

Phys7450: Solid State Physics 2
Lecture 1: Introduction and Overview

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Abstract

In these lecture notes, I will overview the subject of condensed matter physics, review key ideas from Solids 1 and outline the present course of Solids 2.

I. INTRODUCTION

A. Condensed matter physics

Condensed matter physics (CMP) is the largest broadly defined area of physics that studies phenomena of strongly *interacting, macroscopic* (even as large as an Avagadro, 10^{23}) number of degrees of freedom.

1. *Solid state physics*

After quantum mechanics and its many-degrees of freedom successor, quantum field theory were developed in the first quarter of the 20th century, attention turned to application of this scientific breakthrough to the study of solid state materials. The problem is the the quantum mechanical description of an Avagadro number of electrons, carrying spin and charge, moving in the periodic potential ions, that in principle are also a macroscopic number of quantum mechanical degrees of freedom. Since solid state systems are materials with well-packed array of atoms, the typical length scale is on the order of an Angstrom (size of an atom and the associated atomic bonds) and typical energy is on the order of an electron-volt (a Rydberg). Early breakthrough came in 1927 with Arnold Sommerfeld's appreciation of the key role of Fermi-Dirac statistics, with the subject of conventional solid state physics well-established by late 60s with the pioneering works of Bravais, Hall, Drude, Einstein, Debye, Kamerlingh Onnes, Max von Laue, Bragg brothers, Meissner, Pauli, Bethe, Wigner, Slater, Bloch, Feynman, Bardeen, Cooper, Schrieffer, Peierls, Seitz, Froelich, Kondo, Hubbard, Gutzwiller, Pines, Anderson, Kapitsa, Bogoluibov, Landau and his school including Abrikosov, Gorkov, Dzyaloshinski in the Soviet Union.

Since then much of the effort has been directed at understanding the effects of deviation from a perfect crystalline lattice, namely the effect impurities and lattice defects, referred to as quenched disorder. These, together with the studies of strong quantum and thermal fluctuations and strong interactions, that drive phase transitions between different states of matter continue to form a central subject of modern solid state physics.

2. *Soft condensed matter physics*

In early 70s, with an establishment of Exxon research laboratory a new field of the so-called “soft” condensed matter physics was established in an effort to understand the phenomenology and develop new entirely different class of non-solid state materials. These include polymers (plastics), colloids (micro-size polymeric particles), emulsions (paints, milk), liquid crystals (modern displays), surfactants (soaps, detergents), biological materials (DNA, membranes), and a wealth of many other materials that dominate today’s modern synthetic material technology, medicine, etc. These materials are characterized by much larger (as large as microns) length scales and much lower (room thermal) energy, with their phenomenology controlled by classical ($\hbar = 0$), entropic ($k_B T$) effects responsible for their softness.

To do justice to this vast rich subject (“hard” [solid state] + “soft”) of condensed matter physics would take several semesters to cover properly. This is why in this course we will focus on a small subset of the CM field, namely the subject of crystalline materials.

B. “Standard model” of solid state physics

The study of crystalline materials demands a quantum-mechanical description of a macroscopic number of interacting electrons moving in a crystal of ions, latter also treated as quantum degrees of freedom. The problem is succinctly stated as a Schrodinger’s equation

$$H\Psi = i\hbar\partial_t\Psi,$$

for a many-body electron and ion wavefunction, $\Psi(\{\mathbf{r}_i\}, \{\mathbf{R}_j\})$ in terms of the “standard model” Hamiltonian

$$H = H_{electron} + H_{ion} + H_{ion-electron} \quad (1)$$

where,

$$H_{electron} = \sum_i^{N_e} \frac{(\hat{\mathbf{p}}_i + e\mathbf{A}_i)^2}{2m} + \frac{1}{2} \sum_{i,j}^{N_e} \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} - g_e\mu_B \sum_i^{N_e} \mathbf{B} \cdot \mathbf{s}_i + H_{SO} \quad (2)$$

is the electronic Hamiltonian that consists of the kinetic energy (with minimal coupling representing interaction with the electromagnetic field, characterized by a vector potential

\mathbf{A} and $\mathbf{B} = \nabla \times \mathbf{A}$), electron-electron Coulomb interaction, interaction of electron spin with external magnetic field \mathbf{B} ($\mu_B = e\hbar/(2m)$, $g \approx -2$ are the electron's Bohr magneton and gyromagnetic ratio) and spin-orbit interaction

$$H_{SO} = \frac{1}{2m^2c^2} \frac{1}{r} \frac{dU(r)}{dr} (\mathbf{r} \times \mathbf{p}) \cdot \mathbf{s} \propto \mathbf{l} \cdot \mathbf{s}, \quad (3)$$

arising as a relativistic correction that couples spin and orbital degrees of freedom; there are a number of other such corrections (quartic correction to parabolic dispersion and the so-called Darwin term) that we may return to later in the course.

