UNIVERSITY OF CAMBRIDGE

NATURAL SCIENCES TRIPOS Part II

Friday 29 May 2015 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 **four** *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) For a hole in GaAs at the centre of the Brillouin zone $\mathrm{d}^2E(k)/\mathrm{d}k^2 = 2.44 \times 10^{-38}\mathrm{m}^4\,\mathrm{kg}\,\mathrm{s}^{-2}$. Find the corresponding cyclotron frequency for a magnetic field $B = 1$ T. [4]

(b) For a one-dimensional solid with atoms aligned along the x-direction, sketch the tight-binding band structure for a band based on p_z orbitals, and also for a band based on p_x orbitals. [4]

(c) The semiconductor germanium has a relative permittivity $\varepsilon_r = 16$ and an electron effective mass $0.2\,m_e$. Estimate the doping concentration level above which this material has non-zero conductivity even at zero temperature. [4]

(a)

$$\mathrm{d}^2E(k)/\mathrm{d}k^2 = \hbar^2/m = 2.44 \times 10^{-38}\mathrm{m}^4\,\mathrm{kg}\,\mathrm{s}^{-2} \quad \Rightarrow \quad m = 0.45 \times 10^{-30}\,\mathrm{kg}$$

$$\omega_c = \frac{qB}{m} = 3.5 \times 10^{12}\,\mathrm{rad/s} = 2\pi \times 0.6 \times 10^{12}\,\mathrm{Hz}$$

(b)

p_z orbital has a minimum at $k = 0$, while the p_x one is “inverted", with the maximum at $k = 0$.

Last mark: the absolute value of the tunnelling matrix element is larger for p_x, so the band is wider.

(c)

From the standard Bohr model, the size of the orbit is:

$$r = \varepsilon_r \frac{m_e}{m^*} a_0 = 80\,a_0 \approx 4\,\mathrm{nm}.$$

(a_0 is the Bohr radius.)

So critical concentration is

$$n_c \sim 1/r^3 \sim 1.5 \times 10^{25}\mathrm{m}^{-3}$$

(factors of order 1 not important)

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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) heavy-fermion systems;

(b) the Stoner-Hubbard model for magnetism in metals;

(c) Bloch oscillations.

(a)

Fermi-liquid like but with m^* up to $> 100\, m_e$

Generally very large m^* equivalent to very low v_F and very large density of states $g(E_F)$.

One obvious consequence is high low-T heat capacity, but large $g(E_F)$ will also, for example, enhance chances of magnetic ordering and superconductivity....

Origin: narrow bands and strong interactions, usually linked to partially filled (and very localised) f-orbitals

Advanced: Mixing of broad s/p/d bands and narrow f-ones, which are pinned to E_F by strong Coulomb interactions that make them always half-filled. Heavy-fermion state (with f electrons incorporated in the Fermi surface) seems to fully develop only at low T; at high T f-electrons seem to behave more like localised magnetic moments.

(b)

Magnetic ordering driven by strong Coulomb interactions.

Competition between the kinetic energy (E_F) and the on-site repulsion between electrons of opposite spin (U)

Physically, creating a spin imbalance (magnetisation) costs kinetic energy, but reduces the Coulomb repulsion

Mathematically, instability seen as the divergence of the susceptibility

Basic result: instability for $Ug(E_F) \sim 1$, where $g(E_F)$ is the density of states per electron, or $U \sim E_F$, since $g(E_F) \sim 1/E_F$

Advanced: there's a few quotable lines of derivation of the susceptibility in the notes...

(c)

What are: AC current from DC applied electric field.

Frequency (detectable through microwave radiation) proportional to applied DC field.

Explanation: semiclassical dynamics of wave packets; key: applied force leads to constant time derivative of the *quasi* (or crystal) momentum.

Actual microscopics: transfer of the momentum to the lattice, Bragg scattering

Adanced: Experimentally actually hard (impossible) to see in normal crystals, because it would require no scattering... but seen in “artificial" superlattices (with large period, hence small Brillouin zone).

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

Explain why a material with an even number of electrons per unit cell can be a band insulator. [3]

The quantisation of states from the boundary conditions gives that the number of discrete k states in the Brillouin zone is equal to the number of unit cells [1]. The total number of states is double because of the electron spin [1]. For an even number of electrons per unit cells an integer number of bands can be fully occupied [1].

