



MAASAI MARA UNIVERSITY

REGULAR UNIVERSITY EXAMINATIONS

2017/2018 ACADEMIC YEAR

FIRST YEAR SECOND SEMESTER

SCHOOL OF SCIENCE

MASTER OF SCIENCE IN PHYSICS

COURSE CODE: PHY 8212

COURSE TITLE: ENERGY BANDS, MAGNETISM

AND AMORPHOUS MATERIALS

DATE: 5th September 2018

TIME: 1100-1400

INSTRUCTIONS TO CANDIDATES

1. Answer Question **ONE** and any other **TWO** questions
2. Use of sketch diagrams where necessary and brief illustrations are encouraged.
3. Read the instructions on the answer booklet keenly and adhere to them.

*This paper consists of **three** printed pages. Please turn over.*

Question one (30 marks)

- a) If an iron crystal were totally magnetized spontaneously, estimate the resulting magnetization using plausible values for the parameters required. (specific weight of iron = 7.9, atomic weight of iron = 56, Bohr magneton = 9.3×10^{-24} Am²) (5mks)
- b) Discuss the Bloch theorem and its relation to the symmetry of the crystal lattice. (5mks)
- c) What is an iteration process (2mks)
- d) Briefly describe a magnon (3mks)
- e) How does study of amorphous solids differ from one that obeys Bloch condition (3mks)
- f) State the Hartree equations, what were the strengths and weaknesses of these equations. (4mks)
- g) i. Magnetism in condensed matter manifests itself in various forms for different materials and at different temperatures. Name the different types of magnetic behaviour. (4mks)
ii. Using magnetic susceptibility, distinguish between the different types of magnetisms in (i) above. (4mks)

Question Two (20 marks)

Figure 1.1 shows a hypothetical two-dimensional crystal consisting of atoms arranged on a square grid.

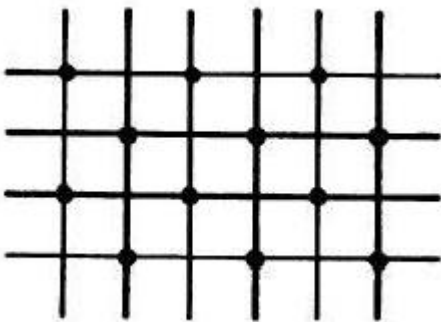


Fig 1.1

- a) Describe and show on the grid an example of a primitive unit cell. (3mks)
- b) Define "the reciprocal lattice" and explain its relation to Bragg reflection. (3mks)
- c) Show the reciprocal lattice and the first Brillouin zone. How is this zone related to Bragg reflection? (4mks)
- d) State and explain the theorem due to Bloch that says an electron moving in the potential of this lattice has traveling wave functions. What boundary conditions must be used with this theorem? (6mks)
- e) The free electron wavefunctions are plane waves of the form $\psi_k = e^{ik \cdot r}$. Show that a combination of wavefunctions of electrons in a periodic potential are standing waves (3mks)

Question Three (20 marks)

The method of orthogonalized plane waves (OPW, closely associated with the method of pseudo-potential) is very often used to make band structure calculations for electron states in metals. It explains successfully why the nearly free electron approximation can be used although the actual lattice potential acting on the electrons is not weak at all. Discuss the essential physical ideas and mathematical steps in this method by including, among others, descriptions of a

- a) Construction of Bloch function out of core states and its properties, **(4mks)**
- b) Construction of the orthogonalized plane wave states and their properties, **(4mks)**
- c) Construction of the pseudopotential and its non-uniqueness, **(8mks)**
- d) Physical explanation why the pseudopotential can be treated as small. **(4mks)**

Question Four (20 marks)

- i. The orienting tendency of an electric field E on a permanent dipole is opposed by thermal agitation.
 - a) Using classical statistical mechanics, calculate the total polarization of a gas of N independent permanent dipoles of moment P . **(6mks)**
 - b) Show that for small fields, the orientational polarization per dipole is inversely proportional to the temperature. **(3mks)**
 - c) Discuss the effect of this phenomenon on the dielectric constant of water, a polarizable molecule, at high frequencies and at low frequencies. **(7mks)**
- ii. The spin susceptibility has a weak temperature dependence of the form $\chi(T) = \chi(0)(1 + \alpha T^2)$. Would you expect α to be positive or negative? (Qualitative arguments only are expected.) **(4mks)**

Marking scheme PHY 8212

Question one (30 marks)