In addition to the latter electron spin crucially enters through Pauli principle requiring the electron many-body wavefunction to be totally antisymmetric under the interchange of both orbital and spin electron coordinates. As we will see soon enough, in the presence of Coulomb interaction this quantum statistical constraint on the electronic wavefunction will give rise to the so-called spin exchange interaction $J\mathbf{S}_i \cdot \mathbf{S}_j$ between spins i and j and will lead to the dominant mechanism of magnetism in nature.

The ionic Hamiltonian is given by

$$H_{ion} = \sum_i^N \frac{\hat{\mathbf{P}}_i^2}{2M_i} + \frac{1}{2} \sum_{i,j}^N \frac{Z_i Z_j e^2}{4\pi\epsilon_0 |\mathbf{R}_i - \mathbf{R}_j|} \quad (4)$$

consisting of the ions' kinetic and Coulomb interaction energies for charge $Z_i e$, and we neglected nuclear spin-orbit and electromagnetic interactions.

The final crucial part of the Hamiltonian is the Coulomb interaction between the electrons and ions,

$$H_{electron-ion} = - \sum_{i,j}^{N,N_e} \frac{Z_i e^2}{4\pi\epsilon_0 |\mathbf{R}_i - \mathbf{r}_j|}. \quad (5)$$

Despite a seeming simplicity of the Hamiltonian and the statement of the problem, even with modern-day computers an exact solution of the above Schrodinger's equation can only be done for at most ten interacting electrons (that's even when ions are treated as frozen). A classical computer of the size of the universe could at best solve a problem of a pathetic number of 200 electrons[2]. Thus, because of the exponential growth of the Hilbert space with the number of degrees of freedom, a frontal attack on this problem is unimaginable.

C. Approximations to the solid-state problem

Thus to make progress serious imaginative physical insight is needed to inspire appropriate approximate treatments. These include:

- **simplified models:** building and analyzing simplified models that maintain key physical ingredients but neglect some qualitatively inessential microscopic details
- **mean-field and variational approximations** that treat this many-body problem as an effective noninteracting single electron system
- **perturbation theory** in electron-ion and electron-electron interaction
- **numerical methods**, using quantum Monte-Carlo, molecular dynamics, and exact diagonalization

1. Crystal lattice

In the case of heavy ions ordered into a perfect crystal lattice, one can approximately ignore their quantum character, taking \mathbf{R}_i as classical variables forming a lattice:

$$\mathbf{R}_{n,s} = \mathbf{R}_n + \mathbf{r}_s, \quad (6)$$

where

$$\mathbf{R}_n = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \quad (7)$$

spans a Bravais lattice with lattice vectors \mathbf{a}_i and a p -atom basis \mathbf{r}_s , with $s = 1, \dots, p$. The corresponding reciprocal lattice is spanned by $\mathbf{G}_h = h_1 \mathbf{b}_1 + h_2 \mathbf{b}_2 + h_3 \mathbf{b}_3$, with reciprocal lattice vectors \mathbf{b}_i , defined by $\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}$ or equivalently $e^{i\mathbf{G}_h \cdot \mathbf{R}_n} = 1$, solved by $\mathbf{b}_1 = 2\pi \mathbf{a}_2 \times \mathbf{a}_3 / v$, where $v = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ is the unit-cell volume.

All the possibilities in two dimensions (5-types) and three dimensions (14 Bravais lattices types and 7 crystal structure classes, characterized by one of the 230 3D space groups) have been completely classified.

Examples of current interest of 2D Bravais lattice with a basis are the honeycomb lattice of graphene and the kagome lattice, illustrated in Figs.(3),(4) and in 3D the diamond lattice which is a face-centered cubic Bravais lattice with a 2-atom basis.

Five Bravais Lattices in 2D

In 2-D, it is possible to have 4 crystal systems and 5 different lattice types (UNIT cell) .

