Solid State Chemistry
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Lecture - 55
Summary of Week 11, Practice Questions

Now, I will go to the last lecture of week 11 of this course. This will be the penultimate week of this course, and after this week you just have one more week. And in this lecture what we typically do is to summarize what we learnt during the week and then do a couple of practice problems. So, in this lecture I will do the same; so, Summary of Week 11 and Practice Problems.

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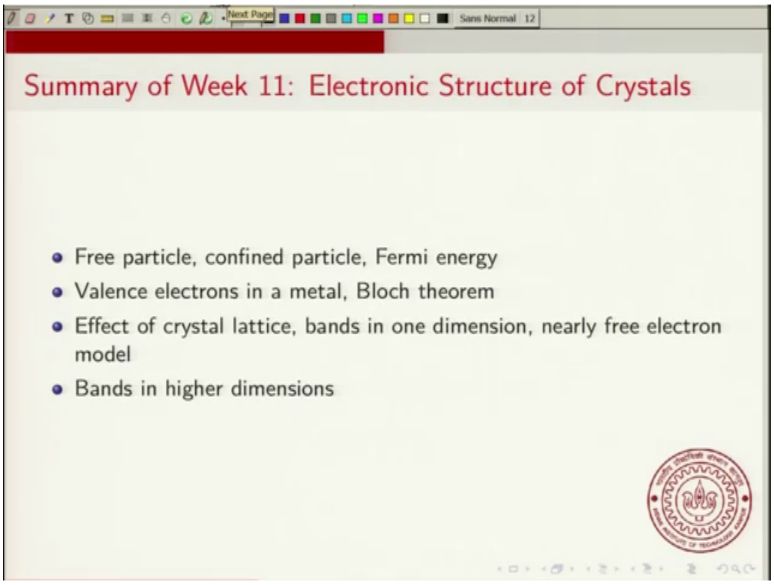

So, in week 11 we learnt about the electronic structure of crystals, ok. You should be familiar with the term electronic structure, if the electronic structure refers to the wave functions of the electrons and the energies of the electrons, and so in this week we took a few steps towards that, ok.

We started by discussing a free particle and a confined particle, a particle that is confined to be within some region and we saw how we could write the energy expressions for the free particle and the confined particle. And then we talked of the concept of Fermi energy, and then we looked at valence electrons in a metal and we described them, we described the behaviour of valence electrons using Bloch theorem and Bloch equations.

And we saw the effect of the crystal lattice we studied how this leads to bands in one dimension, ok. And then and then we saw the nearly free electron model which allows us to see the concept of a band gap and then we briefly looked at bands and higher dimensions, ok.

Now, I should mention that throughout this week I have sort of given you the main features of band theory of solids, ok. But I mean they obviously, each of these requires a lot more work if you really want to understand, and it takes a lot of time to master, but at least with these basic with this basic knowledge you can understand how bands come. And, then we will see in the next week we will see how to use the band theory of solids to understand properties of materials, ok.

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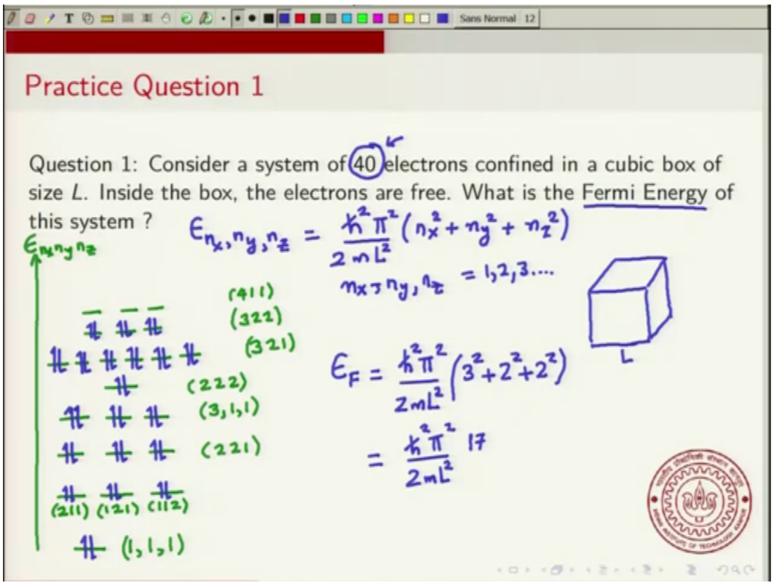

So, I will just do a couple of simple exercises simple questions. So, the first question asked the following. So, consider a system of 40 electrons confined in a cubic box of size L. Inside the box, the electrons are free. What is the Fermi energy of this system? So, basically the idea is the following that you look at the you look at these electrons in a box of size L, a cubic box of size L and you ask what are the possible energy states that you can get and then you say and then you start filling the electrons into the energy states, ok.