- a) The number of atoms per unit volume of iron crystal is

$$n = \frac{\rho N_A}{A} = \frac{7.9}{56} \times 6.02 \times 10^{23} = 8.5 \times 10^{22} \text{ cm}^{-3} = 8.5 \times 10^{28} \text{ m}^{-3} \quad \checkmark 1$$

where ρ is the specific weight of iron, A is its atomic weight and N_A is Avogadro's number. The magnetic moment per iron atom is $\mu_o \approx 2.2\mu_B$, $\checkmark 1$ μ_B being the Bohr magneton. Hence the magnetic moment per unit volume, or the magnetization, is

$$\begin{aligned} M &\approx n\mu_o = 2.2n\mu_B \quad \checkmark 1 \\ M &= 2.2 \times 8.5 \times 10^{28} \times 9.3 \times 10^{-24} \quad \checkmark 1 \checkmark 1 \\ &= 1.74 \times 10^6 \text{ Am}^{-1} \end{aligned}$$

- b) The Bloch theorem applies to the wave function of an electron moving in a crystalline solid in which its potential is periodic:

$$V(r) = V(r + R) \quad \checkmark 1$$

R being a lattice vector, i.e., the potential has the same translational symmetry as the lattice. The motion of the electron is described by the Schrödinger equation,

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r) = E\psi(r).$$

The Bloch theorem states that the solution, $\psi(r)$, the wave function of the electron, has the form:

$$\psi_k(r) = e^{ik \cdot r} u_k(r), \quad \checkmark 1$$

where the function $u_k(r)$ has the same translational symmetry as the lattice:

$$u_k(r) = u_k(r + R) \quad \checkmark 1$$

and the vector k is related to the momentum p of the electron by $p = \hbar k$.

The Bloch theorem is a consequence of the translational symmetry of the lattice. The solution of the Schrödinger equation can always be written as,

$$\psi(r) = f(r)u(r),$$

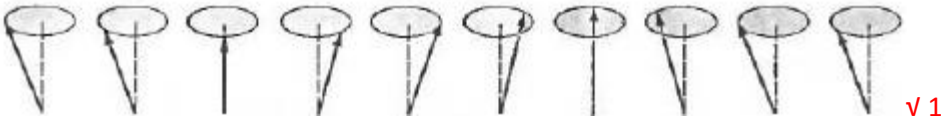
where $u(r)$ has the above-mentioned symmetry.

Since the potential $V(r)$ is periodic, all observable quantities associated with the electron must be periodic also, in particular the probability density $|\psi(r)|^2$, hence

$$|f(r + R)|^2 = |f(r)|^2. \quad \checkmark 1$$

The only function satisfying this relation for all R has the exponential form $e^{ik \cdot r}$, as required by the Bloch theorem. $\checkmark 1$

- c) A computation process in which a form is guessed for the one electron potential. $\checkmark 1$ A new U^{el} is then computed from the resulting wave functions, $\psi_i(r)$, and a new Schrödinger equation is solved. Ideally, the procedure is continued until further iterations do not materially alter the potential. $\checkmark 1$
- d) A magnon is a quantized spin wave, $\checkmark 1$ a quasiparticle, a collection of excitation of electrons spin structure in a crystal lattice as shown in the figure below. Spin waves do not rigorously obey the superposition principle. $\checkmark 1$



- e) Periodicity, amorphous solids lack crystal periodicity. ✓ 1

Many of the concepts used in the theory of amorphous solids are borrowed, with little if any justification from the theory crystalline solids, even though they are only well understood as a consequence of lattice periodicity. ✓ 1

Studying amorphous solids is difficult. Amorphous solids and liquids have about the same density as crystalline solids, and are therefore also susceptible to probing with X-rays. However, the discrete, sharp peaks, of scattered radiation characteristic of crystals are not found. ✓ 1

- f) It is the one-electron equations; ✓ 1

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_i(r) + U^{ion}(r) \psi_i(r) + \left[e^2 \sum_j \int dr' |\psi_j(r)|^2 \frac{1}{|r-r'|} \right] \psi_i(r) = \epsilon_i \psi_i(r) \quad \checkmark 1$$

It tries to solve the effects of electron-electron interactions, a subject that is ignored by working in the independent electron approximation. ✓ 1

The Hartree approximation ignores electron correlations; i.e., the N -electron probability distribution factors into a product of N one-electron distributions. ✓ 1

The Hartree approximation fails to represent the way in which the particular (as opposed to the average) configuration of the other $N - 1$ electrons affects the electron under consideration ✓ 1

- g) i. Diamagnetism ✓ 1

Paramagnetism ✓ 1

Ferromagnetism ✓ 1

Antiferromagnetism ✓ 1

- ii. Diamagnetism: $\chi < 0$ Generally χ is of the order 10^{-5}cm^{-3} , and is hardly affected by temperature, ✓ 1

