Electronic Theory of Solids
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Lecture - 29
Magnetism: Quantum Theory

Hello and welcome, we have started working on Magnetism. So, as I said the other day that magnetism is one of the oldest known macroscopic quantum phenomenon. And of course, after the discovery of quantum mechanics we now know that it is a quantum phenomenon.

And the existence of permanent magnet only in quantum mechanics was shown by Niels Bohr and his collaborator Miss Van Leeuwen As I showed the other day its a very straightforward calculation and what she showed they showed was that if you just take the partition function and in classical mechanics then your integral just vanishes.

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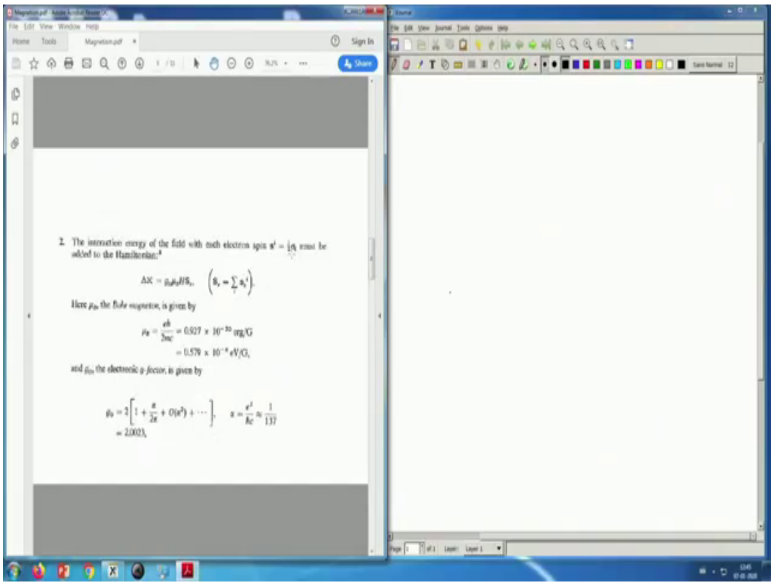

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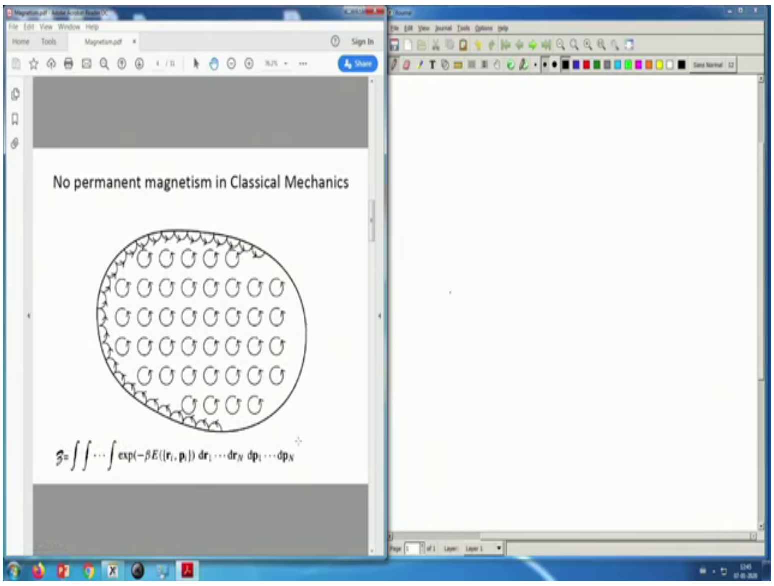

This is the integral for the partition function and since it is an infinite integral over momentum and space and so, continuous integral it is an integral which is basically assumes continuous r and p. Then of course, you can just shift the origin of the momentum to absorb your vector potential and then of course, the final result will not reflect any magnetic field in the dependence of z.

