electrons. [1]

(TURN OVER)

The wavefunction of two electrons in overlapping orbitals must to be antisymmetric. [1]

Considering both the orbital and spin part of the wavefunction, the antisymmetric requirement is fulfilled by four arrangements: a symmetric spatial part with antisymmetric (singlet) spin part; and an antisymmetric spatial part with three possible symmetric (triplet) spin parts. [2]

Bonus mark: give the equations

$$\frac{1}{2} (|ab\rangle + |ba\rangle) (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$\frac{1}{\sqrt{2}} (|ab\rangle - |ba\rangle) \begin{pmatrix} |\uparrow\uparrow\rangle \\ (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2} \\ |\downarrow\downarrow\rangle \end{pmatrix}$$

The Coulomb interaction depends only on the spatial part of the wave function. The antisymmetric arrangement is energetically preferred because of the lower probability of finding the two electrons in close proximity. In general, this favours a symmetric spin arrangement (triplet state). [2.5]

Bonus mark: if the overlapping orbitals are not orthogonal however, the exchange interaction term may be negative and the lowest energy is then the single state.

Bonus marks: give explicit formulae for the expectation value of the Coulomb interaction; introduce E_{Coul} , E_{ex} ; discuss the short range case $E_{\text{Coul}} = E_{\text{ex}}$.

(c) In strong magnetic fields, the electron energies are quantised. [1]

Bonus mark: give the explicit formula

$$E = \frac{\hbar^2 k_z^2}{2m} + (\ell + 1/2)\hbar\omega_c \quad \omega_c = \frac{eB}{m^*}.$$

The density of states acquires a strongly peaked energy dependence, and as the magnetic field is increased, the peaks shift through the chemical potential, causing the thermodynamic properties of the metal to oscillate as a function of $1/B$. [2.5]

Therefore, properties such as magnetic susceptibility, resistivity, heat capacity, etc. oscillate as a function of the applied magnetic field. [1]

The large applied field introduces energy levels that are cylindrical in reciprocal space, with axis parallel to the direction of the field. The oscillatory response signal is strongest for cylindrical states that are locally tangential to the Fermi surface. Therefore, one can use the oscillations to infer the shape of the Fermi surface. Furthermore, their temperature dependence can be used to obtain the effective mass of the carriers. [2]

Bonus mark: brief discussion of the de Haas-van Alphen oscillations (susceptibility) and/or the Shubnikov de Haas oscillations (resistivity).

3 Attempt either this question or question 4.

Discuss the notion of *effective mass* for electrons moving in a periodic potential. [6]

In the free electron energy $\varepsilon = \hbar^2 k^2 / 2m$ we see that the inverse mass $1/m$ determines the curvature of ε as a function of k . [3]

For electrons in a band, there can be regions of unusually large curvature, in particular near the band gap at the Brillouin zone boundary. This curvature can be interpreted as the electrons having an effective mass $m^* \neq m$. [3]

Bonus mark: if the energy gap E_g is small compared to the free electron energy λ at the boundary, the curvature is enhanced by a factor λ/E_g .

Show how Bloch's theorem follows from the fact that, in a lattice, the Hamiltonian \hat{H} commutes with the translation operator \hat{T}_a , where a is a Bravais lattice vector. Hence, or otherwise, show that Bloch's theorem implies that a wave function ψ_{nk} of wave vector k and band index n must take the form $\psi_{nk} = e^{ik \cdot r} u_{nk}(r)$, where $u_{nk}(r)$ has the same periodicity as the lattice. [8]

If H and T_a commute, they can be simultaneously diagonalised, i.e., we can choose simultaneous eigenvectors of both operators. [2]

Plane waves are a complete basis set of eigenvectors of T_a and they satisfy $T_a |k\rangle = e^{ik \cdot a} |k\rangle$. Therefore, it must be possible to choose a set of eigenvectors $|\psi\rangle$ of H such that $T_a |\psi\rangle = e^{ik \cdot a} |\psi\rangle$. This is one of the forms of stating Bloch's theorem. [3]

Given a wavefunction of the form $\psi_{nk} = e^{ik \cdot r} u_{nk}(r)$, where $u_{nk}(r)$ has the same periodicity as the lattice,

$$T_a \psi_{nk} = e^{ik \cdot (r+a)} u_{nk}(r+a) = e^{ik \cdot a} e^{ik \cdot r} u_{nk}(r) = e^{ik \cdot a} \psi_{nk}. \quad [3]$$

BOOKWORK UP TO HERE. UNSEEN HEREAFTER.