For a free two-dimensional (2D) electron gas, show that the Fermi wavevector is

$$k_{\mathrm{F}} = \sqrt{2\pi n}\,,$$

where n is the electron density. [2]

Could integrate, but faster to just divide the area of a circle, πk_F^2, with the unit area in k space, $(2\pi)^2/A$, and remember the factor of 2 for spin:

$$2 \times \pi k_F^2 A/(2\pi)^2 = N \quad \Rightarrow \quad k_F = \sqrt{2\pi N/A} = \sqrt{2\pi n}$$

A 2D electron gas is subject to a periodic potential

$$V(x, y) = -V_0 \left[\cos(Qx) + \cos(Qy)\right],$$

where $Q = \alpha\sqrt{2\pi n}$, with $\sqrt{2} < \alpha < 2$, and $V_0 \geq 0$. Sketch the shape of the 1st Brillouin zone, clearly labelling its dimensions. [2]

A square $Q \times Q$

Sketch the Fermi surface for the cases $V_0 = 0$ and $V_0 > 0$, labelling the electron and hole pockets for the case $V_0 > 0$. [4]

Since

$$Q/2 < k_F < Q/\sqrt{2}$$

the circle of radius k_F intersects the square of side Q, so have electron pockets on the sides and hole pockets in the corners.

For $V_0 > 0$, the Fermi surface cuts the the Brillouin zone at right angles.

ESSENTIALLY BOOKWORK DOWN TO HERE

For $\alpha = \sqrt{3}$ find the electron and hole carrier densities in the limit of very small V_0. [6]

Geometry... it's all just areas of equilateral triangles and $\pi/3$ pie segments...

$$\bar{n} = \frac{k_F^2}{2\pi^2}\frac{2\pi - 3\sqrt{3}}{3} = n\frac{2\pi - 3\sqrt{3}}{3\pi} \approx 0.12\,n$$

$$\bar{p} = \frac{k_F^2}{2\pi^2}\frac{9 - 3\sqrt{3} - \pi}{3} = n\frac{9 - 3\sqrt{3} - \pi}{3\pi} \approx 0.07\,n$$

Could ask as a check:

$$\bar{n} - \bar{p} = n\frac{\pi - 3}{\pi} \approx 0.05\,n$$

NOT SEEN

Find the value of α for which the electron and hole carrier densities are equal. With help of a sketch of the dispersion relations along different directions, explain the conditions under which the material becomes an insulator. Include in your discussion a rough estimate of the minimal value of V_0 necessary for this to occur. [8]

For a "compensated" metal the areas of the Fermi circle and the Brillouin square are equal:

$$Q^2 = \pi k_F^2 \quad \Rightarrow \quad \alpha = \sqrt{\pi} \qquad [2].$$

An insulator only if (a) $\alpha = \sqrt{\pi}$ *and* (b) the bottom of the second band is higher in energy than the top of the first. The sketch should show dispersion relations along different directions and the effect of the opening of the gap [4].

The size of the gap is $\sim V_0$ so the critical value of V_0 is

$$V_0 \sim \hbar^2 Q^2/2m \sim \hbar^2 n/2m. \qquad [2]$$

NOT SEEN

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

Show that in a semiconductor in which the charge carriers are non-degenerate the electron and hole concentrations, n and p, satisfy the law of mass action

$$np = A\,(k_{\mathrm{B}}T)^3 \exp\left(-\frac{E_{\mathrm{g}}}{k_{\mathrm{B}}T}\right),$$

where E_{g} is the band gap energy and A is a constant that you should explicitly calculate. [9]
[*You may find one of the following results useful:* $\int_0^\infty \sqrt{x}\,\mathrm{e}^{-x}\,\mathrm{d}x = \sqrt{\pi}/2$,
$\int_0^\infty x^2\,\mathrm{e}^{-x^2}\,\mathrm{d}x = \sqrt{\pi}/4$.]

Density of states, including spin:

$$g(k) = 2\frac{1}{(2\pi)^3}4\pi k^2 \qquad [2]$$

For non-degenerate electrons with band-bottom E_c:

$$n = \frac{1}{\pi^2}\int k^2 \left[\exp\left(\frac{E_c + \hbar^2k^2/2m_e - \mu}{k_BT}\right) + 1\right]^{-1} dk \approx \frac{1}{\pi^2}\int k^2 \exp\left(\frac{-E_c - \hbar^2k^2/2m_e + \mu}{k_BT}\right) dk$$

$$n \approx \frac{1}{\pi^2}\int k^2 \exp\left(\frac{-\hbar^2k^2/2m_e}{k_BT}\right) dk \exp\left(\frac{-E_c + \mu}{k_BT}\right) = \frac{1}{\pi^2}\left(\frac{2m_ek_BT}{\hbar^2}\right)^{3/2}\int x^2 \exp\left(-x^2\right) dx \exp\left(\frac{-E_c + \mu}{k_BT}\right)$$