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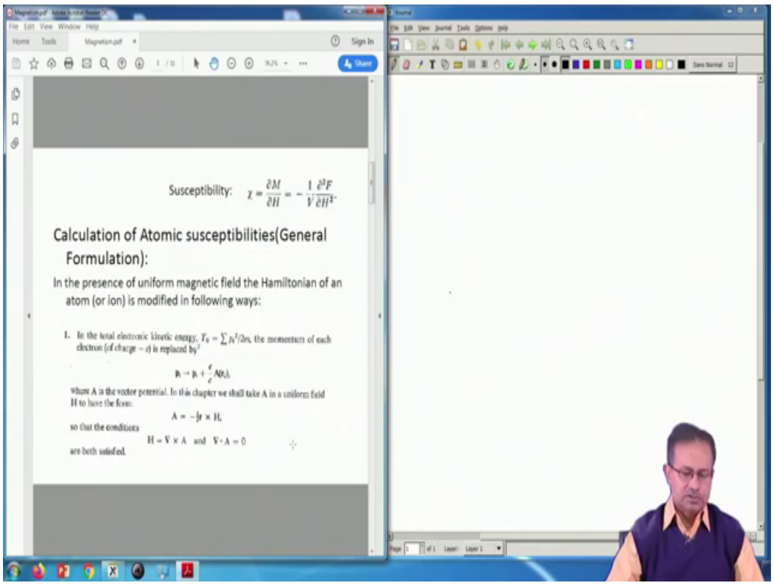

And then therefore, if you take a derivative if you just calculate the free energy.

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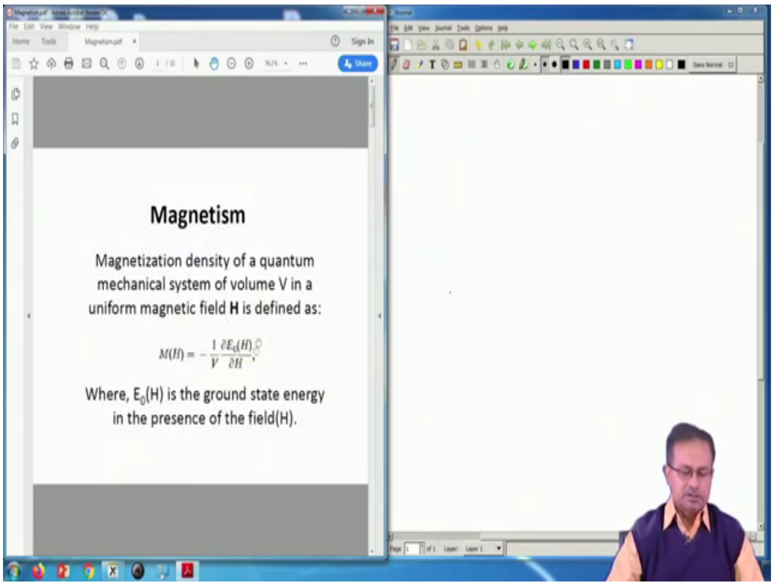

And take derivative with like this.

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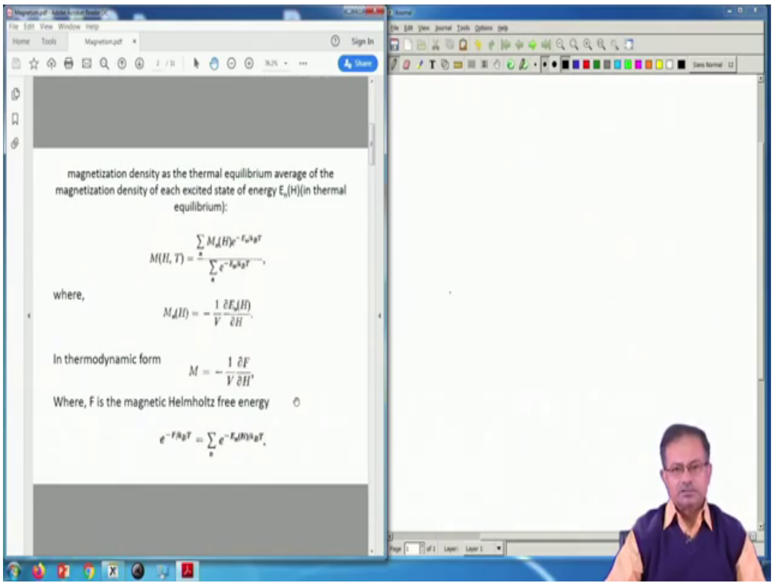

Then you will not find any magnetism in any permanent magnetism in classical theory of solids. Of course, the as I said the devil lies in the details because, the in quantum mechanics of course, you do not integrate you sum over states and these are discrete states so, you have to sum. And, that some actually gives rise to magnetism and there is a pictorial way of looking at it which is this, that I mentioned that the classical description is like electrons orbiting around the field, if the field is coming out of this board.

