***Condensed Matter Physics Option* – C3**

Condensed-matter Structure and Dynamics

Formal Syllabus*

Symmetry. Crystal structure, reciprocal lattice, Brillouin zones — general treatment for non-orthogonal axes. X-ray, neutron and electron diffraction. Disordered materials.
Lattice dynamics. Measurement of phonon dispersion. Thermal properties of crystals. Phase transitions. Soft modes.

Electronic structure of solids. Semiconductors. Transport of heat and electrical current. Fermiology. Landau quantisation. Low-dimensional structures.

Lorentz oscillator model. Optical response of free electrons and lattice. Optical transitions in semiconductors. Excitons.

Isolated magnetic ions. Crystal field effects. Magnetic resonance. Exchange interactions. Localized and itinerant magnets. Magnetic ordering and phase transitions, critical phenomena, spin waves. Domains.

Conventional and unconventional superconductors. Thermodynamic treatment. London, BCS and Ginzburg–Landau theories. Flux quantization, Josephson effects, quantum interference.

*The sections marked in **bold** are covered in the "Structure and dynamics" section of the C3 course.

General

- Particularly important material and equations are enclosed in **boxes.**
- Students should be familiar with "boxed" equations and should be able to apply them. Equations in **double-thickness boxes** should be memorised. An equation sheet will be provided for the other equations if they are required to solve exam questions.

Lecture 1 - Symmetry in the solid state – part I: Simple patterns and groups

- Elements of group theory
- Operator composition and conjugation – equivalence classes.
- Discrete symmetries around a fixed point: proper and improper rotations.
- The symmetry of the translation set in 2 dimensions: 2D lattices.
- 2D "wallpaper" groups.

At the end of this section, the students should understand the concepts of symmetry operators, their composition and the important concept of conjugation, which will enable them to construct classes of symmetry-equivalent operators (conjugation classes). Using this knowledge in a practical way, they should be able to recognise the 10 2D point groups and the 17 wallpaper groups. <u>Opportunities for exam questions will include</u>: composition and conjugation of symmetry operators; identification *of symmetry elements in a pattern (e.g., an Escher drawing); interpretation of the group symbols (e.g., "p4gm").*

Lecture 2 - Symmetry in the solid state – part II: Crystallographic coordinates and Space Groups

- Crystallographic coordinates
- Distances and angles
- The "dual" basis: construction and applications.
- Point groups in 3D.
- Crystallography in 3D: screws, glides, notation in the International Tables for Crystallography.

At the end of this lecture, the students should understand crystallographic coordinates and be able to measure distances and angles for generic (non-orthogonal) lattices . They should be able to construct the dual basis and be able to calculate dot products between real-space and reciprocal-space vectors. They should also understand the new generalised rotations and roto-translation symmetry operators in 3D and should be able to interpret the key symbols on the ITC entry for space groups. <u>Opportunities for exam questions will include</u>: a variety of calculations employing the metric tensor; demonstrate understating of the 3D symmetry operators; use of the International Tables in a practical way, e.g., to calculate equivalent positions.

Lecture 3 - Symmetry in the solid state – part III: The reciprocal lattice and its symmetry

- Fourier transform and the Reciprocal Lattice.
- The "weighed" reciprocal lattice and its symmetry – "normal" and "anomalous" conditions.
- Laue classes.
- Extinction conditions.
- Examples of "real" crystal structures.

At the end of this lecture, the students should understand that Fourier transforms of periodic functions in real space are non-zero only at the reciprocal-lattice nodes. They should also understand why "extra" reciprocal lattice vectors are generated by the use of "conventional" unit cells, and why the Fourier transforms are zero on these vectors. They should understand the concept of atomic radii and how it leads to different types of crystal structures. <u>Opportunities for exam questions will include</u>: calculation of extinction conditions for specific Bravais lattices and operators.

Lecture 4 - Symmetry in the solid state – part IV: The reciprocal lattice and its symmetry

- The Wigner-Seitz and Brillouin constructions.
- Brilluin zones and the symmetry of the band structure

Students should be able to understand and carry out in a practical way the Wigner-Seitz and Brillouin constructions. <u>Opportunities for exam questions will include</u>: specific examples of the Wigner-Seitz and Brillouin constructions; symmetry constraints on group velocities at different points of the Brillouin zone.

Lecture 5 - Wave and particle beams

- Elements of the theory of scattering of X-rays: scattering from a quasi-free electron, and from an atom – atomic scattering factors.
- Polarisation of X-ray beams and its effect on the scattering amplitudes.
- X-ray absorption and anomalous scattering.
- Scattering of neutrons – basic principles and formulas.
- Production and detection of X-rays and neutrons – synchrotrons and neutron sources.