Using the given integral ($\sqrt{\pi}/4$):

$$n \approx \frac{1}{\sqrt{2}}\left(\frac{m_ek_BT}{\pi\hbar^2}\right)^{3/2} \exp\left(\frac{-E_c + \mu}{k_BT}\right) \qquad [4]$$

Repeat the same for holes with band-top E_v, or just deduce/quote:

$$p \approx \frac{1}{\sqrt{2}}\left(\frac{m_hk_BT}{\pi\hbar^2}\right)^{3/2} \exp\left(\frac{E_v - \mu}{k_BT}\right) \qquad [2]$$

So finally

$$np = \frac{1}{2}\,(m_{\mathrm{e}}m_{\mathrm{h}})^{3/2}\left(\frac{k_{\mathrm{B}}T}{\pi\hbar^2}\right)^3 \exp\left(-\frac{E_{\mathrm{g}}}{k_{\mathrm{B}}T}\right),$$

$$A = \frac{1}{2}\,(m_{\mathrm{e}}m_{\mathrm{h}})^{3/2}\left(\frac{1}{\pi\hbar^2}\right)^3 \qquad [1]$$

BOOKWORK

In a particular material, the chemical potential $\mu = 0$ is fixed at the bottom of a conduction band. Other states, not further considered here, ensure that $\mu = 0$ independent of T. The bottom of the conduction band $E_{\mathrm{c}}(k) = \hbar^2k^2/(2m)$ is separated

by E_g from the top of a valence band, $E_\mathrm{v}(k) = -E_\mathrm{g} - \hbar^2 k^2/(2m)$. Explain why in this case the law of mass action is not valid. [2]

Still needs work!

In the derivation of the law of mass action we explicitly assume that the carriers are non-degenerate and replace the Fermi occupation number with the Boltzmann one. Here the electrons are degenerate and this approximations does not hold.

A SMALL CHECK THAT THEY UNDERSTOOD THE BOOKWORK

Find and sketch the T dependence of both n and p for $\mu = 0$. Without doing any detailed calculations, comment on how you expect the product np to differ from the prediction of the law of mass action. [7]

Electrons degenerate but specifically for $\mu = 0$ we can still factor out the T dependence and make the integral dimensionless:

$$n = \frac{1}{\pi^2} \int k^2 \left[\exp\left(\frac{\hbar^2 k^2/2m}{k_B T} \right) + 1 \right]^{-1} dk$$

$$n = \frac{1}{\pi^2} \left(\frac{2mk_B T}{\hbar^2} \right)^{3/2} \int x^2 \frac{1}{e^{x^2}+1} dx \propto T^{3/2} \qquad [2]$$

+ simple sketch [1].

Holes are still non-degenerate, so the above calculation still works with $\mu = 0$ and $E_v = -E_g$:

$$p \approx \frac{1}{\sqrt{2}} \left(\frac{mk_B T}{\pi\hbar^2} \right)^{3/2} \exp\left(\frac{-E_g}{k_B T} \right) \propto T^{3/2} \exp\left(-\frac{E_\mathrm{g}}{k_\mathrm{B} T} \right) \qquad [1]$$

+ reasonable sketch [1].

np is reduced compared to the law of mass action. Physics: Pauli exclusion, n is lower than classical result for $\mu = 0$. Maths:

$$\frac{1}{e^{x^2}+1} < e^{-x^2} \qquad [2]$$

NOT SEEN

Now suppose that μ is instead fixed at a slightly positive value, $0 < \mu \ll E_\mathrm{g}$. Find n at $T = 0$ and sketch the T dependence of n that you would expect. [7]

At $T = 0$ filled Fermi sea up to μ.

$$\hbar^2 k_F^2/2m = \mu \quad \Rightarrow \quad k_F = \sqrt{2m\mu/\hbar^2}$$

Standard integration, or simply dividing the volume of the Fermi sphere, $(4\pi/3)k_F^3$, with the unit volume in k space, $(2\pi)^3/V$, and remembering the factor of 2 for spin, gives

$$n = \frac{k_F^3}{3\pi^2} = \frac{1}{3\pi^2}\left(\frac{2m\mu}{\hbar^2}\right)^{3/2} \qquad [3]$$

n will be $\approx$ constant for $k_B T \ll \mu$ [2] and cross over to $\sim T^{3/2}$ behaviour at $k_B T \sim \mu$ [2].

NOT SEEN

NOTE THAT BOTH QUESTIONS HAVE 11 MARKS FOR (ESSENTIALLY) BOOKWORK AND 14 FOR UNSEEN STUFF.

END OF PAPER