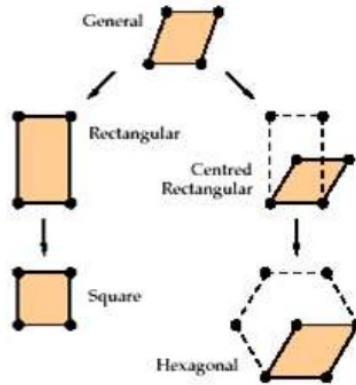


FIG. 1: 2D Bravais lattices.

Bravais lattices in 3D: 14 types, 7 classes

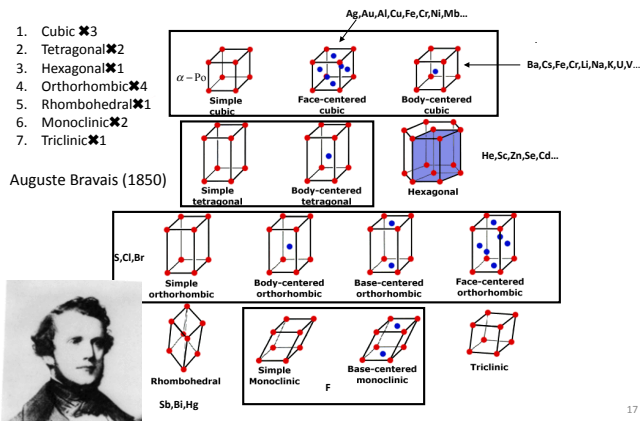


FIG. 2: 3D Bravais lattices.

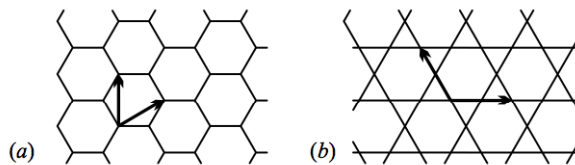


FIG. 3: 2D non-Bravais “lattices” with a basis, (a) honeycomb, (b) kagome.

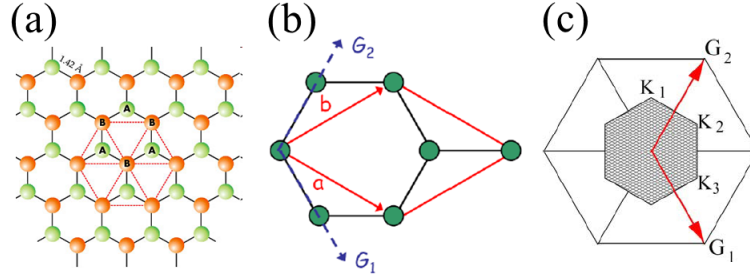


FIG. 4: Details of the honeycomb lattice structure illustrating in (a) and (b) its real space triangular unit cell with a 2-atom basis. In (c) its reciprocal lattice and the corresponding Wigner-Seitz cell, i.e., the 1st Brillouin zone is indicated in gray.

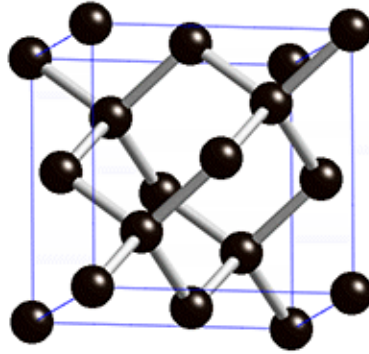


FIG. 5: A 3d non-Bravais diamond lattice, which is an FCC Bravais lattice with a 2-atom basis.

2. Band structure: metals and insulators

Using such crystalline lattice positions inside $V(r) \equiv H_{electron-ion}[\mathbf{R}_{n,s}]$, defines a periodic ion potential $V(r)$ that the electrons move in. This still leaves electron-electron interaction to contend with that is the main challenge of solid state physics. As we will see, it can be treated in mean-field approximation, perturbation theory (Hartree and Hartree-Fock approximation being the lowest order), or through other inspiring approximations (large-N, order parameter decoupling, numerically). If as a crudest approximation, we ignore the

electron-electron interaction, we are left with a single electron band structure problem

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + V(r) + \dots\right) \psi_n(\mathbf{r}) = E_n \psi_n(\mathbf{r}) \quad (8)$$

for a single-electron wavefunction $\psi_n(\mathbf{r})$, with the many-body wavefunction give by the antisymmetric Slater determinantal

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}) = \frac{1}{\sqrt{N_e!}} \mathcal{A} \prod_n^{N_e} \psi_n(\mathbf{r}_{P\{n\}}),$$

encoding the Pauli principle.

