

Lecture 3

Although there were few successes of Drude model, some of them came out as pure luck. Along with them, the inconsistencies in the theory led people to search for the correct description. One of the main drawbacks of Drude's theory was that he considered electrons to be classical particles which follows Maxwell-Boltzmann velocity distribution,

$$f_{MB}(\vec{v}) = n \left(\frac{m}{2\pi k_B T} \right)^{3/2} e^{-\frac{mv^2}{2k_B T}}$$

where $f_{MB}(\vec{v}) dV_x dV_y dV_z$ gives the number of electrons per unit volume in the range of velocity between \vec{v} and $\vec{v} + d\vec{v}$ (meaning v_x and $v_x + dv_x$, v_y and $v_y + dv_y$, v_z and $v_z + dv_z$). However, with the advent of quantum theory people soon found that electrons are not classical particles, and should then be treated according to quantum theory. This let Sommerfeld to use the correct velocity distribution of the electrons - the Fermi-Dirac velocity distribution given by,

$$f_{FD}(\vec{v}) = \frac{(m/\hbar)^3}{4\pi^3} \frac{1}{e^{[\frac{1}{2}mv^2 - E_F]/k_B T_0}} + 1$$

where T_0 is a temperature found by the normalization constant,

$$n = \iiint f(\vec{v}) dN_x dN_y dN_z$$

Sommerfeld applied the FD distribution to the free electron gas in metal, and in most applications Sommerfeld's theory is nothing but the single modification. This indeed removed few of the anomalies of Drude theory of metal.

Using the Fermi-Dirac statistics the specific heat of the electron gas turns out to be proportional to temperature, which correctly explains the negligible contribution to the specific heat of the metal at room temperatures. Also, the Lorentz number comes out to be $2.44 \times 10^{-8} \text{ W}\cdot\text{ohm}/\text{K}^2$, which is in excellent agreement with the Wiedemann-Franz law, although now with any luck and correct measures. Along with that, the thermopower is also found to be in excellent agreement with the

Observed values.

However, the large part of the problems still remain unresolved. The mystery of Hall co-efficient, magnetic field dependent magneto-resistance, temperature dependence of DC electrical conductivity has no proper explanation in either of the theories. Also, Drude model considers the kinetic theory of gases and calculates wrong specific heat of $\frac{3}{2} n k_B$, which is temperature independent and ~~is only valid at~~ ^{not observed at all.} very high temperatures. Although Sommerfield model provides a temperature dependent specific heat, the specific heat here is ~~really~~ linearly dependent on T , which is only valid in the low temperature limit.

To account for these inconsistencies, one should get back to the basic approximations and try fixing them. What both Drude and Sommerfield model have in common is that both of them are free electron theories, meaning, they take the free electron approximation. The metallic ions play a very minor role. The effects of the ions in between the collisions

is totally ignored. Drude considered the ions as the source of collision, however, didn't explain the exact role that the ions play as a source of collision. And for the most important part, the possibility that the ions themselves, as independent dynamical entities, contribute to the physical phenomena (such as the specific heat, thermal conduction etc.) is totally ignored. Also, the ions are considered to be stationary. However, they are not really stationary and one needs to incorporate the ionic motion to properly understand the role of them as ~~a~~^{the} source of collision.

We will now then introduce the movement of the electrons in the presence of a specified potential due to fixed arrays of static stationary ions. Then we may talk about the consequences of the ionic movement from the static array.

The important fact to consider here that the ions are not distributed at random. Rather, they are arranged in a regular periodic array, called lattice. This was first directly confirmed by the

X-ray diffraction experiment, and later reconfirmed by neutron diffraction, electron microscopy and other direct measurements. The existence of this periodic lattice is at the heart of modern solid state physics. So, our primary focus will now turn to the subject of periodic arrays — the crystal lattices. In the next few lectures we will try to investigate the fundamental properties of such lattices. After that, we will come back to the Sommerfeld model again, and explore it in detail. Then we will use our knowledge of crystal lattice to account for the proper model of electrons in a solid.

Crystal structures

We use the word crystal in many of our encountered objects like quartz, diamonds, rock salts etc. They form their very plane faces and those are at sharp angles with each other. Although we do not see metals like these crystals, the metals that occur naturally are quite often found in crystalline forms.

However, the definition of crystal in Solid State

Physics is not dependent on the macroscopic shape of a solid, rather on the underlying microscopic structure. If on the microscopic level the ions are arranged in a periodically ordered manner, then the group of such ordered ions/atoms is referred to as crystals. The fact that observed crystals are made up of periodic structures was long hypothesized to account for the geometric regularities of macroscopic crystals, in which plane faces make only definite angles with each other. It was only with the advent of ~~X~~¹ X-ray diffraction in 1912 that the confirmation came in.