And then of course, you have this circulating currents, each of them will produce a moment and that moment adds up to give you a total magnetization. And that is what we have learned in our classical theory of magnetism, but then as I showed that there is this large loop which survives finally, from the all the internal currents.

Because, all of them cancel internally inside, only the large loop at the boundary survives, but then at the boundary exactly at the boundary there are these skipping orbits. These orbits which do not complete. So, the electrons in such orbits will actually provide a magnetization which is just if you provide a current actually which is just the opposite of in sense of the net magnetic net current that you get from this internal small loops, some of them.

So, you add these up, you get a large current loop, you add these you just look at this these skipped orbits in incomplete orbits, then you will find that they just exactly cancel each other. So, that is how one rationalizes the fact that there is no magnetism classically.

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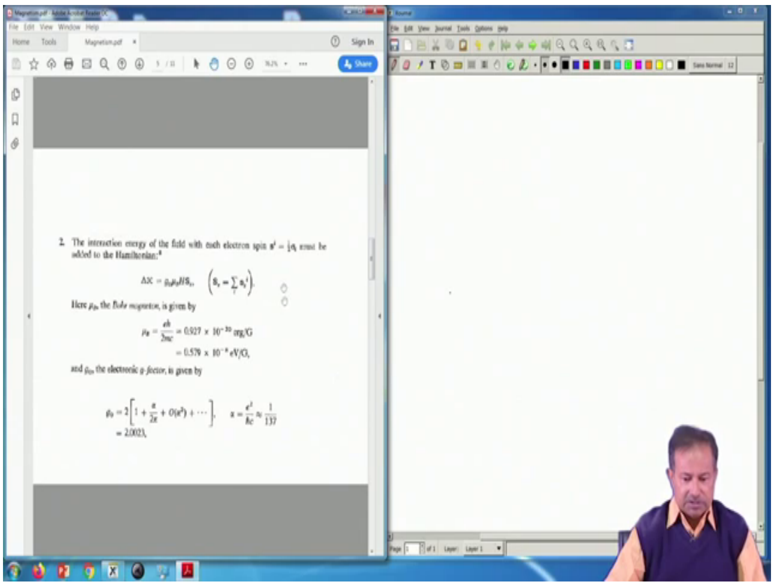

As I said the resolution lies in quantum mechanics ok. So, the things that one actually need to calculate is that there is this change in interaction energy change in energy for example, if you calculate the Hamiltonian in the absence of magnetic field. Then you calculate the Hamiltonian in presence of the to write down the Hamiltonian presence of the magnetic field then this additional term that you see that comes from the spin.

So, this is well known g mu B times the magnetic field dot S, here the magnetic field is taken in the z direction. So, the plot product is h dot S and mu B is the more Bohr magneton which is given by e h cross by twice m c whose magnitude is extremely important. Because, that is the scale about which where the d which determines the energy that is change in energy due to a magnetic field for coming from the magnetic field interacting with the spin.

So, this is typically the h e h cross by twice m c is an extremely small energy scale. For example, its 10 minus of the order of half into 10 minus 8 eV per Gauss. Typically, one works with 10 to the power 4 Gauss for example, in the laboratories. So, even then it will be like 10 to the power minus 4 electron volt. So, that is extremely small energy compared this with electronic energies in a solid which is like electron volt, the Fermi energies are typically 2 to 5 electron volts.

So, this is about a factor of 10 minus 5 lower than that even at a field of tesla. So, that has to be borne in mind because the magnetic energies are far-far smaller than the electric energy is coming from Coulomb interactions. Or for example, in combination of Coulomb interaction and the quantum mechanics because, Pauli principle provides you the e of f. So, that is energy that is far bigger than the magnetic energies.