The solution of the single particle Schrodinger's equation, (8) can be laborious, but, because it is afterall a single electron problem, it can in principle be straightforwardly done numerically. Its eigenfunctions satisfy the famous Bloch Theorem,

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}), \quad (9)$$

with the Bloch function periodic, $u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}_n) = u_{\mathbf{k}}(\mathbf{r})$ and its eigenvalues

$$E(\mathbf{k}) = E(\mathbf{k} + \mathbf{G}_h)$$

over the Brillouin zone, leading to the band structure (illustrated in Figs.6,7)), filled accord-

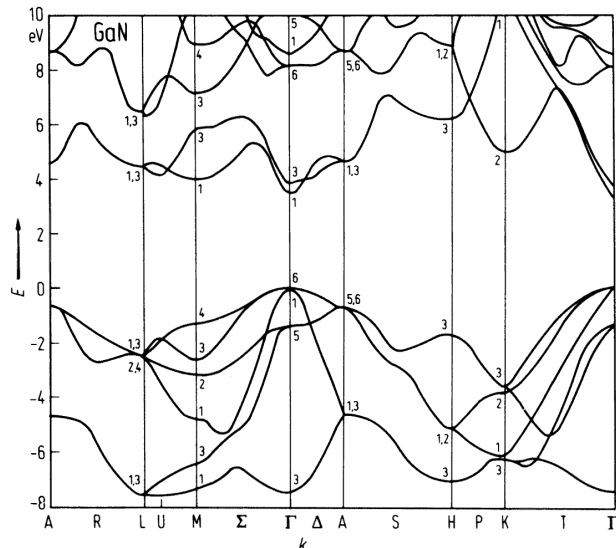


FIG. 6: Band structure of Gallium Nitride, GaN.

ing to Pauli principle, controlling noninteracting properties of the corresponding material.

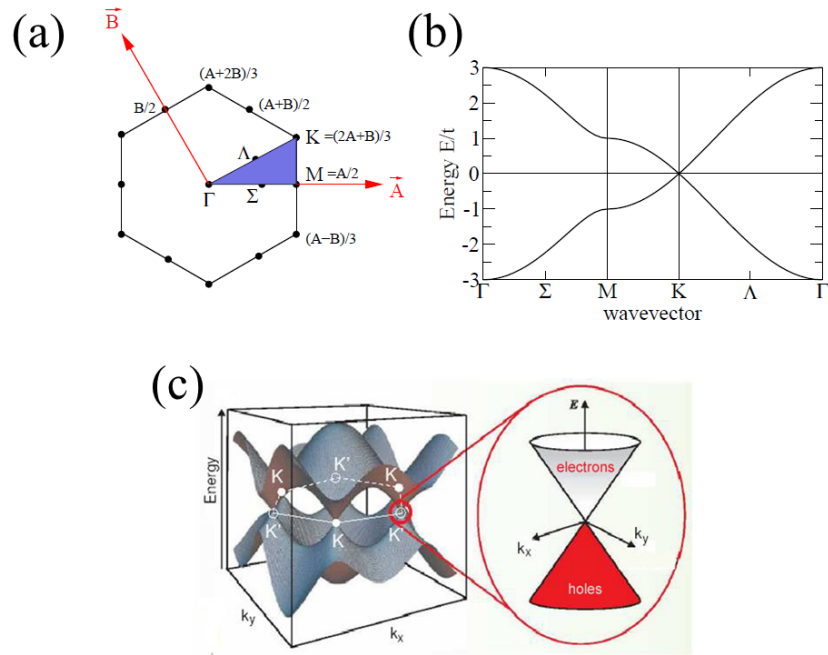


FIG. 7: Band structure of graphene as a Dirac material.

