UNIVERSITY OF CAMBRIDGE

NATURAL SCIENCES TRIPOS Part II

May–June 2020 **1 hour 15 minutes**

PHYSICS (7)
PHYSICAL SCIENCES: HALF SUBJECT PHYSICS (7)

QUANTUM CONDENSED MATTER PHYSICS

*Candidates offering this paper should attempt a total of **four** questions: **three** questions from Section A and **one** question from Section B.*

*The approximate number of marks allocated to each question or part of a question is indicated in the right margin. This paper contains **four** sides, including this coversheet. You may use the formula handbook for values of constants and mathematical formulae, which you may quote without proof.*

You have 75 minutes (plus any pre-agreed individual adjustment) to answer this paper. Do not start to read the questions on the subsequent pages of this question paper until the start of the time period.

Please treat this as a closed-book exam and write your answers within the time period. Downloading and uploading times should not be included in the allocated exam time. If you wish to print out the paper, do so in advance. You can pause your work on the exam in case of an external distraction, or delay uploading your work in case of technical problems.

Section A and the chosen section B question should be uploaded as separate pdfs. Please name the files 1234X_Qi.pdf, where 1234X is your examination code and i is the number of the question/section (A or 4 or 5).

STATIONERY REQUIREMENTS
Master coversheet

SPECIAL REQUIREMENTS
Mathematical Formulae handbook
Approved calculator allowed

QUANTUM CONDENSED MATTER PHYSICS

SECTION A

*Attempt **all** questions in this Section. Answers should be concise and relevant formulae may be assumed without proof.*

A1 Consider a hole formed by removing an electron from a particular Bloch state in an otherwise filled band. What are the momentum, energy, velocity, effective mass and charge of the hole compared with those of an electron occupying this particular Bloch state in an otherwise empty band? [4]

$k_h = -k_e$

$E_h(k_h) = -E_e(k_e)$ (measuring energy from the top of valence band)

the velocity does not change

$m^*(h) = -m^*(e)$

$q = -e$

A2 Calculate the cyclotron frequency for a hole in GaAs at the centre of the Brillouin zone for a magnetic field $B = 1$ T, assuming $\mathrm{d}^2E(k)/\mathrm{d}k^2 \approx 2.44 \times 10^{-38}\,\mathrm{m^4\,kg\,s^{-2}}$. [4]

At band centre we can assume (for the 'usual' parabolic band)

$$E(k) = E_0 + \frac{\hbar^2 k^2}{2m^*} \text{ hence }, \quad \frac{\mathrm{d}^2E(k)}{\mathrm{d}k^2} = \frac{\hbar^2}{m^*}, \text{ so } m^* = \frac{\hbar^2}{\mathrm{d}^2E(k)/\mathrm{d}k^2} \approx 0.5m_e$$

So we found the effective mass. Then the cyclotron frequency (not forgetting the 2π) is

$$\nu = \frac{\omega}{2\pi} = \frac{eB}{2\pi\, m^*} \approx 5.65 \times 10^{10}\mathrm{Hz}$$

A3 A current is passed through an n-doped semiconductor for which the electron mobility is $0.2\,\mathrm{m^2\,V^{-1}\,s^{-1}}$. At what magnetic field, applied perpendicular to the current flow, does the Hall field reach 1% of the electric field along the current flow? [4]

$j_\parallel = \sigma E_\parallel$ with conductivity $\sigma = ne\mu$.

$E_H = R_H j_\parallel B$ Hall field is perpendicular to $E_\parallel$ and $R_H = \dfrac{1}{ne}$, hence $E_H = \mu E_\parallel B$.

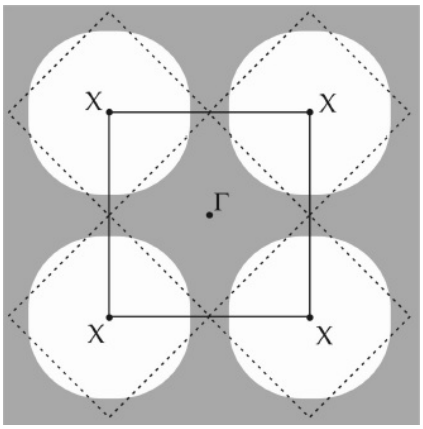
[Or: $0 = j_y \propto neE_y - Bj_x$ with $j_x = \sigma E_x$, so $B\sigma E_x = neE_y$, hence $E_y/E_x = \mu B$ since $\sigma = ne\mu$.]