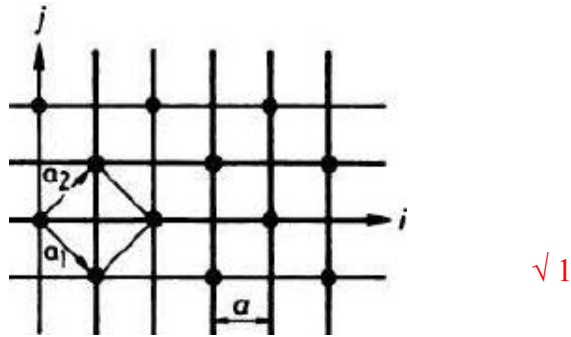
Paramagnetism: $\chi \propto \frac{1}{T}$ ✓ 1

Ferromagnetism: $\chi \propto \frac{1}{T - T_C}$, below the Curie temperature T_C , a ferromagnetic material is spontaneously magnetized; at T above T_C , it is paramagnetic. ✓ 1

Antiferromagnetism: At T higher than the Neel temperature T_N , $\chi \propto \frac{1}{T + \Theta}$ where Θ is a positive constant; at $T < T_N$, χ decreases with decreasing temperature. ✓ 1

Question Two (20 marks)

- a) A primitive unit cell is a unit cell that contains lattice points at corners only $\sqrt{1}$, such as shown in Fig.1 below.



The basis vectors of the unit cell are

$$a_1 = a(i - j), \quad \sqrt{1}$$

$$a_2 = a(i + j),$$

where a is the edge of the square lattice.

- b) If $a_i (i=1,2)$ are the basis vectors of the direct lattice, vectors $b_i (j=1,2)$ satisfying the relation $\sqrt{1}$

$$a_i \cdot b_j = 2\pi\delta_{ij} = \begin{cases} 2\pi, & i = j \\ 0, & i \neq j \end{cases} \quad \sqrt{1}$$

are the basis vectors of the reciprocal lattice. In the reciprocal space the condition for Bragg reflection is that the difference between the reflected wave vector k and the incident wave vector k_0 is an integer multiple n of a reciprocal lattice vector k^*

$$k - k_0 = nk^* \quad \sqrt{1}$$

- c) From the direct basis vectors

$$a_1 = a(i - j), \quad \sqrt{1}$$

$$a_2 = a(i + j),$$

the reciprocal basis vectors are obtained as

$$b_1 = \frac{\pi}{a}(i - j), \quad \sqrt{1}$$

$$b_2 = \frac{\pi}{a}(i + j).$$

The reciprocal lattice and the first Brillouin zone are shown in Fig. 2.

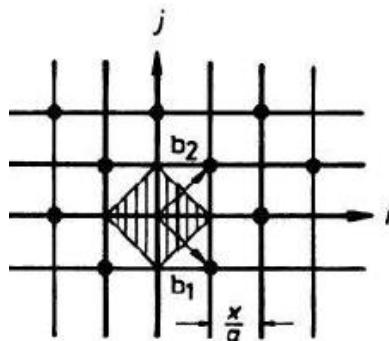


Fig. 2 $\sqrt{1}$

Bragg reflection takes place at the boundaries of the Brillouin zone. ✓ 1

- d) The wave representing an electron moving in the periodic potential field $V(r+R)=V(r)$, R being a lattice vector. ✓ 1 The lattice has the form of a Bloch function

$$\psi_k(r) = e^{ik \cdot r} u_k(r),$$

where the function $u_k(r)$ has the same translational symmetry as the lattice: ✓ 1

$$u_k(r) = u_k(r+R) \quad \checkmark 1$$

It is a plane wave modulated by the periodic potential field. This is Bloch's theorem. ✓ 1

The exponential part of the Bloch wave is a plane wave which describes the global behaviour of electrons in a crystal lattice, while the periodic function describes the local motion of those electrons around the nuclei. ✓ 1

Therefore, Bloch waves characterize the motion of the electrons in a crystal.

The Born- von Karman periodic boundary condition must be employed with Bloch's theorem. ✓ 1

Question Three (20 marks)

- a) In a metal the valence electrons are nearly free, but inside a core the wave function oscillates very rapidly. ✓ 1 In regions outside the cores, the electron wave is essentially a plane wave

$$|k\rangle = \frac{1}{\sqrt{N\Omega}} e^{ik \cdot r},$$

$$|k+k_i\rangle = \frac{1}{\sqrt{N\Omega}} e^{i(k+k_i) \cdot r}, \quad \checkmark 1$$

where N is the number of unit cells in the crystal, Ω is the volume of a unit cell, k_i is a reciprocal lattice vector.