So, in a solid magnetic energies are in anywhere in a charge when you are dealing with spin half electron for example, you typically are giving an energy even for a tesla field which is exceedingly small 10 minus 5, 10 minus 4 electron volt. The g 0 factor is of course, the g factor g 0 is the famous g factor which is typically taken almost for all practical purposes to be 2 although there are corrections.

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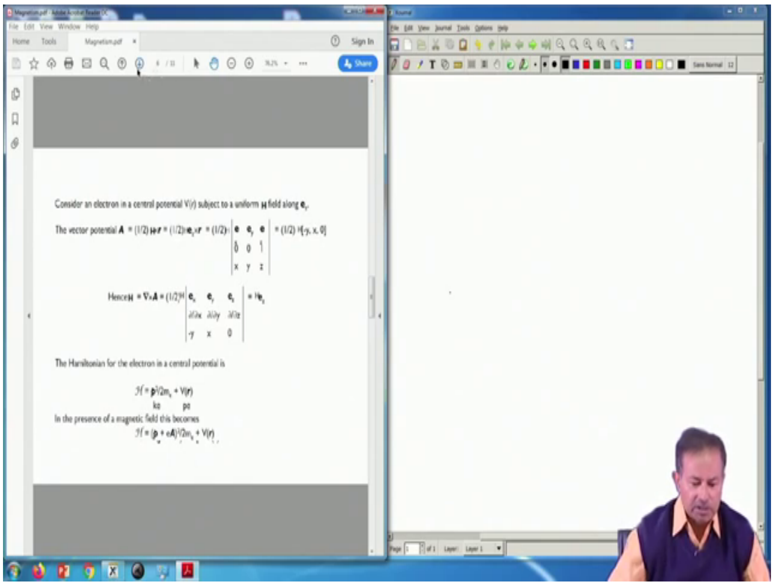

So, let us just now understand how an electron in a magnetic field, a free electron in a magnetic field behaves, how does its how is how does its Hamiltonian change from when there was no field. So, that is what we are after now. So, we put a magnetic field in the z direction and then the usual arguments that we also used in the Landau problem when we did quantum Hall effect is that this half H cross r is the vector potential.

And so, that gives me a vector potential which is half H minus y along x direction x along z direction and 0, x along y direction and 0 along z direction. So, this is a trivial, this we have already done. The interesting thing to remember that this vector potential will now go and change the p the momentum.

So, you have to write the canonical momentum. So, by already you can see that there are two contributions of magnetic field to even a free electron. One is that straight forward interaction S dot h kind of a term which interacts with spin. So, that is an energy that gets changed, that is the interaction energy with the spin. Then of course, the orbital angular momentum couples to the electron field, electronic field.

And, that comes from changing the momentum to its canonical momentum p plus p minus e a by c and that is exactly what we are after now. So, both the terms have to be included in your Hamiltonian to find out the change from the case when there was no magnetic field. So, let us just go through it, see the typical Hamiltonian is p square by twice m plus some central potential say Coulomb potential or whatever. You can neglect this for the time being because, we are only interested in the magnetic part of it. So, just put a V of r anyway.

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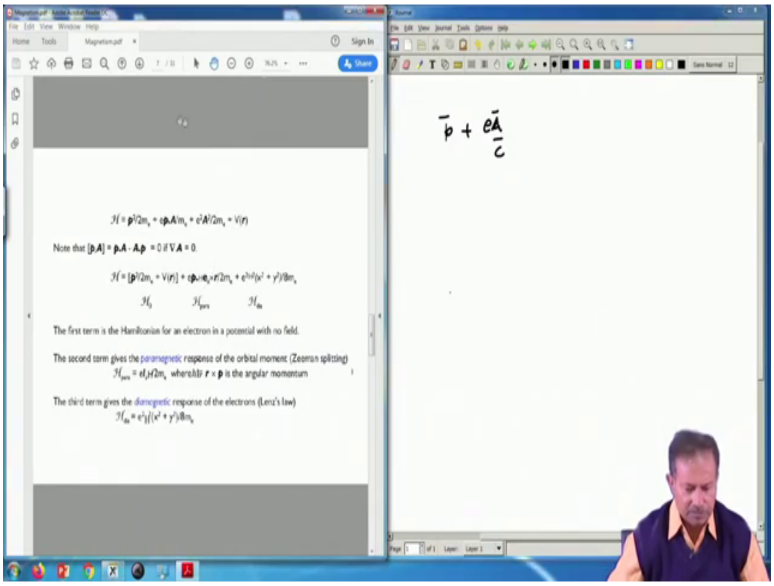

So, in the presence of magnetic field this will become the p minus again the typical p minus e A by c. So, which a here is p plus A by c and sorry p plus e A by c and this is the change in the Hamiltonian. So, let us just go ahead and so, there will be two terms.