For the given ratio $\frac{E_H}{E_\parallel} = 0.01$, n cancels, and μ is given in the question $\Rightarrow B = 5 \times 10^{-2}$T

SECTION B
Attempt one question from this section

B4 (a) Explain why a Fermi surface can normally only cross the Brillouin-zone boundary at right angles. Sketch the expected Fermi surface for a two-dimensional metal for different values of the conduction electron density, indicating clearly the electron surfaces, hole surfaces, and van Hove singularities. [6]

A copper-oxide high-temperature superconductor, P, can be modelled as a metal with conductivity in only two dimensions, with a single approximately cylindrical Fermi surface for holes, centred at the corners X of the first Brillouin zone. The Brillouin zone is shown by the solid square in the figure with its centre at Γ:



(b) The superconductor P has a square lattice with lattice constant $a = 0.386$ nm. In a magnetic field B, it exhibits quantum oscillations with the period $\Delta_P(1/B) = 5.5 \times 10^{-5}\ \mathrm{T}^{-1}$. Using the Onsager relation for the extremal cross-sectional area A_k of the Fermi surface,

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

deduce the hole concentration per site in the superconductor. [3]

(c) Another type of copper-oxide superconductor, Q, with the same lattice constant as P, has a hole concentration $p = 1.1$ per site, and exhibits quantum oscillations with a period $\Delta_Q = 1.85 \times 10^{-3}\ \mathrm{T}^{-1}$. Assuming Q has a single cylindrical Fermi surface, as in P, compare the expected periodicity of quantum oscillations in Q with the measured periodicity Δ_Q, and comment on your result. [2]

(d) It is suggested that there may be a doubling of the unit cell in Q, causing the Brillouin zone to fold back, giving the Brillouin-zone scheme indicated by the dashed lines in the figure above. Obtain the number of holes per site implied by this suggestion, and discuss the validity of the modified Brillouin zone as an explanation for the observed quantum- oscillation periodicity Δ_Q. [8]

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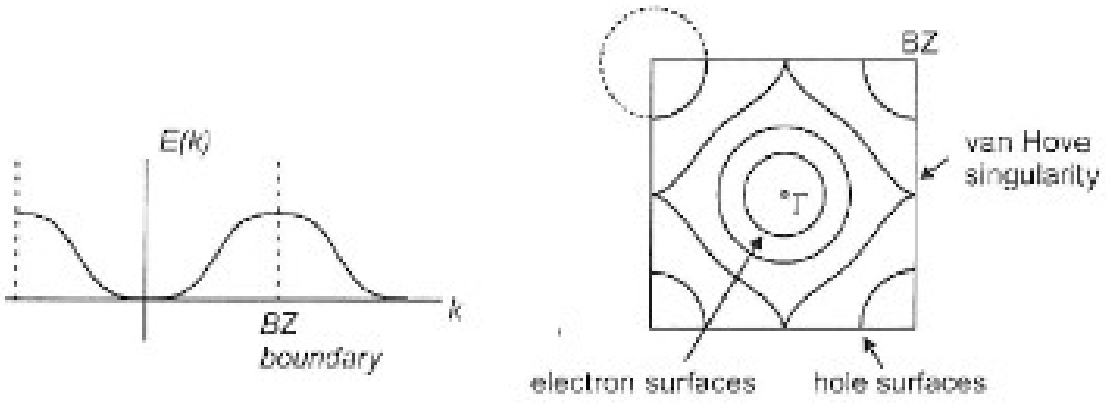
Fermi surface perpendicular to the Brillouin zone (BZ) boundary, i.e. $E(k)$ is periodic, such that $E(k+g) = E(k)$ where g is the reciprocal lattice vector. At the BZ boundary, the dispersion $E(k)$ is flat, due to hybridisation with states near $(k-g)$. For the group velocity we have $v_g = \nabla_k(E/\hbar)$, and it has zero projection perpendicular to BZ boundary. Thus v_g lies in the BZ boundary plane. The sketches below [6]



Calculate the hole density with Onsager: first find the area of Fermi surface

$$A_k = \frac{2\pi e}{\hbar}\frac{1}{\Delta(1/B)} \approx 1.73 \times 10^{20}\mathrm{m}^{-2}$$