The wave function ψ_{nk} satisfies the equation $[\hat{p}^2/(2m) + \hat{V}(r)] \psi_{nk} = \varepsilon_n(k) \psi_{nk}$, where $\hat{p} = -i\hbar \nabla$. Show that this reduces to

$$\left[\frac{1}{2m} (\hat{p} + \hbar k)^2 + \hat{V}(r) \right] u_{nk}(r) = \varepsilon_n(k) u_{nk}(r). \quad [2]$$

By direct substitution, using $p e^{ik \cdot r} u_{nk}(r) = \hbar k e^{ik \cdot r} u_{nk}(r) + e^{ik \cdot r} p u_{nk}(r)$ and $p^2 e^{ik \cdot r} u_{nk}(r) = (\hbar k)^2 e^{ik \cdot r} u_{nk}(r) + 2\hbar k \cdot p e^{ik \cdot r} u_{nk}(r) + e^{ik \cdot r} p^2 u_{nk}(r) = e^{ik \cdot r} (p + \hbar k)^2 u_{nk}(r)$, the result follows straightforwardly. [2]

Divide the Hamiltonian into the two terms

$$\hat{H}_0 = \frac{1}{2m} \hat{p}^2 + \hat{V}(r) \quad \text{and} \quad \hat{H}_1 = \frac{\hbar^2 k^2}{2m} + \frac{\hbar k \cdot \hat{p}}{m}.$$

(TURN OVER)

At $\mathbf{k} = 0$, $u_{n0}(\mathbf{r})$ is the solution of $\hat{H}_0 u_{n0} = \varepsilon_n(0) u_{n0}$. For a general (small) value of \mathbf{k} , \hat{H}_1 can be treated as a perturbation of the $\mathbf{k} = 0$ case. Use the results from second order perturbation theory to show that the energy at small \mathbf{k} is

$$\varepsilon_n(\mathbf{k}) = \varepsilon_n(0) + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2} \sum_{n' \neq n} \frac{|\langle u_{n0} | \mathbf{k} \cdot \hat{\mathbf{p}} | u_{n'0} \rangle|^2}{\varepsilon_n(0) - \varepsilon_{n'}(0)},$$

where the sum is over all other states $\psi_{n'\mathbf{k}}$ at $\mathbf{k} = 0$ (you may assume that the n -th state is nondegenerate; you may also quote second order perturbation theory formulae without deriving them). [5]

The first contribution in H_1 is a c-number, hence its contribution to the energy is straightforwardly $\hbar^2 k^2 / 2m$. [1]

For the second contribution in H_1 we need to apply the formula for the energy correction in second order perturbation theory:

$$\sum_{n' \neq n} \frac{|\langle u_{n0} | V | u_{n'0} \rangle|^2}{\varepsilon_n(0) - \varepsilon_{n'}(0)}, \quad [2]$$

where V is the perturbing potential (in this case $V = \hbar \mathbf{k} \cdot \mathbf{p} / m$). The expression for $\varepsilon_n(\mathbf{k})$ then follows from a line of algebra. [2]

Derive the ratio m/m^* of the electron mass to the effective mass at $\mathbf{k} = 0$. You may use the formula $m^* = \hbar^2 [\nabla_{\mathbf{k}}^2 \varepsilon_n(\mathbf{k})]^{-1}$. [4]

Using the formula for the effective mass $m^* = \hbar^2 [\nabla_{\mathbf{k}}^2 \varepsilon_n(\mathbf{k})]^{-1}$, and recalling that \mathbf{k} is a c-number and thus $\langle u_{n0} | \mathbf{k} \cdot \mathbf{p} | u_{n'0} \rangle = \mathbf{k} \cdot \langle u_{n0} | \mathbf{p} | u_{n'0} \rangle$, we obtain [2]

$$\frac{m}{m^*} \simeq 1 + \frac{2}{m} \sum_{n' \neq n} \frac{|\langle u_{n0} | \mathbf{p} | u_{n'0} \rangle|^2}{\varepsilon_n(0) - \varepsilon_{n'}(0)}. \quad [2]$$

4 Attempt **either** this question **or** question 3.

Briefly state the assumptions used in Drude theory.

[2]

The Drude model considers the metal to be formed of static positively charged ions and free electrons scattering ballistically off them. [1]

The Drude model neglects long-range interactions between the electron and the ions or between the electrons. It only considers instantaneous collisions between electrons and ions. [1]

BOOKWORK UP TO HERE. PART BOOKWORK, PART UNSEEN HEREAFTER.

Within Drude theory, show that the resistivity tensor for currents within the x - y plane and for an applied magnetic field B along the z -direction is:

$$\begin{pmatrix} \frac{1}{\sigma_0} & -\frac{B}{nq} \\ \frac{B}{nq} & \frac{1}{\sigma_0} \end{pmatrix}$$

and give an expression for σ_0 in terms of n , q , m and τ . Explain the meaning of each of these five symbols.