In the core zone the electrons are tightly bound. ✓ 1 The tight-binding approximation gives the wave function as

$$|\Phi_{jk}(k)\rangle = \frac{1}{N} \sum_i e^{ik \cdot R_i} \varphi_j(r - R_i),$$

where $\varphi_j(r - R_i)$ is the j th state orbital of the atom located at R_i , and the summation extends over all the atoms in the lattice. ✓ 1

- b) Taking a plane wave with wave vector k as basis, construct a function $\chi_i(k, r)$ orthogonal to all the electron wave functions with wave vector k in the core zone:

$$\chi_i(k, r) = |k+k_i\rangle - \sum_{j=1} \mu_{ij} |\Phi_{jk}\rangle, \quad \checkmark 1$$

where the coefficient μ_{ij} is determined by the orthogonal condition

$$\int \Phi_{jk} \chi_i(k, r) d^3r = 0. \quad \checkmark 1$$

The wave function $\chi_i(k, r)$, called an orthogonalized plane wave function, is orthogonal to the electron wave function in the core zone. It behaves as a plane wave at large distances from an atom, but oscillates rapidly near a core. ✓ 1

This makes such functions suitable for construction of the wave function of a valence electron in the crystal, in the form a linear combination of several orthogonalized plane waves:

$$\psi_k = \sum_i C_i \chi_i \quad \checkmark 1$$

c) As

$$\chi_i = |k + k_i\rangle - \sum_{j=1} |\Phi_{jk}\rangle \langle \Phi_{jk} | |k + k_i\rangle, \quad \checkmark 1$$

denoting

$$\hat{p} = \sum_j |\Phi_{jk}\rangle \langle \Phi_{jk} | \quad \checkmark 1$$

we have

$$\psi_k = (1 - \hat{p}) |k + k_i\rangle. \quad \checkmark 1$$

and substituting it in the Schrödinger equation, we have

$$-\frac{\hbar^2}{2m} \nabla^2 \varphi + W \varphi = E \varphi, \quad \checkmark 1$$

where

$$\begin{aligned} W &= V(r) - \left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \hat{p} + E \hat{p} \\ &= V(r) + \sum_j (E - E_j) |\Phi_{jk}\rangle \langle \Phi_{jk} | \end{aligned} \quad \checkmark 1$$

is known as a pseudopotential. The pseudopotential is not unique. For if we substitute

$$W' = V(r) + \sum_j f(E, E_j) |\Phi_{jk}\rangle \langle \Phi_{jk} |, \quad \checkmark 1$$

where $f(E, E_j)$ is an arbitrary function, in the Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \varphi + W' \varphi = E' \varphi, \quad \checkmark 1$$

and take the inner product of its both sides with ψ_k^* , it can be shown that $E' = E$. $\checkmark 1$ Thus W' is also a pseudopotential.

d) Now write

$$W = V(r) + \sum_j (E - E_j) |\Phi_{jk}\rangle \langle \Phi_{jk} | = V(r) + V_B, \quad \checkmark 1$$

where $V(r)$, the real crystal potential, is an attractive potential, and

$$V_B = \sum_j (E - E_j) |\Phi_{jk}\rangle \langle \Phi_{jk} |.$$

In a crystal the energy E of a valence electron is higher than that of an inner electron, E_j , $\checkmark 1$ so that V_B has the property of repulsing electrons and is a repulsive potential. $\checkmark 1$ Thus V_B tends to cancel $V(r)$. This cancellation of the crystal potential by atomic functions is usually appreciable, leading to a very weak and quite smooth pseudopotential W . $\checkmark 1$

Question Four (20 marks)

a) In a gas of independent dipoles, the latter are able to rotate freely. The potential energy of a dipole of moment \mathbf{p} in an applied electric field \mathbf{E} is

$$V = -\mathbf{p} \cdot \mathbf{E} = -pE \cos \theta \quad \checkmark 1$$

where θ is the angle it makes with the direction of the field.