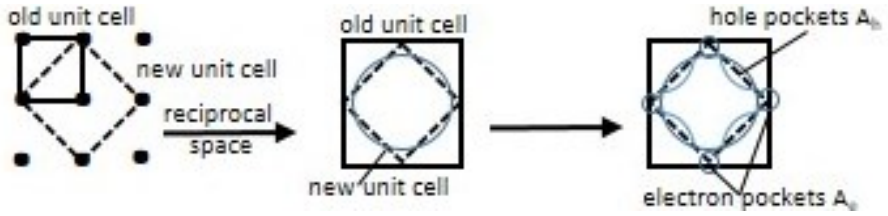
using $\Delta(1/B) = \Delta_P$ from the question. Then calculate the area of BZ for the given lattice spacing a: $(2\pi/a)^2 \approx 2.65 \times 10^{20}\mathrm{m}^{-2}$. For the two (spin up-down) degenerate states per site, the hole concentration is

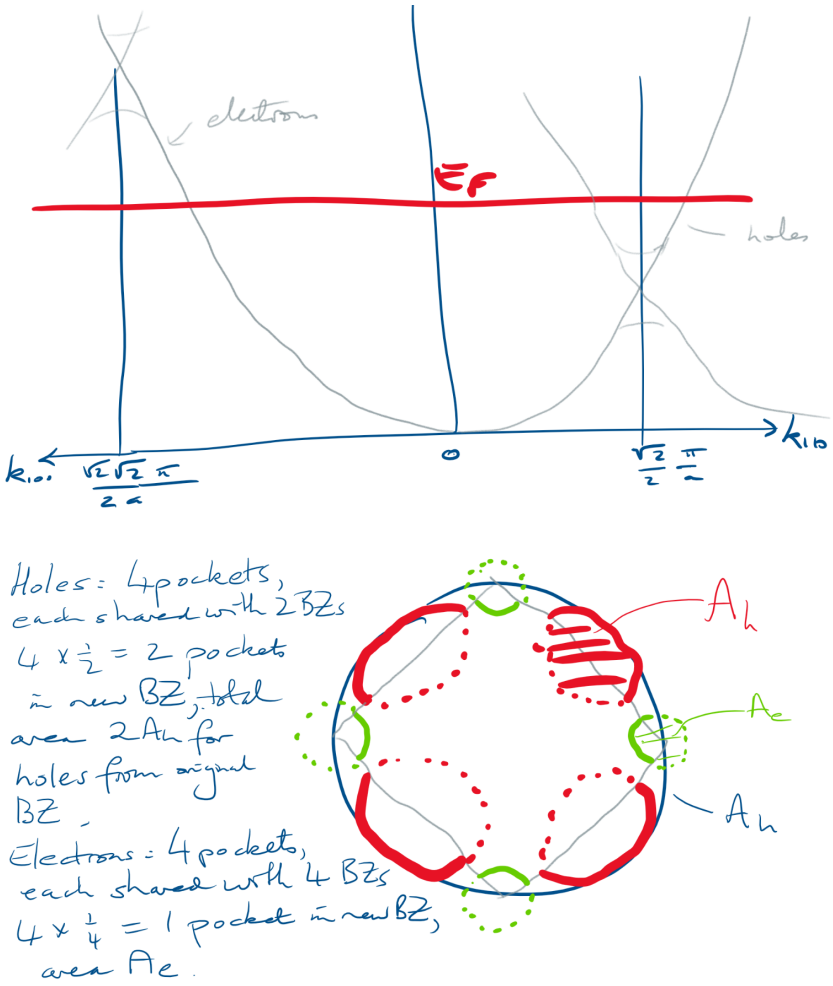
$$p = 2 \cdot \frac{A_k}{A_{NBZ}} = 2 \cdot \frac{1.73}{2.65} = 1.3 \text{ per site} \quad [3]$$

We are told the other superconductor has $p = 1.1$ per site. Since $p \propto A_k \propto 1/\Delta$, we can estimate the expected oscillation periodicity from the comparison with the previous case:

$$\Delta_Q \approx \Delta_P \frac{1.3}{1.1} \text{ which is much smaller than what we are told, } 1.85 \times 10^{-3}\ \mathrm{T}^{-1}. \quad [2]$$