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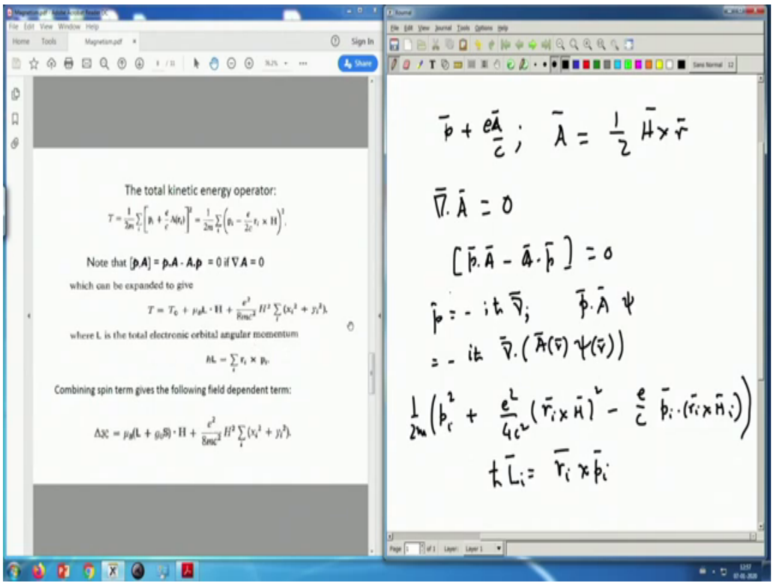

So, let this is what it is total kinetic energy operator for example, changes and it gives you this term ok. And which we just saw that this A of course is so, you write A as half H cross r, H is the magnetic field remember and that is what this term will give you. So, this is what you have to calculate now of course, remember that p is a quantum mechanical operator; so, one has to be a bit careful.

So, one chooses a gauge here which is called the Landau gauge or the sorry the Coulomb gauge or the transverse gauge which is this. So, as I showed in the previous calculations for quantum Hall effect, integer quantum Hall effect that this your choice of gauge really does not matter. So, you just choosing transverse gauge here and then of course, you can easily show that p dot A minus A dot p is actually 0, this is 0.

So, the commutator of A and p is 0, if divergence a is 0, it is very straightforward. We write p as minus i h cross del operator and then just to use say p dot A operating on psi. So, that is minus i h cross del operating on A r psi of r and you can see that there are two terms out of which del dot A term will be gone and you are left with grad of a dot grad psi which is A dot p.

So, p dot A is basically A dot p. So, if you do that then of course. This can be expanded. So, there will be terms like p square p i square 1 by twice m p i square plus e square by 4 c square r i cross h square and then there is this A dot p plus p dot A. And so, we will we can combine them and we will we will have e dot.

So, the term that we will get is e by c p i dot r i cross H i. So, this kind of a term is; so, you even now write this in terms of the well known angular momentum operator which is L i for example, is r i cross p i ok. So, if you do that of course, then what you will get is that there is a and remember your mu B was e h cross by twice m c.