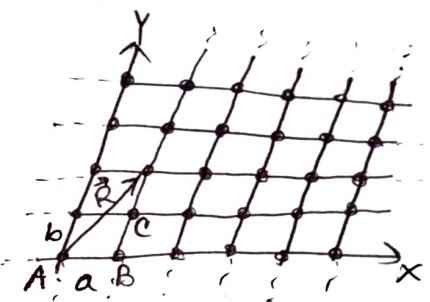
We will start with some basic geometric properties of this periodic crystal structure, before going into the detailed picture of X-ray diffraction and how this periodic structure helps understanding properties of solid.

The crystalline state

A solid is said to be a crystal if the atoms/molecules/ions are arranged in such a way that their positions are exactly periodic. The following figure captures the concept. The distance between any two nearest neighbours in the x -direction is a and in y -direction is b . A perfect crystal will be such a crystal for which the periodicity is maintained in both x - and y -directions from $-\infty$ to $+\infty$. To an observer located at any of the atomic sites, the crystal appears the same if it is perfect.

The idea is often expressed by saying that a crystal possesses translational symmetry, meaning, if the crystal is translated by any vector joining two atoms, say \vec{R} , the crystal remains invariant under such translation.

In reality, one can't make a perfect crystal. For example, the surface of a crystal is an imperfection, because it breaks the periodicity. The atoms very



near the surface "see" the environment differently than the atoms deep within the crystal. Also, there are almost always impurities (foreign atoms) that breaks the perfect crystal structure. Even with all ~~perfection~~ the perfection, there are thermal vibrations of the atom ions ~~that~~ for $T > 0 \text{ K}$, which distorts the crystal structure. However, we can isolate a crystal so large that the ratio of surface atoms to all atoms is small. We can neglect the very small impurities, and at a very low temperature, the vibrations are weak and one can speak of a "perfect" crystal.

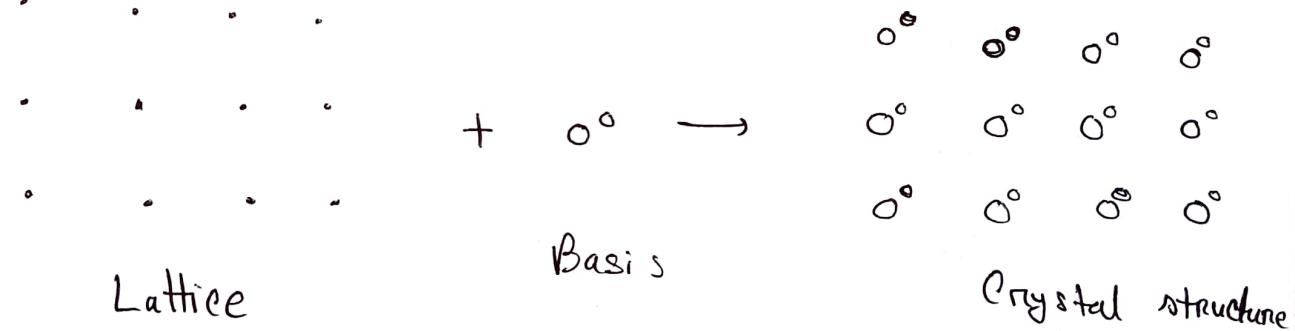
We will study the perfect crystals here. Imperfections are often the main subject of interest. For example, crystal defects cover a huge part of Solid State Physics. We will treat the imperfections as small perturbation in the crystalline structure. For now, let's concentrate on the perfect crystals.

We will define few quantities related to crystal structure. Although these definitions apply to one, two- or three dimensional crystals, we will start with 2D crystals and restate them for 3D crystals.

The crystal lattice

Any crystal structure can be represented geometrically by forming a crystal lattice. What we do is, we replace the repeating unit of the crystal structure just by a point. The ~~repeat~~ repeating unit (which can be an atom, group of atoms, molecule or ion etc.) is called the basis. So, for forming the crystal structure, we assign the basis at each lattice point.

$$\therefore \text{Lattice} + \text{Basis} = \text{Crystal Structure}$$



There are two types of lattices - Bravais and non-Bravais lattice. Bravais lattice are those where all lattice points are equivalent, which mean there is only one type of basis. In a non-Bravais lattice all the lattice points are ~~not~~ simply not equivalent.

For example, as shown in the figure, A, B, and C are equivalent. A', B' and C' are equivalent as well. However, A and A', B and B', or A and B' are not equivalent. So, the whole lattice is a non-Bravais lattice. However, lattice ABC and lattice A'B'C' will constitute Bravais lattice individually.