From this we must conclude that this is not a simple cylindrical Fermi surface, additional periodic potential could lead to doubling of unit cell as suggested in the question. This means that the Fermi surface now intersects BZ at right angles, which leads to the formation of pockets for electrons and holes [1]. Here are sketches (below/next page, 3 marks for sensible diagrams/understanding): The actual sizes of the pockets depend on the size of the hybridisation





gap, but the hole density dictates the difference in area. Total number of holes in the sample:

$$N_h = 2(2A_h - A_e + A_{NBZ})\frac{A_{\text{sample}}}{(2\pi)^2}$$

where we have 2 holes per site. Now we get $A_{\text{sample}} = a^2N$ and $A_{NBZ} = \frac{1}{2}(2\pi/a)^2$, so

$$1.1 = \frac{N_h}{N} = \frac{2(2A_h - A_e + A_{NBZ})}{2A_{NBZ}} = \frac{2A_h}{A_{NBZ}} - \frac{A_e}{A_{NBZ}} + 1\ , \text{ so } \frac{2A_h}{A_{NBZ}} - \frac{A_e}{A_{NBZ}} = 0.1.$$

For the material P we had $p = 1.3$ and the oscillation period Δ_{P}. The observed oscillation period is

$$\Delta_{\text{Q}} = \Delta_{\text{P}}\frac{1.85 \times 10^{-3}}{5.5 \times 10^{-5}} \approx 33.6\Delta_{\text{P}}.$$

Therefore density per unit cell in the Q band is $\frac{1.3}{33.6} = 0.0386 = \frac{2A_k}{2A_{NBZ}}$. So $A_k = 0.0386A_{NBZ}$. Given that $2A_h - A_e = 0.1A_{NBZ}$, we know $A_h > 0.05A_{NBZ}$ and $A_e > 0$. So if Δ_{Q} comes from the electron pockets of area $A_e = A_kA_{NBZ}$, then $A_h = \frac{0.1+0.0386}{2}A_{NBZ} = 0.693A_{NBZ}$, which looks plausible.

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B5 (a) What is meant by 'screening' of electrostatic fields inside a conductor? Explain how screening arises and why it is not possible for the conductor to perfectly screen an electric field at short ranges. [2]

(b) Outline the approximations made in the Thomas-Fermi theory of screening and explain why the chemical potential μ is expressed in this theory as

$$E_{\mathrm{F}}(\mathbf{r}) = \mu + eV(\mathbf{r}) \,, \qquad [2]$$

where E_{F} is the Fermi energy calculated within the free-electron model for the local electron density $n(\mathbf{r})$, e is the electronic charge and $V(\mathbf{r})$ is the electrostatic potential.

(c) Certain three-dimensional materials have a linear dispersion relation for the conducting electrons: $E(\mathbf{k}) = \hbar v|\mathbf{k}|$, where v is a constant. Show that within the Thomas-Fermi approximation and for small changes in $n(\mathbf{r})$ from its value n_0 found when V is zero, the excess local charge density induced by the electrostatic potential V is given by

$$\rho_{\mathrm{ind}}(\mathbf{r}) = -e[n(\mathbf{r}) - n_0] \approx -\frac{3e^2 n_0}{E_{\mathrm{F0}}} V(\mathbf{r}) \,,$$

where E_{F0} is the Fermi energy of free electrons with number density n_0 in this material. [6]

(d) Poisson's equation for the electrostatic potential associated with the charge distribution $\rho(\mathbf{r})$ in the presence of additional induced charges $\rho_{\mathrm{ind}}(\mathbf{r})$ is given by

$$\nabla^2 V(\mathbf{r}) = -\frac{1}{\varepsilon_0 \varepsilon} [\rho_{\mathrm{ind}}(\mathbf{r}) + \rho(\mathbf{r})] \,.$$

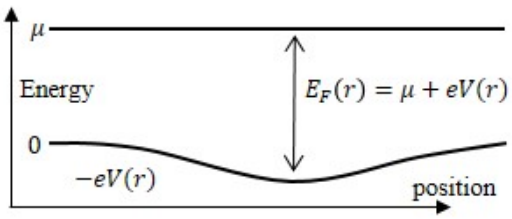
Show that, within the Thomas-Fermi approximation, a screened potential around a point charge of the form $V(r) \propto 1/r \, \exp(-r/\xi)$ satisfies Poisson's equation, and show that the Thomas-Fermi screening length ξ is given by

$$\xi = \sqrt{\frac{\varepsilon_0 \varepsilon E_{\mathrm{F0}}}{3e^2 n_0}} \,. \qquad [4]$$

(e) Evaluate ξ for a material that has a density of $2000\,\mathrm{kg\,m^{-3}}$, relative atomic mass of 65, one valence electron per atom, $\varepsilon = 20$ and $v = 80\,\mathrm{km\,s^{-1}}$. To what extent are the approximations that underlie the Thomas-Fermi theory valid for such a material? [5]