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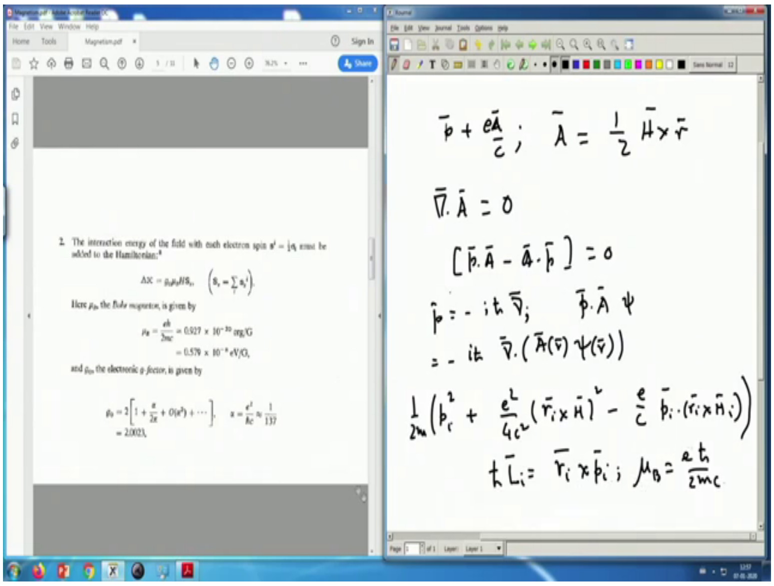

So, mu B equal to e h cross by twice m c. So, I put this all in and you will get a Hamiltonian which is exactly this what is written here which is change in Hamiltonian.

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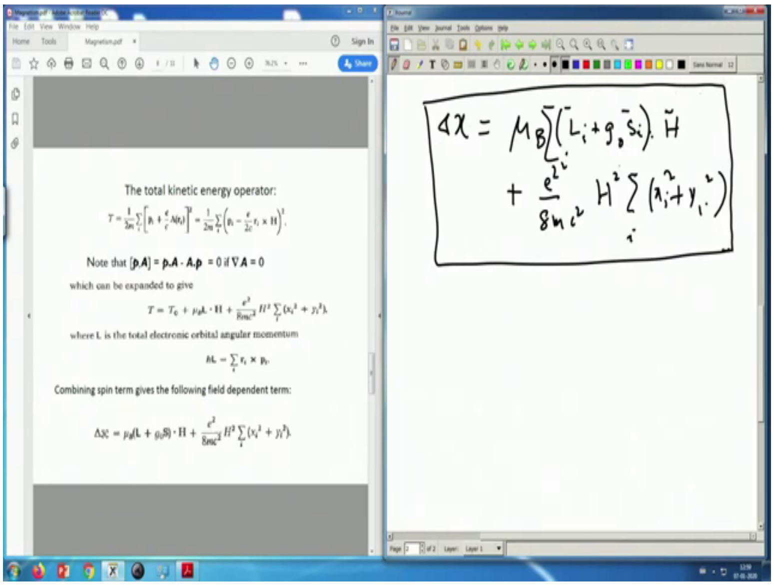

So, the Hamiltonian will be the current see the changes in the kinetic energy plus there is mu dot mu B dot g dot S term S dot h term. So, all that if you combine your change in Hamiltonian is just mu B into L plus g 0 S dot H. So, these L i and S i dot H; so, I have summed over all i's so, this is the total plus e square by 8 m c square into H square into all of these x i square plus y i square.

So, I could put an L i plus g i here also to make it consistent with this L i plus S i sum over i and that sum over L i is total L sum over a size is total S. So, that will give me L plus g 0 S dot H; so, that is the; that is the; that is the term. So, this is the change in delta H is written on the left hand side also so, that has to be calculated now.

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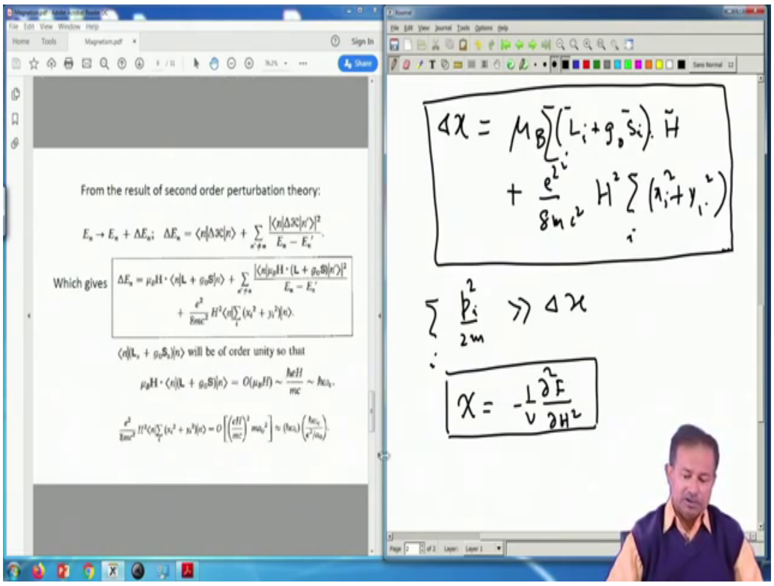