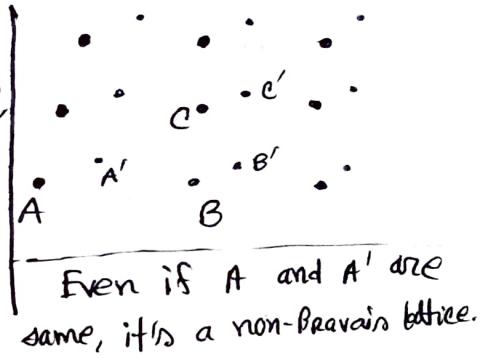
We can give two equivalent definition of a Bravais lattice.

- A Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever array the point is viewed.
- A three dimensional Bravais lattice consists of all points with position vector \vec{R} of the form,

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

where \vec{a}_1, \vec{a}_2 and \vec{a}_3 are any three vectors not on the same plane, and n_1, n_2 and n_3 are integral values (positive, negative or zero).

The vectors \vec{a}_i appearing in definition b) are called



Even if A and A' are same, it's a non-Bravais lattice.

the primitive or basis vectors.

In two-dimension, definition (a) still holds, but definition (b) is modified to having a vector $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2$ where \vec{a}_1 and \vec{a}_2 are not on the same line or parallel (non-collinear).

Here, in the example, \vec{a}_1 and \vec{a}_2 are the primitive vectors. The position of lattice point C is

$$\text{then, } \vec{R}_C = \vec{a}_1 + \vec{a}_2. \text{ For lattice point F, } \vec{R}_F = 3\vec{a}_1 + \vec{a}_2.$$

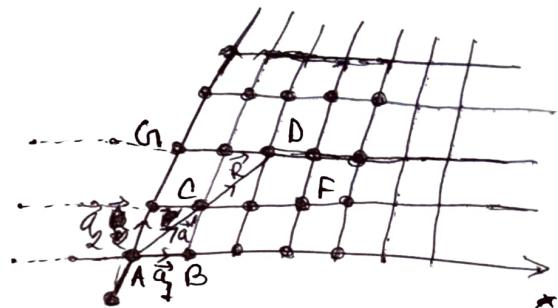
We call \vec{R} the lattice translation vector. If we perform any translation through \vec{R} , the lattice will look exactly the same.

The choice of the primitive vectors are not at all unique. For example, in the same lattice shown in the previous figure we could choose ~~\vec{a}_1~~ or \vec{a}'_1 and \vec{a}'_2 as the primitive vectors. In that case,

$$\vec{R}_C = \vec{a}'_2, \quad \vec{R}_F = \vec{a}'_2 + 2\vec{a}'_1, \quad \vec{R}_{G_1} = -2\vec{a}'_1 + 2\vec{a}'_2$$

and again you can express any point in the lattice of the form $\vec{R} = n_1 \vec{a}'_1 + n_2 \vec{a}'_2$.

A two-dimensional Bravais lattice is also called a net.

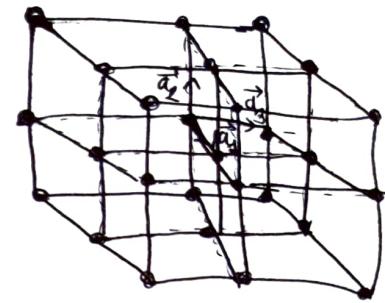


$$\begin{array}{c} \vec{a}'_1 \\ \vec{a}'_2 \end{array} \quad ; \quad ;$$

$$\vec{a}'_2 = \vec{a}_1 + \vec{a}_2$$

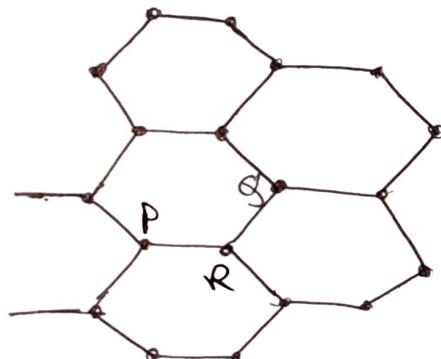
We can construct a simple cubic Bravais lattice as an example of 3D Bravais lattice.

The lattice can be spanned by three mutually perpendicular primitive vectors of equal length.



It is important that not only the arrangement, but also the orientation must appear the same from every point in a Bravais lattice. Here is a ~~pic~~ figure of a honeycomb lattice.

This is the lattice structure of graphene (a very thin layer of carbon atoms, ~~is~~ said to be 2D).



Is this a Bravais lattice? For point P and Q, the orientation ~~is~~ are perfectly identical. However, the orientation found from point R, you see that the structure seems rotated, and not the same as P and Q. So, the honeycomb lattice is not a Bravais lattice.