Classical statistical mechanics gives that the probability of finding the dipole along the θ direction is given by the Boltzmann distribution function

$$f(\theta) = e^{-V/k_B T} = \exp\left(\frac{pE \cos \theta}{k_B T}\right). \quad \checkmark 1$$

The average value of p along the direction of the field is then

$$\langle p \cos \theta \rangle = \frac{\int_0^\pi p \cos \theta \exp\left(\frac{pE \cos \theta}{k_B T}\right) 2\pi \sin \theta d\theta}{\int_0^\pi \exp\left(\frac{pE \cos \theta}{k_B T}\right) 2\pi \sin \theta d\theta} \quad \checkmark 1$$

Let $x = \cos \theta$ and $\beta = \frac{pE}{k_B T}$, $\checkmark 1$

$$\langle p \cos \theta \rangle = \frac{\int_{-1}^1 e^{\beta x} x dx}{\int_{-1}^1 e^{\beta x} dx} = \frac{p}{\beta} (\coth \beta - 1). \quad \checkmark 1$$

As there are N independent dipoles in the gas the total polarization is

$$P = N \langle p \cos \theta \rangle = \frac{N k_B T}{E} \left(\frac{pE}{k_B T} \coth \frac{pE}{k_B T} - 1 \right). \quad \checkmark 1$$

b) For small fields, $\beta = \frac{pE}{k_B T} \ll 1$ $\checkmark 1$ and

$$\coth \beta = \frac{1}{\beta} + \frac{\beta}{3} - \frac{\beta^3}{45} + \dots \approx \frac{k_B T}{pE} + \frac{pE}{3k_B T}. \quad \checkmark 1$$

By definition, the orientational polarizability per dipole is

$$\alpha = \frac{P}{EN} \approx \frac{p^2}{3k_B T} \propto T^{-1}. \quad \checkmark 1$$

c) If the electric field oscillates, the dipoles, following the field, will flip back and forth as the field reverses its direction during each cycle. $\checkmark 1$ However, the dipole may experience friction due to its collision with other molecules in the gas, causing some loss of energy known as dielectric loss. $\checkmark 1$ This means that a relaxation time τ is involved, as well as a phase lag between the field and the polarization, and that the dielectric constant $\epsilon = \epsilon_0 + \alpha n$ where ϵ_0 is the vacuum permittivity and n the number of dipoles per unit volume, $\checkmark 1$ is complex:

$$\epsilon = \epsilon_1 + i \epsilon_2.$$

The variations of ϵ_1, ϵ_2 with $\omega\tau$ are shown in Fig. 3. The imaginary part, ϵ_2 , is proportional to the dielectric loss.

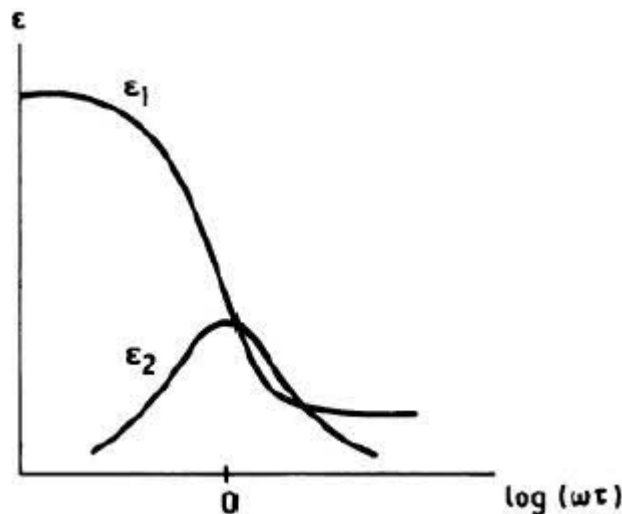


Fig. 3 $\checkmark 1$

At low frequencies ($\omega\tau \gg 1$) dielectric loss is small and $\epsilon \approx \epsilon_1 \approx \epsilon_s$, the static permittivity. $\checkmark 1$

As the frequency increases to the vicinity of ($\omega\tau \approx 1$) dielectric loss becomes appreciable and the real part of the dielectric constant decreases with increasing frequency in that region. ✓ 1
At high frequencies ($\omega\tau \ll 1$), the flippings of the dipoles are unable to follow the rapid oscillations of the field and dielectric loss again becomes small. In this region the real part ϵ_1 tends to a constant ϵ_∞ , the dielectric constant for high frequencies. ✓ 1

ii. When $k_B T \ll \epsilon_F$, the excited electrons will lie within a range $k_B T$ above the Fermi surface. ✓ 1

For those electrons whose magnetic moments are exactly parallel to the applied magnetic field, $\epsilon + (k)_{\max}$ is greater and so the fraction of such excited electrons is relatively small and the reduction of their chemical potential is less. ✓ 1

In order to maintain equilibrium, some of the electrons whose magnetic moments are almost parallel to the magnetic field will orientate so that their moments are more parallel to the magnetic field. ✓ 1

Hence we expect $\alpha < 0$ (negative). ✓ 1