So, inside a box inside this cubic box of size L, the energy is given by a set of 3 quantum numbers, you can say n x, n y and n z. And we already saw this it should be h cross square pi square by 2 m L square into n x square plus n y square plus n z square. And the condition is that n x, n y and n z can all take values 1, 2, 3 and so on up to infinity, ok. So, and we have told that there are 40 electrons, and the Fermi energy is the highest energy that the electron can have in this system, ok.

So, let us try to let us try to do this. Now, if you take this and you and you look at the energy level, so the ground state the lowest energy state. So, let me put an axis of energy here, energy, and it is a function of n x, n y, n z, ok, function of these 3 quantum numbers. And if you see the lowest energy level, ok, so that corresponds to n x equal to 1, n y equal to 1, n z equal to 1 that is the lowest energy level, ok; the next highest energy level, ok. Now, in this case you need to find the next highest value of n x, n y and n z and in this case the next highest energy corresponds to n x equal to 2, n y equal to 1, n z equal to 1 or n x equal to 1 and n y equal to 2, n z equal to 1 or n x equal to 1, n y equal to 1 n z equal to 2.

So, so you can have you can have 3 different levels, you can have I will just write it as 211; that means, n x equal to 2, n y equal to 1, n z equal to 1 or you can have 121 or you can have 112. And since the electrons are indistinguishable you really cannot tell you really cannot distinguish between these states. So, basically there are 3 states that you cannot really distinguish between, ok. The next highest energy level will also be will also have 3 states and I will just write it as 221, that also includes 212 and 122.

The next highest energy level, now 2 square plus 2 square plus 1 square is 9, then you can have 2 square plus 2 square plus 2 square which is 12, or you can have 3 square plus 3 square say 3 square plus 1 square plus 1 square which is 11. So, the next highest energy level is actually 311. And again, any of them can be 3 and any of them can be 1. So, you have 3 states. So, you can have 311, 131 and 113.

After this the next highest energy level is 222 which is just where we just has one energy states, ok. You cannot you cannot have any other combination, ok. Now, let us just count how many states you have had so far. So, we, so if we count the total number of states we have 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, and since we have 40 electrons we should go at least up to 20 states, we need at least 20 states to fill 40 electrons, ok.

So, the next one is actually 321 and now, so this 321, now if you do different combinations there are actually 6 combinations. So, you can have 321, 312 or you can have 231, 213 or you can have 132, 123, so, there are 6 combinations here, ok. And subsequent to this is the 322, ok. In this case you can have only 3 and so, 322, 3 square plus 2 square plus 2 square that is 17, the next one is actually 411, and this is also triply degenerate, ok.

So, so I think I think we have enough levels now, ok. Now, let us fill the electrons. So, we will start from the lowest energy. We have to fill 40 electrons. So, 1, 2, 3, 4, 5, 6, 7, 8 that makes it 14, 20, 22. Now, there are 12 electrons here that makes it 34. So, you have 2, 4, 6, 8, 10 you have 34 so far and then we can have up to 40. So, then this is how 40 electrons be filled. The 411 state will be vacant.

So, at low temperature, all the this is a lowest energy state, ok, only the lowest energy state will be seen. At higher temperatures you will also have states where some of the electrons are excited. So, the Fermi energy is equal to h cross square pi square by 2 m L square, and then you have 3 square plus 2 square plus 2 square, and in units of h cross square pi square by 2 ml square into 9 plus 4 plus 4 that is 17, ok. So, this is the value of the Fermi energy of this system, ok.

Now, again this concept of first building up the energy levels and then filling them up starting from the lowest energy is very important, ok. And, it is something that we use even when you are doing the band theory of solids, we have all the energy levels ok, we have all the energy bands and then you start filling them from the bottom we will see this in the following week. We start filling them up from the lowest energy onwards and that is how you determine the Fermi level for any given band structure.

So, what is important is that for the Fermi level you need to know the number of electrons. So, if you do not know the number of electrons you cannot determine the Fermi energy, ok. So, that was the first problem, first practice question.