An electric field inside a conductor causes charges to move. In macroscopic electrostatics (where there is no long-term electric current) the charges move until the field inside the conductor is exactly cancelled out. This does not take into account the Pauli exclusion principle, which means that in the ground state a range of states will be occupied by charge carriers, and these include a lot of kinetic energy. If we increase the charge density in response to an electric field in the conductor, this kinetic energy will rise, and there is a trade-off between reducing the energy stored in the electrostatic field and increasing the kinetic energy of the carriers. So on the atomic scale the lowest energy corresponds to only imperfect screening at short distances, whereas at large distances perfect screening is obtained – if there is an electric field at large distances, the electrostatic energy diverges and it is energetically worth for the system to move the charge to screen it. [2]

TF theory assumes independent particles, so the electrons move in the mean field provided by the other electrons and the ion cores. The ion core potential is thus represented by a uniform positive background. It assumes that the potential changes only slowly over the length scale of the Fermi wavevector, so the kinetic energy of the electrons may be expressed in terms of a local Fermi energy derived from the free-electron model (in this material with its particular band structure). The zero of the local energy is offset by the electrostatic potential, so the local Fermi energy is given by $E_{\rm F}(\mathbf{r}) = \mu + eV(\mathbf{r})$. [2]



We need to calculate the Fermi energy in a linearly dispersed sytem, in 3D. This starts from

$$N = V\int_0^{E_{\rm F}} \frac{4\pi k^2 dk}{(2\pi)^3} = \frac{V}{6\pi^2 v^3 \hbar^3} E_{\rm F}^3,$$

$$\text{Then}\quad E_{\rm F} = \left(6\pi^2 v^3 \hbar^3 n\right)^{1/3} = \alpha n^{1/3} \quad\Rightarrow\quad \frac{dE_{\rm F}}{dn} = \frac{1}{3}\alpha n^{-2/3} = \frac{1}{3}\frac{E_{\rm F}}{n}.$$

So for small changes in the Fermi level: $\delta E_{\rm F} = (E_{\rm F}/3n)\delta n$. Now, since $E_{\rm F}(\mathbf{r}) = \mu + eV(\mathbf{r})$, then for small V we can say that $\delta E_{\rm F} = eV(\mathbf{r})$.

$$\text{Then, inverting:}\quad n(\mathbf{r}) - n_0 = \frac{3n_0}{E_{\rm F0}} eV(\mathbf{r})\ ,\quad \text{which gives the required answer.}$$

Note, we are assuming there is no induced charge density due to polarisation of the ion cores, but this approximation is within the TF theory, since we are replacing those by a uniform background. [6]

Substituting $\rho_{\rm ind}$, Poisson's equation becomes

$$\nabla^2 V - \frac{3e^2 n_0}{\varepsilon_0 \varepsilon E_{\rm F0}} V = -\frac{1}{\varepsilon_0 \varepsilon}\rho(\mathbf{r})\ ,$$

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or in Fourier space: $(k^2 + 1/\xi^2)V_k$ = rhs. For a point charge located at $r = 0$, the solution is the same as for the Green's function: ρ_{free} is zero everywhere except at $r = 0$. Although many students will be familiar with this problem via Fourier transformation route, it is easiest to verify by direct substitution that this linear differential equation (in 3D spherical coordinates, with only r-dependence present) is satisfied by

$$V \propto \frac{1}{r}\exp\left[r/\xi\right] \ , \quad \text{where} \ \ \xi^2 = \frac{\varepsilon_0 \varepsilon E_{\text{F}}}{3n_0 e^2}. \qquad [4]$$

$$\text{For this 'model material'} \ \ n_0 = \frac{2000}{65 \times 10^{-3}/6 \times 10^{23}} = 1.85 \times 10^{28}\text{m}^{-3}$$

and substitution of numbers gives $k_{\text{F}} = (3\pi^2 n_0)^{1/3} = 8.16 \times 10^9 \text{m}^{-1}$, $E_{\text{F}} = \hbar v k_{\text{F}} = 6.79 \times 10^{-20}$J $= 0.424$ eV, and $\xi \approx 8 \times 10^{-11}$m. This is a very short screening length!

Since the wavelength corresponding to the Fermi wavevector is $\lambda_{\text{F}} = 2\pi/k_{\text{F}} \approx 6 \times 10^{-10}$m, the theory is applied far outside limits of TF approximations (i.e. $\xi \gg \lambda_{\text{F}}$). Clearly, the accurate value of screening length predicted is meaningless. All one is left with is a general assessment that the screening length has to be of the order of the size of the atom. [5]
