PHY HC 5026: Solid State Physics: Lecture 01

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1 Introduction

1.1 Why study solid state physics?

Solid State Physics is the study of solids (especially crystalline solids) using combinations of techniques originally from crystallography, metallurgy and engineering, along with the theoretical tools of quantum mechanics, statistical mechanics, thermodynamics, and electromagnetism. The goal is to try to understand how the macroscopic properties of solids emerge from their microscopic, atomic scale properties. Therefore, Solid State Physics forms the theoretical basis of Materials Science. It also has direct applications to technology, you probably have heard about "solid state hard-drives in computers", in fact all of electronics is due to solid state physics! Semiconductors are perhaps the biggest gift of this subject. "Solid State Physics" is the largest branch of Materials Science, a very popular field of current physics research.

Once we have a basic understanding of the crystalline solids at their very microscopic level, that is how they are structured geometrically, we can later on derive many physical properties easily. Therefore, let us start with crystal structure.

2 Crystal Structure

Lattice: a lattice is a geometrical object, it is a regular repeated three-dimensional arrangement of points (Fig. 1) that extends up to infinity in all directions.

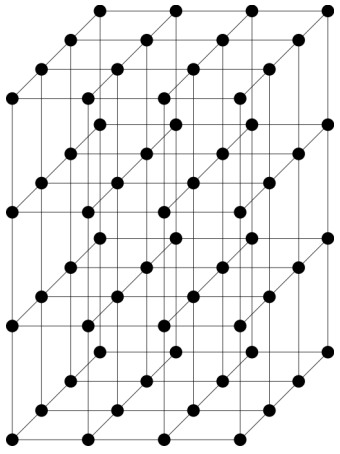

Figure 1: A piece of a lattice: repeated arrangement of points in 3D. A lattice of course is infinite in size and therefore, cannot be drawn entirely on this piece of paper!

If you stand on one of those points, the surrounding always appear to be identical. **Question:** Would it really be true if the lattice was not infinite?

Such ordered structures are everywhere in nature, for example the hexagonal lattice pattern of a bee-hive (Fig. 2).

Figure 2: A typical beehive surface structure.

Question: Can you guess why do bees like particularly this hexagonal shape? Why not squares, or triangles?

Crystal: a crystal is a physical object unlike the mathematical lattice. A crystal or crystalline solid is a solid material whose constituents (atoms, molecules, or ions) are arranged in a *lattice structure*.

Of course real crystals won't be infinite in size, but consider the distance between two atoms $\sim 10^{-10}$ meters, and consider the size of a piece of a crystal several centimeters ($\sim 10^{-2}$ meters), so, that's like a football on the surface of earth, isn't it effectively infinite? But, we have to be careful, we should be always considering the bulk, the interior of the crystal. The infinity (large) approximation will fail if we considering a location very close to the edge of a real crystal.

Experimental evidence of crystals: originally mineralogists found that the "index numbers" (will be defined later) that define the orientations of the faces of a crystal are exact integers! This discovery was supported by the 1912 x-ray diffraction of crystals, when ***Max von Laue*** developed the theory of x-ray diffraction by a periodic array, and his colleagues verified his theoretical results through diffraction experiments. The x-ray diffraction experiment decisively proved that crystals at their microscopic level, are built of periodic array of atoms or molecules. **Question:** can you guess why x-ray was used for this diffraction experiment and not other kind of light wave? For example, why not microwave or ultraviolet light?

Basis: a **basis** is either a single atom or a packed group of atoms (molecule) that when attached to each point of a geometrical (mathematical) lattice, produces the physical crystal. Symbolically:

$$\texttt{LATTICE} + \texttt{BASIS} = \texttt{CRYSTAL STRUCTURE} \tag{1}$$

Imagine the "H 32" classroom tile-floor is a mathematical lattice, if you put a frog (all identical frogs) on each corner, the physical structure consisting of those frogs, would be a crystal structure. That frog is your "basis". Instead of a frog, if you placed a "chalk and a duster" at every corner, provided all chalk-duster pairs are identical, that would still produce another crystal structure, this time your basis would be that chalk-duster pair. This was just a 2D example though, crystals are 3D structures.

Therefore, we can redefine crystal as the infinite repetition of a **basis**. The set of mathematical points to which a basis is attached, is called a "lattice".

Lattice Translation Vectors Just like to span the whole normal 3D space, we need 3 unit vectors ($\hat{i}$, $\hat{j}$, $\hat{k}$), we can construct any vector in space using these 3, all we have to do is multiply each of them by desired random real numbers (+ve or −ve) and combine them, e.g., $0.5\hat{i} - 2.3\hat{j} + 1000.4\hat{k}$ will be a vector, or any combination, and we can get a vector with any magnitude and direction. Similarly, to span the 3D space space of lattice, we will need 3 such (linearly) independent vectors, they may or may not be orthogonal, but that's OK as long as they are linearly independent, we can build the whole lattice space using them. But what's the catch here? Can we really build any vector with them? Remember, a lattice space is a discrete space, a space of discrete points! You cannot build any arbitrary vector here! The (position) vector must start on one of the lattice points and must end on another lattice point, how will you achieve that?