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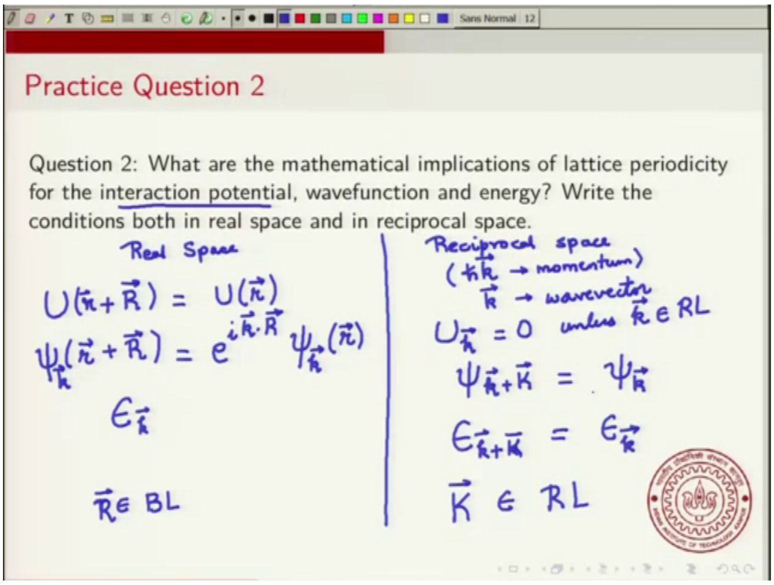

Now, the next practice question is the following what are the implications of lattice periodicity for the interaction potential, wave function and energy and write the conditions both in real space and a reciprocal space, ok; so now, because of the lattice periodicity.

So, the lattice periodicity implies, ok. So, let me write the real space conditions on this side, ok. So, clearly starting with the interaction potential; so, if I call it U of r, ok. Now, because of the lattice periodicity you have U of r should be U of r plus R, where r belongs to the r, r is a vector in the Bravais lattice R is R is a lattice translation vector. So, it belongs to the Bravais lattice. So, I mean it is a lattice translation vector.

Now, what about what about the wave function? Now, the wave function, let me write this a little differently I will just write it in the reverse order, just to emphasize the periodicity. So, the effect of translation by R is nothing, ok. Now, let us look at the let us look at the wave function. So, the wave function, now for the, now this wave function, can be expressed as linear combination of various of different K functions, of wave functions with different values of K, ok.

So, we index it with the letter K, to say the wave vector. So, corresponding to so you can you can you can express it in terms of these functions are depend on wave vector, ok. And what you get now is that this is equal to e to the i k vector dot capital R multiplied by psi k, ok. I am not writing the band index I am not writing the n before the k, but if you want you can put that also, ok. So, it is related to psi of R through this factor, through this through this e to the i k dot r.

What about the energy? Now, the energy is of course, independent of r. So, the energy is just dependent on k, and there is no you do not see any effect of periodicity on the energy in real space, we will see the periodicity the effect of periodicity on energy in the momentum space, ok. So, now, let us take look at the reciprocals place or the momentum space or the wave vector or momentum space, ok. So, note that h cross k is momentum and k is a wave vector. So, up to a constant this is reciprocal space is either called k space or wave vector space or momentum space, ok.

So, now what happens? So, if you take this if you take this potential, and you ask because the potential is a periodic function, if you look at U of k, and this is the this is something called the Fourier transform, ok. So, you are transform it, and you write U of k, then U of k will be 0 unless k belongs to reciprocal lattice, ok. So, unless k is a vector of the reciprocal lattice, and so that means, that means this is only non-zero if the corresponding wave vector. So, what is meant by U of k is a Fourier transform of U of r, I will not get into the details of that, ok, but you can take any function of R and convert it to a function of k and this function will be 0 unless K belongs to the reciprocal lattice, ok. I am not I am not doing the detailed mathematical derivation of the 4ier transform, but this is what it implies.

Now, in the case of, now if you look at the wave function, ok. Now, this is exactly equal to psi of k. So, because of the periodicity in real space the wave function is a periodic function in reciprocal space, and we have the energy which is also a periodic function in reciprocal space equal to epsilon k. I am now again, I am not writing the end band index, what is important is that k is contained in the reciprocal lattice, ok. So, the periodicity in real space implies a periodicity in reciprocal space and if you recall it is this periodicity in reciprocal space that we used to construct the bands in a solid, ok.

So, with this I will conclude this lecture and we will conclude the week 11 of this course. Now, in the last week we are just going to build up a little bit and see how to use the band theory of solids, ok. It will be a little less mathematical than this week ok, but we will see simple applications of band theory of solids to understand both the electrical properties and the optical properties of solids.

Thank you.