*At the end of this lecture, the student should understand and be able to apply the basic equation governing the scattering from individual centres (atoms for X-ra*y and electron beams, nuclei and unpaired electrons for neutrons). *They should also have a general understanding of how these beams are attenuated in condensed matter and of the main techniques employed to produce these beams and detect them. It is very important that the students develop a good understanding of the* ***length-scales*** *and* ***orders of magnitudes*** *involved in these phenomena. Opportunities for exam questions will include: application of the scattering formulae, often in the context of the calculation of a diffraction cross section (lecture 5); general knowledge of the relevant material.*

Lecture 6 – Scattering geometries

- Cross section for a small "perfect" single crystal.
- The effect of atomic vibration - Debye-Waller factors.
- Laue and Bragg equations.
- Scattering geometries and geometrical factors.
- Elastic and inelastic scattering triangles.
- Structural solution from diffraction data – the phase problem.
- Basic ideas of dynamical scattering.

At the end of this section, the students should be able to understand the use of formulas to calculate cross sections, scattering rates in different geometries. They should be able to determine crystal orientations and scattering angles to observe particular brag peaks. They should also understand the limits of the kinematic approximation. Opportunities from exam questions will include: employing the scattering triangle construction to calculate rotation angles to reach scattering conditions; calculating structure factors; calculating scattering rates in different geometries from formulas provided in equation sheets.

Lecture 7 – Defect in crystals and non-crystalline solids

- Crystal size effects.
- Diffuse scattering.
- Extended defects - dislocations.
- Scattering from liquids and glasses.

At the end of this lecture, the students should understand how deviations from perfect periodicity affect the cross sections – in particular how scattering is generated outside the reciprocal lattice *nodes. The main equations for disordered materials scattering will also be presented. Opportunities from exam questions will include: knowledge of the specific topics; application of the relevant equations (provided in equation sheets) to solve realistic problems.*

Lecture 8 – Introduction to lattice modes and their symmetry.

- Lattice modes: a unified way to describe electron densities, wavefunctions, displacements and vibrations, magnetic structures and much more.
- Decomposing generic modes into normal modes.
- A simple example: normal modes of a square molecule and their applications to solve the dynamical equation.
- Extended lattices: mode decompositions of lattice fields.
- Normal modes of vibration of a crystal.
- Techniques to measure molecular and lattice dynamics: Infra Red absorption/reflectivity; Raman scattering; Inelastic Neutron Scattering.
- Selection rules: IR and Raman-active modes.
- Translational symmetry: the Bloch theorem.
- Generalisation of the Bloch theorem: the symmetry of the Hamiltonian.
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At the end of this lecture, the students should appreciate the importance of symmetrised modes in various classes of problems, and be able to use symmetry in an intuitive way to solve simple problems. Opportunities from exam questions will include: construction of simple invariant modes. Symmetry analysis of a specific problem (e.g., the vibration of a molecule) leading to predictions of its Raman, IR and neutron signatures (selection rules).

Lecture 9 – Phonons and anharmonic phenomena.

- Normal mode quantization.
- Use of the Brillouin zone construction to classify phonon modes.
- Linear momentum vs. crystal momentum.
- Beyond the harmonic approximation.
- Thermal expansion
- Thermal conductivity
- Normal and Umklapp processes

At the end of this lecture, the students should be able to employ the Wigner-Seitz and Brillouin constructions (lecture 3) to classify phonon modes. They should understand the difference between linear momentum and crystal momentum, and how it can lead to a variety of phenomena, particularly related to electron-phonon and phonon-phonon scattering and to the deviations from the harmonic approximation. Opportunities from exam questions will include: application of the concepts and formulae to solve realistic problems.

Lecture 10 – Phase transitions.

- An example of a phase transition illustrated with an Escher drawing.

- Symmetry changes and their effects on the macroscopic properties of a crystal: the Neumann's principle.
- Electrical polarisation and magnetisation. Time reversal symmetry (basic illustration).
- "Phenomenological" description of phase transitions: a brief introduction to Landau theory.
- Phase transitions by soft modes condensation.

At the end of this lecture, the students should understand how a phase transition leads to the loss of certain symmetry operators, and how this may lead in certain cases to the appearance of macroscopic observable such as electrical polarisation and magnetisation. A few basic concepts relating to the Landau theory of phase transitions will also be introduced, enabling the students to understand why most phase transitions involve the "activation" of a single mode. <u>Opportunities from exam questions will include</u>: Determine whether polarisation/magnetisation is allowed in a given space group symmetry and analysis of what happens at a phase transition. Simple forms of the Landau free energy and their use to determine the behaviour of the order parameters.