Assume that we got 3 such vectors, $\vec{a_1}$, $\vec{a_2}$, and $\vec{a_3}$, the condition would be: if we start from a lattice point represented by a position vector $\vec{r}$, and would want to jump to another lattice point represented by $\vec{r'}$, these two points must be related as:

$$\vec{r'} = \vec{r} + u_1\vec{a_1} + u_2\vec{a_2} + u_3\vec{a_3} \tag{2}$$

where u_1, u_2, u_3 must be all integers (+ve or -ve). Just like the normal continuous 3D space, if you choose all possible (infinite of them!) random integer values of these u's, you can fill the whole discrete space of lattice, in other words, r' can construct the whole lattice if you supply all possible integer values to those u's. Those $\vec{a}$'s are such that no lattice points will be missed if you choose all possible u integer values.

Unit Cell: a unit cell is a like a building block of a lattice, that when repeated infinitely, builds the whole lattice. It is the cell formed by 3 vectors $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ that span a lattice space. There are two types of *unit cells*:

1. **primitive unit cell:** a primitive unit cell or just a primitive cell is the smallest possible unit cell. It must contain only one lattice point (the meaning of that will be clear soon).
2. **conventional unit cell:** a conventional cell may contain more than one lattice points. It is used because usually a primitive cell may not display all the symmetries of the lattice, so we choose a unit cell that does.

The lattice point counting rule: when we say a primitive cell contains exactly one lattice point, what do we really mean? What is the counting rule of 1, 2, 3 etc lattice points contained in a cell? The general formula (in 3D) of total number of lattice points (N) contained within a unit cell is given by:

$$N = N_{internal} + \frac{N_{corner}}{8} + \frac{N_{edge}}{4} + \frac{N_{face}}{2} \tag{3}$$

where the meanings of various N's in the right side of Eq. (3) are apparent from their names in the suffixes. For example, N_{corner} is the number of points located at the corners of a cell, in 3D, such a corner-point is shared by 8 cells, therefore, for one such cell, we must consider only $1/8^{\text{th}}$ of one such corner-point. If a point was located at one of the faces of a 3D cell (imagine a cube), it is shared by just an adjacent cell, therefore, only 2 cells share such a face-point, therefore, such a point must be counted as half for a single cell. **Question:** can you explain the other two kinds of points?

Lattice Translation Vector: the *primitive translation vectors* $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ that spans the volume of a primitive cell of a lattice can be used to construct a special vector on that lattice: $\vec{T}$, called a *lattice translation vector*, defined as (Eq. (4)):

$$\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3 \tag{4}$$

this is the vector that can take you to every possible lattice point if you supply the desired integers: u_1, u_2, u_3. This vector operation also leaves the lattice *invariant*, meaning: if you are standing on a lattice point located by a position vector $\vec{r}$, and I apply a translation on you by $\vec{T}$, that is I move you to a new location $\vec{r'}$ such that:

$$\vec{r}' = \vec{r} + \vec{T} \tag{5}$$

you will not be able to tell if are still standing at the old location $\vec{r}$ or the new location $\vec{r}'$ by looking around you, everything will appear the same! That means, the operation $\vec{T}$ is a symmetry of the lattice, a translation symmetry to be precise.

The volume of a *primitive cell* is given by:

$$V_p = |\vec{a_1} \cdot (\vec{a}_2 \times \vec{a}_3)| \tag{6}$$

this is just a consequence of simple vector algebra, remember the formula of a volume enclosed by 3 vectors? It's just that.

Wigner-Seitz cell: it is easy to check that primitive cells are not unique, for a given lattice, you can come up with different shapes of primitive cells, examples are shown in Fig. (3)

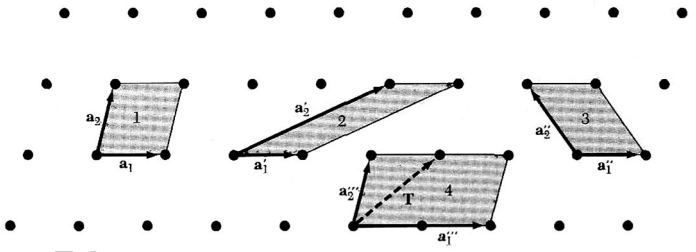

Figure 3: Here we see 4 kinds of cells, defined by the vector pairs: $(\vec{a}_1, \vec{a}_2)$, $(\vec{a}_1', \vec{a}_2')$, $(\vec{a}_1'', \vec{a}_2'')$, and finally $(\vec{a}_1''', \vec{a}_2''')$, out of these only the first 3 are primitive cells and the corresponding vector pairs are primitive translation vectors. The last one, that is the vectors $\vec{a}_1''$ and $\vec{a}_2''$, are not primitive translation vectors because you cannot form that translation vector $\vec{T}$ using these two, can you?

but there is a standard and unique way of finding a special kind of *primitive cell* called a "*Wigner-Seitz*" cell. Let us define it through construction:

- **Step-1:** choose a lattice point (any).
- **Step-2:** draw lines to all its nearest neighbors.
- **Step-3:** draw perpendicularly bisecting lines (planes in 3D, lines in 2D) to the above drawn lines.

area (volume in 3D, area in 2D) enclosed by those perpendicular bisectors will be a *Wigner-Seitz* primitive cell (a 2D example in Fig. (4)). **Question: check that it does contain only one lattice point using the formula given by Eq. (3).**

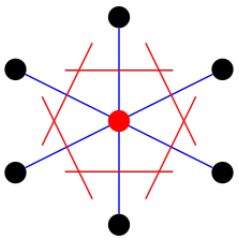

Figure 4: A Wigner-Seitz primitive cell in 2D.

References

Charles, K. (2005), *Introduction to Solid State Physics*, Wiley.