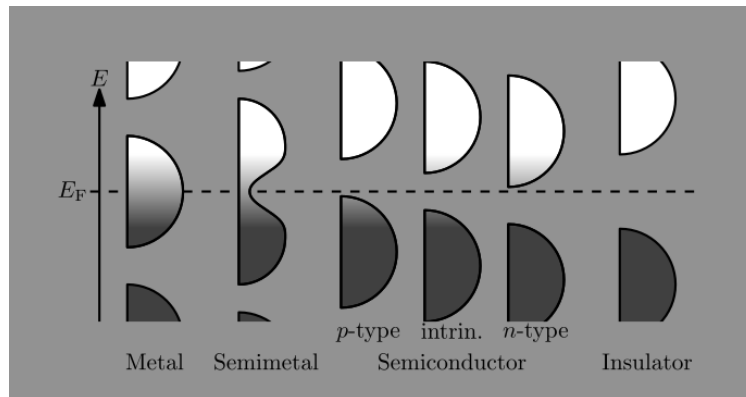


FIG. 8: A schematic of a band structure and corresponding noninteracting states of matter ranging from a metal (where the Fermi level is inside a partially-filled band) and a band insulator (where the Fermi energy is in the interband gap).

In particular, as illustrated in Fig.8, the band structure and its electron filling determines the nature of the noninteracting electron state, with a metal for a Fermi level inside a partially-filled band and a band insulator for a Fermi energy in the interband gap.

D. Experimental probes

To study this intricate and rich behavior “hidden” inside the material, a large array of experimental probes is employed. Among the primary ones that we will study (some discussed in the introductory course on solid state physics) include:

- **thermodynamics**, which primarily focusses on the heat capacity $C_v = T\partial S/\partial T = \partial E/\partial T|_V$.
- **transport**, which can be purely thermal, purely electrical or mixed, and in the presence of a magnetic field includes longitudinal (current along the electric field) and transverse Hall (current perpendicular to the electric field). It can also be dc (at vanishing frequency $\omega = 0$) or ac (at finite tunable frequency)
- **scattering** can include a variety of particles, with neutrons and x-rays (and more generally, photons of various wavelengths from microwaves to x-rays) being the primary sources. These allow measurements of static and dynamic correlation functions of charge and spin densities.
- **nuclear magnetic resonance, NMR** uses a combination of a strong dc and weak ac magnetic fields to directly probe magnetic spin susceptibility and therefore magnetic order.

E. Solids 2: Advanced solid state physics overview

In this course we will build on the introductory background material outlined above, with a focus on advanced topics that require treatment of interactions and quantum and thermal fluctuations. We will develop and utilize methods of statistical mechanics and quantum-field theory to study a range of phenomena. The outline of the course is as follows.

Course outline:

- Review and Introduction
 - scope and states of condensed matter physics: "More is Different"
 - band structure: insulators and conductors
 - "standard model" of thermodynamics
 - experimental probes
- Elasticity, fluctuations and thermodynamics of crystals
 - elasticity of Goldstone modes
 - quantum field theory of lattice vibrations: phonons
 - thermodynamics of phonons
 - thermal expansion and melting
 - correlation functions and x-ray scattering
 - Hohenberg-Mermin-Wagner theorem
- Bosonic matter
 - Bose gases thermodynamics and BEC
 - Bogoliubov theory of a superfluid
 - Lee-Huang-Yang thermodynamics
 - Ginzburg-Landau theory and Landau's quantum hydrodynamics
 - XY model, 2d order, vortices and the Kosterlitz-Thouless transition
- Magnetism in charge insulators
 - Paramagnetism
 - Spin exchange vs dipolar interaction
 - Heisenberg model and crystalline anisotropies
 - Hosten-Primakoff and Schwinger bosons

- Jordan-Wigner transformation and XXZ chain
- Coherent-spin states and Berry phases
- Mean-field and Landau theory of FM and AFM states

- Electron liquid
 - Fermi gas thermodynamics
 - Hartree-Fock theory of interactions
 - Response functions
 - Landau Fermi liquid theory
 - Pauli magnetism
 - Landau diamagnetism

- Superconductivity
 - Cooper instability
 - BCS and Bogoliubov theory
 - BCS-BEC crossover
 - Ginzburg-Landau theory
 - Vortex physics

- Quantum Hall and related effects
 - Hall effect
 - Landau levels and Integer QHE
 - de Haas-van Alphen oscillations
 - Fractional QHE

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- [1] *More Is Different*, P. W. Anderson, Science, New Series, Vol. 177, No. 4047. (Aug. 4, 1972), pp. 393-396.
- [2] *Quantum Field Theory of Many-body Systems*, by Xiao-Gang Wen.
- [3] *Fundamentals of the Physics of Solids I*, Electronic Properties, J. Solyom.