[10]

The meaning of the symbols is:

[1]

- σ_0 : conductivity
- n : carrier density
- q : charge of the carrier species
- m : mass of the carrier
- τ : relaxation time, or average time between collisions for a given electron.

[In the following, the resistivity and conductivity tensors are worked out in full, but students are only expected to focus on the x - y part of the tensors.]

Assuming a uniformly applied electric field \mathbf{E} and a magnetic field in the z -direction $\mathbf{B} = B\hat{z}$, the (infinitesimal) momentum $\Delta\mathbf{p}$ accumulated on average between collisions is given by

$$\Delta\mathbf{p} = (q\mathbf{E} + q\mathbf{v} \times \mathbf{B}) \tau. \quad [2]$$

Bonus mark: an electron at a given time will on average have been traveling for time τ since its last collision and consequently will have accumulated momentum $\Delta\mathbf{p}$. Because of the random nature of the ballistic scattering with the ions, any prior contributions to the momentum before a scattering event are lost and therefore the net momentum of the electrons at a given time is in fact the accumulated momentum: $\mathbf{p} = \Delta\mathbf{p}$.

In components, the vector equation above can be written as (recall $\mathbf{p} = m\mathbf{v}$)

[2]

$$\begin{aligned} v_x - \frac{qB\tau}{m}v_y &= \frac{q\tau}{m}E_x \\ \frac{qB\tau}{m}v_x + v_y &= \frac{q\tau}{m}E_y \\ v_z &= \frac{q\tau}{m}E_z \end{aligned}$$

(TURN OVER)

which in turn can be cast in matrix form (re-expressing $\mathbf{v} = \mathbf{J}/nq$):

$$\begin{pmatrix} 1 & -qB\tau/m & 0 \\ qB\tau/m & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} J_x \\ J_y \\ J_z \end{pmatrix} = \frac{q^2\tau n}{m} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}.$$

Dividing by the diagonal DC conductivity $\sigma_0 = q^2\tau n/m$, we obtain the resistivity tensor: [1]

$$\begin{pmatrix} \sigma_0^{-1} & -B/nq & 0 \\ B/nq & \sigma_0^{-1} & 0 \\ 0 & 0 & \sigma_0^{-1} \end{pmatrix} \begin{pmatrix} J_x \\ J_y \\ J_z \end{pmatrix} = \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix},$$

in agreement with the result anticipated in the question. [4]

A material has equal numbers of electron and hole carriers. Assuming that the *conductivity* tensors associated with the two carrier types add, and that both carrier types contribute the same DC conductivity in zero applied field σ_0 , find the resistivity tensor of the material. [4]

Since we are told that the *conductivity* tensors add, we firstly need to find the conductivity tensor for each of the carrier species. By inverting the vector relation in the previous part of the question, we obtain [2]

$$\begin{aligned} E_x + \frac{qB\tau}{m}E_y &= \frac{m}{q\tau} \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right] v_x = \sigma_0^{-1} \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right] J_x \\ -\frac{qB\tau}{m}E_x + E_y &= \frac{m}{q\tau} \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right] v_y = \sigma_0^{-1} \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right] J_y \\ E_z &= \frac{m}{q\tau} v_z = \sigma_0^{-1} J_z, \end{aligned}$$

and therefore [1]

$$\begin{pmatrix} \sigma_0 \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right]^{-1} & \sigma_0 \frac{qB\tau}{m} \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right]^{-1} & 0 \\ -\sigma_0 \frac{qB\tau}{m} \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right]^{-1} & \sigma_0 \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right]^{-1} & 0 \\ 0 & 0 & \sigma_0 \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} = \begin{pmatrix} J_x \\ J_y \\ J_z \end{pmatrix}.$$

The two carrier species differ only in the sign of their charge, since we are told that they have the same DC conductivity in zero field, σ_0 . Therefore, upon adding the electron and hole conductivities, the off-diagonal terms cancel and we are left with a diagonal conductivity tensor for the material: [1]

$$\begin{pmatrix} 2\sigma_0 \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right]^{-1} & 0 & 0 \\ 0 & 2\sigma_0 \left[1 + \left(\frac{qB\tau}{m} \right)^2 \right]^{-1} & 0 \\ 0 & 0 & 2\sigma_0 \end{pmatrix}.$$

Show that the diagonal components ρ_{xx} and ρ_{yy} of the *resistivity* tensor of the material approach the value $\sigma_0 B^2 / (2n^2 q^2)$ in the limit of large magnetic fields. Compare the value of B needed to achieve this limit to that required to observe quantum oscillations caused by the quantisation of cyclotron orbits.

