
FIP10601 – Text 1

Introduction

Solid State Physics, as the name suggests, aims to study properties of matter in the solid state. Any piece of such matter is generically referred to as a **solid**. Oversimplifying, a solid may be viewed as a **macroscopic** “bunch of atoms” held together by interactions of **electromagnetic** origin.

Our study will focus primarily on **crystalline** solids, or *crystals*. They are characterized by the existence of **long-range positional order** of the atoms, which occurs in a certain number of **crystal structures**. Real solids are usually *polycrystalline*, i.e., they contain crystalline regions, called *grains*, separated by amorphous regions of comparatively small thickness (*grain boundaries*). Even inside the grains, or in synthesized *single crystals*, there exist deviations from the ordered arrangement, which are generically called *defects*. In addition, real solids, being finite in size, are limited by surfaces. Our study will be restricted to *bulk* properties, not focusing on surface effects, and the role of defects will be just mentioned when relevant.

In a solid, characteristics of individual atoms are important, but **emergent** features due to the presence of a large number of atoms are of fundamental importance. For example, concepts such as *conductivity*, *specific heat*, *magnetization*, and many others are meaningless for single atoms. Therefore, Solid State Physics studies **collective** properties of the set of atoms that forms a solid, which means that we have to deal with a **many-body system**. In addition, the microscopic nature of its constituents makes **quantum** effects important, and the high densities that characterize solids ($10^{22} - 10^{23}$ atoms/cm³) lead us to suppose that **interactions** between these constituents must be very relevant. The analysis of such a highly complex system falls in the general subject of **quantum many-body problems**.

Facing this difficult task, we can ask two basic questions:

- How can we describe the ground state (and, more generally, thermodynamic equilibrium states) of a solid?
- How can we describe a solid’s response to external perturbations?

From the point of view of **experimental physics**, in most cases we can only learn about equilibrium properties through the response to perturbations, which disrupt equilibrium! An exception is elastic x-ray or neutron diffraction, that give information about the crystal structure. Experimental perturbations to solids are of a wide variety, like electromagnetic fields, temperature gradients, pressure and tension, photon or particle beams, etc., to which we can add controlled changes of chemical composition.

Many properties that are experimentally accessible (i.e., measurable physical quantities) are **macroscopic**. Understanding the observed phenomena involves interpreting processes that occur at a **microscopic** level. To do this, **theoretical models** must be built up.

In practice, it is **impossible** to describe all features of solids with a single model. Usually, simplified models are employed, taking into account only the relevant degrees of freedom for specific properties. An important point is that models — and theoretical methods used in connection to them — should allow to predict values of measurable quantities for comparison with experiments.

The importance of response to perturbations leads to the unifying concept of *elementary excitations*. Most elementary excitations in a solid involve changes in electron states or motions of the atoms themselves around their equilibrium positions. It is convenient to separate these degrees of freedom, though not neglecting their relationship.

In this sense, we must reformulate our initial view of a solid as a bunch of atoms put together. We begin by noticing that for the energy scale of relevant phenomena in solids we may see each atom as composed by an *ionic core* (or simply *ion*) and *valence electrons* (which we will just call *electrons*). Core states are hardly affected by the presence of neighboring atoms. Valence states are significantly modified, and give rise to *electronic states* of the solid. In the context of an *independent-electron approximation*, these are single-electron states. Their nature (*localized* or *extended*) and their occupation define, for instance, basic characteristics with respect to charge transport (*conductors*, *insulators*, *semiconductors*). Other features, such as magnetic properties or superconductivity, are more heavily dependent on interactions between the electrons.

Viewing a solid as a system of *ions* and *electrons*, one can start with a *first-principles* model, building up the Hamiltonian in terms of degrees of freedom associated to these particles. Such a Hamiltonian can be written as a sum of terms,

$$\mathcal{H} = \mathcal{H}_{\text{ion}} + \mathcal{H}_{\text{el}} + \mathcal{H}_{\text{el-ion}} + \mathcal{H}_{\text{ext}}, \quad (1)$$

taking into account separately the purely ionic (\mathcal{H}_{ion}) and purely electronic (\mathcal{H}_{el}) degrees of freedom, plus their interaction ($\mathcal{H}_{\text{el-ion}}$), and the effect of external fields (\mathcal{H}_{ext}).

In terms of momentum and position of each particle (with their respective masses), we can write

$$\mathcal{H}_{\text{ion}} = \sum_i \frac{P_i^2}{2M_i} + \frac{1}{2} \sum_{ij}' \mathcal{V}_{\text{ion-ion}}(\mathbf{R}_i - \mathbf{R}_j), \quad (2a)$$

$$\mathcal{H}_{\text{el}} = \sum_l \frac{p_l^2}{2m_e} + \frac{1}{2} \sum_{ll'}' U(\mathbf{r}_l - \mathbf{r}_{l'}), \quad (2b)$$

$$\mathcal{H}_{\text{el-ion}} = \sum_{il} V_{\text{el-ion}}(\mathbf{r}_l - \mathbf{R}_i), \quad (2c)$$

where the prime on summations indicate that terms with equal indices are suppressed. As mentioned before, the relevant interactions are electromagnetic. $\mathcal{V}_{\text{ion-ion}}$ is a simple Coulomb potential if the ions are well separated, but must include a short-range repulsive part that prevents them from coming too close; the electron-electron interaction U can be seen as pure Coulomb repulsion, and $V_{\text{el-ion}}$ is again basically a Coulomb potential modified in the core region. Stability of the solid is achieved through a balance between repulsive and attractive effects of these interaction terms.

Many properties of a solid are better described by quite different Hamiltonians, although derived from the above one. For example, magnetic properties of insulators can be obtained from effective Hamiltonians involving only spin degrees of freedom, because the other ones are “frozen”. Note that spin-dependent terms, like spin-orbit interaction or an applied magnetic field, were not explicitly included in Eqs. (2), but the electron spin must surely be taken into account.

Starting from the generic model of Eq. (1), our first simplification will be to take for granted the existence and stability of crystalline solids. This will allow us to study

- the nature of electronic states in thermodynamic equilibrium as well as transport processes for a **given** (static) configuration of ions defining the *crystal structure*;
- motions of the ensemble of ions around the equilibrium configuration;
- interplay between electron and ion motions through their interactions.

This constitutes a part of solid-state theory often referred to as *electrons and phonons*, the latter being elementary excitations associated with ion motion. This is what will occupy most of the present course. Although it is also a subject of introductory courses, our main focus will be on **interactions**, specially electron-electron interactions, which are usually neglected at that level.

For completeness, we will begin (Unit 1) by reviewing the fundamentals of the *independent-electron approximation* applied to crystalline solids, with emphasis on the importance of crystal symmetries. In this context, we will discuss thermal and transport properties of metals and semiconductors, also including consequences of quantum confinement and low-dimensionality. Then we will move on (Unit 2) to a reasonably detailed theoretical analysis of **interactions** between electrons in metallic solids. We will end with a short discussion of the electron-phonon interaction in metals, including its role on the special low-temperature state known as superconductivity.