Solid State Theory

Alejandro Muramatsu
Institut für Theoretische Physik III

Ideally, the aim of a theory of condensed matter physics is to solve a system with nuclei and electrons, taking into account their interactions, such that the starting point would be the following Hamiltonian:

$$H = H_{nuc} + H_{el} + H_{el-nuc} \ , \tag{1}$$

where, still ideally, the input should be the charge of the nuclei Ze, the mass of the nuclei M, the charge of the electron $-e$, and the mass of the electron m. At the energy range we are interested in, somewhere between zero and keV's, only the Coulomb interaction will play a role. This means, that apart from disregarding gravitation, strong, and electroweak interactions, we will in general assume that relativistic effects are not important, and retardation effects can be neglected. Therefore, the different parts of the Hamiltonian above can be written quite generally as follows

$$H_{nuc} = \sum_i^N \frac{\boldsymbol{P}_i^2}{2M_i} + \frac{1}{2}\sum_{i\neq j} \frac{e^2 Z_i Z_j}{\mid \boldsymbol{R}_i - \boldsymbol{R}_j \mid} \ , \tag{2}$$

$$H_{el} = \sum_i^{ZN} \frac{\boldsymbol{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} \frac{e^2}{\mid \boldsymbol{x}_i - \boldsymbol{x}_j \mid} \ , \tag{3}$$

$$H_{el-nuc} = -\sum_{i,j} \frac{e^2 Z_j}{\mid \boldsymbol{x}_i - \boldsymbol{R}_j \mid} \ . \tag{4}$$

To solve the Schrödinger equation with such a Hamiltonian is a formidable task, since nowadays computers can be used to treat the case $N \sim \mathcal{O}(1)$ and $Z \sim \mathcal{O}(1)$, whereas we are interested in the case $N \sim 10^{23}$, i.e. in the thermodynamic limit $N \to \infty$. This means that we are going to be in the realms of statistical mechanics, or to be more precise of quantum statistical mechanics.

Before we really start, let us have a short survey of the sort of things we are going to discuss. The Hamiltonian above is certainly a very general one. It can describe a gas of atoms as well as a liquid or a solid. We will concentrate on the solid, and moreover only consider those which are perfectly ordered in a periodic fashion. Therefore, the first chapter is devoted to

- Crystal structure.

Although this seems to be a big constraint, it turns out that most of the interesting things we know nowadays can be understood by considering ordered structures. Periodicity is a symmetry that will allow us to reduce the complexity from 10^{23} to the number of degrees of freedom that are periodically repeated, such that in many cases it will be possible to solve the problem in the thermodynamic limit.

Once we discussed the general consequences of having a crystalline structure, we allow the atoms to perform small oscillations around their equilibrium positions. This will lead to the description of

- Lattice vibrations.

by means of one of the possible *elementary excitations* of a solid, namely *phonons.* This is another reduction of complexity in the problem. We will call elementary excitations, those modes of the system that at low enough energies (and hence, temperatures), can be considered as eigenmodes of the solid. These modes will be real eigenmodes (i.e. modes with an infinite lifetime) only within certain approximations. However, in this way we will be able to understand the experiments and look for corrections by considering interactions among the elementary excitations, that in general will lead to a finite lifetime, as also seen in experiments. We will be more precise about this in the coming chapters. Here we will have also the first encounter with second quantization, much in the same way as in elementary quantum mechanics, when discussing the harmonic oscillator (creation and annihilation operators).

Next we will focus on the electrons, where in a first round we will consider them as non-interacting, and discuss

- Electrons in a periodic potential.

Since we know that electrons are charged, this may appear at a first sight as a gross simplification. However, at the beginning of quantum mechanics, Sommerfeld considered electrons as non interacting particles and took only into account the fact that they obey the Fermi-Dirac statistics. In such a way he could explain the temperature dependence of the specific heat in metals as well as their magnetic susceptibility. We will come to understand this apparent contradiction only later, when we discuss the effects of interaction. For the moment we will introduce the concept of a *band-structure*, that is very useful to understand simple metals and semiconductors.

In order to complete the picture developed, we will come then, to consider

- Interacting electrons.

Here we will go deeper into the concepts of second quantization and develop a theoretical frame that should allow us to deal in principle with fully interacting electrons. Unfortunately this goal was still not reached and different approaches are the subject of current research. Nevertheless, the theoretical language developed here should be useful to make contact with undergoing research work. On the other hand, it will be usefull to understand the solution of the contradiction mentioned above. We will see that in this case, the elementary excitation is the so-called *quasiparticle*, namely a fermionic excitation with spin 1/2 and charge $-e$ that interacts weakly with the other ones. This concept, introduced by Landau, explains the behavior of most metals. There are however, exceptions like one-dimensional systems or high temperature superconductors, but they are the subject of more advanced lectures and current research.

The subjects above constitute the first half of these lectures. The second half is devoted to diferent subjects that are important in the physical understanding of solids. The first one is

- Collective excitations.

By them we denote those elementary excitations, that arise from the cooperative arrangement of electrons in long-lived modes like *plasmons* and *excitons*. We will discuss them both in the general frame developed before as well as with simple pictures that are helpfull to understand their experimental manifestation.

One of the most dramatic manifestations of quantum mechanics is the realization of a state of matter, where transport of electric current takes place without losses, that is

- Superconductivity.

We will review here the phenomena, concepts, and theory of conventional superconductivity, a knowledge that is indispensable if we would like to understand a new form of superconductivity that is present in the so-called high temperature superconductors, where a different, new state of matter is suspected due to the evidence given by an increasing number of experiments. These new materials that were discovered in 1986 by J. Bednorz and K.A. Müller, who received the Nobel Prize in 1987, became one of the most important subjects of research in condensed matter physics, and continue to be at the center of interest at present.

Finally, the last chapter is devoted to

- Magnetic properties.

Magnetism known to most people due to the surprising effects that arise from the interaction among magnets and of magnets with paramagnetic metals, plays a very important role in new technologies like information storage devices. It also plays a central role in high temperature superconductivity and other so-called strongly correlated materials, where the properties, many of them still to be understood, are determined by strong interelectronic interactions. We will give here a survey of different phenomena related to magnetism, and of theoretical techniques developed to describe them.

It is hoped that at the end of these lectures, a broad view of Solid State Physics is achieved, such that students will be prepared to start their own research project in one of the research groups at Stuttgart, where condensed matter physics constitutes a major area of research.