[5]

The diagonal conductivity tensor can be straightforwardly inverted to obtain the resistivity tensor, and in the large field limit, $B \gg m/q\tau$, it reduces to:

[1]

$$\begin{pmatrix} (2\sigma_0)^{-1} \left(\frac{qB\tau}{m}\right)^2 & 0 & 0 \\ 0 & (2\sigma_0)^{-1} \left(\frac{qB\tau}{m}\right)^2 & 0 \\ 0 & 0 & (2\sigma_0)^{-1} \end{pmatrix},$$

and we arrive at the desired result $\rho_{xx} = \rho_{yy} = \sigma_0^{-1} (q^2 B^2 \tau^2 / 2m^2) = \sigma_0 B^2 / (2n^2 q^2)$.

[1]

From the lecture notes, we see that electron energies become quantised in the presence of strong applied magnetic fields. This quantisation becomes observable when the relaxation time τ is long enough compared to the characteristic time scale set by the cyclotron frequency $\omega_c = qB/m$, namely $\omega_c \gg 2\pi/\tau$. Therefore, we see that the high field limit required to observe quantum oscillations is the same as the one obtained above, $B \gg m/q\tau$.

[3]

Now consider the resistivity $\rho_{xx}(B)$ of the material introduced above for general values of the field B . Assuming that the carrier density n is constant in the range of temperatures and fields of interest, show that $\rho_{xx}(B)$ divided by the longitudinal zero-field resistivity $\rho_{xx}(B=0)$ depends on the parameters of the system only via the product $B\sigma_0$: i.e., $\rho_{xx}/\rho_{xx}(B=0) = F(B\sigma_0)$, where F is a scaling function. Derive the functional form of F .

[2]

In the case of the material, we derived earlier the conductivity tensor and found that it is diagonal. The resistivity tensor can thus be obtained by straightforward inversion and

$$\frac{\rho_{xx}}{\rho_{xx}(0)} = 1 + \left(\frac{qB\tau}{m}\right)^2 = 1 + \frac{(B\sigma_0)^2}{n^2 q^2}.$$

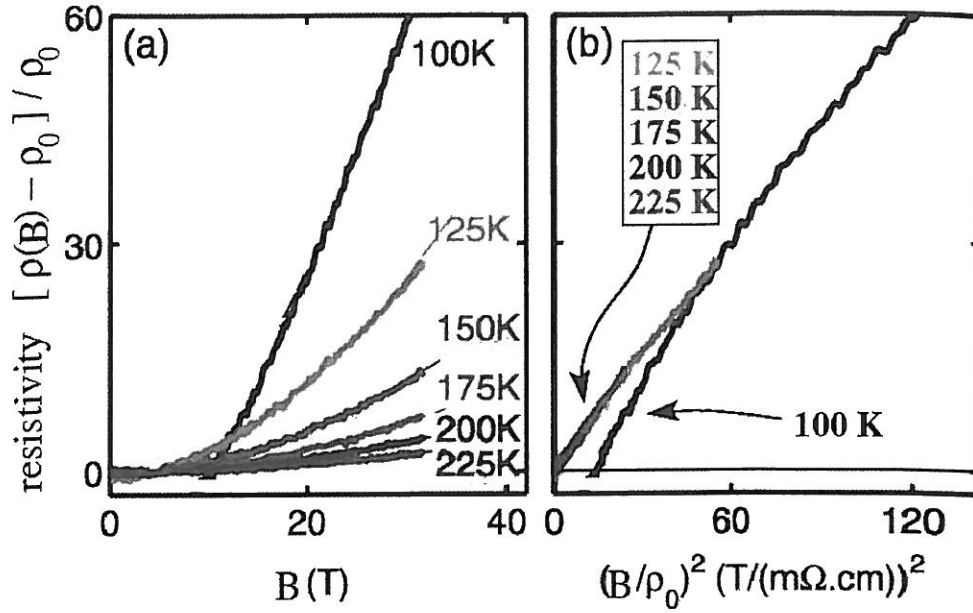
We find that the only dependence on the parameters of the system is via the product $B\sigma_0$. The scaling function F is quadratic (up to an additive constant).

[1]

Consider the two plots at the end of the question, showing the same resistivity data as a function of the applied magnetic field B (left panel) and as a function of $(B/\rho_0)^2$, where $\rho_0 = 1/\sigma_0$. Are the data consistent with the resistivity depending on the parameters of the system only via the product $B\sigma_0$? For what range of temperatures does this dependence hold?

[2]

(TURN OVER)



The data in the figure collapse on top of one another when plotted as a function of $B/\rho_0 = B\sigma_0$, and are therefore consistent with the scaling form, for $125 \text{ K} \leq T \leq 225 \text{ K}$. The collapse is obtained when the data are plotted as a function of $(B\sigma_0)^2$ and the resulting scaling behaviour is linear (note that both axes in the figure are linear). Therefore the behaviour is consistent with the Drude result for the material discussed above. [2]

Note: This scaling behaviour is known as Kohler's rule, and the plot is a Kohler's plot.

END OF PAPER