How do you calculate in quantum mechanics? Well you just so, what you do is that you can do a perturbation theory because this is much much less than the t's p square by twice m term right this term. So, this term is much much bigger than your delta H. So, you can easily do a perturbation theory here taking delta H to be a perturbation. But, how long how many orders do you keep in your perturbation theory?.

First of all the first order has to be kept because that is the leading order. Do you need the second order? Because, its much smaller in energy because the as you increase the order the energy becomes smaller and smaller, contribution becomes smaller and smaller. But, you have to keep up to the second order; remember that your susceptibility was minus del 2 F del H 2. So, that is to calculate susceptibility you at least need up to order second order.

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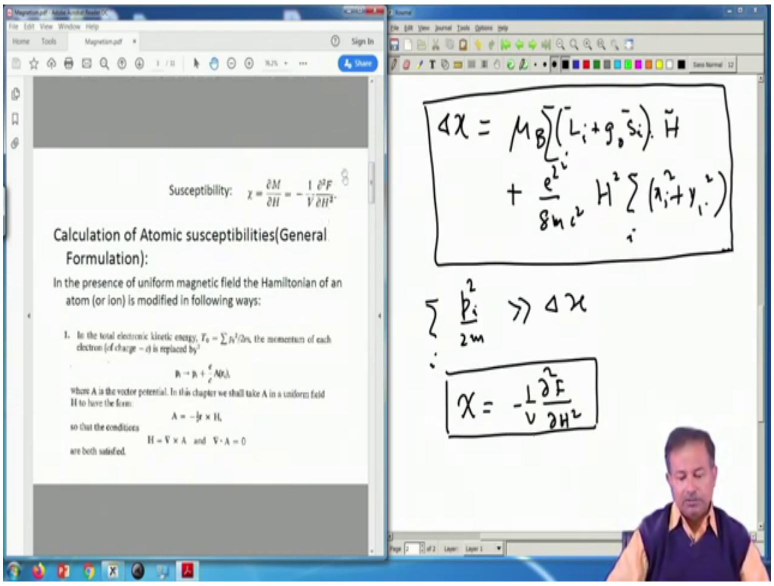

Remember this formula that chi is minus 1 by V del 2 F del H 2 and then of course, you need up to second order in H. So, that you can actually calculate the susceptibility.

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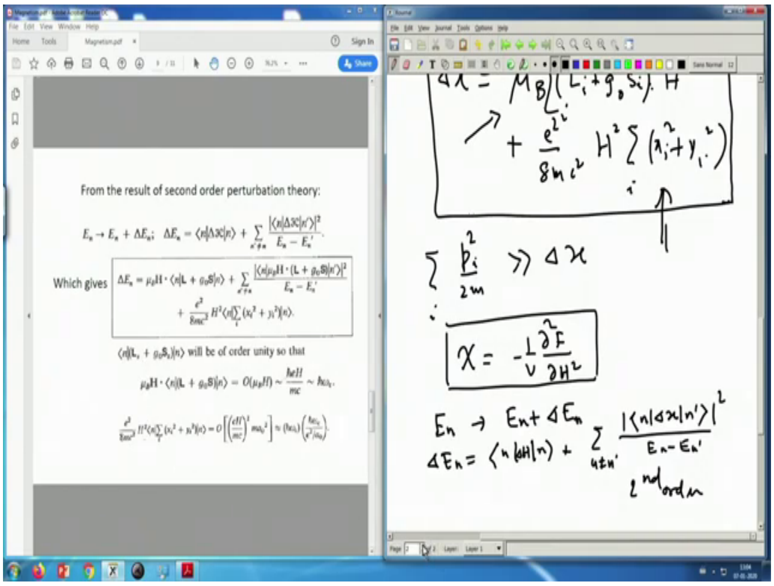

So, that is exactly what is shown here. The perturbation theory just changes the nth level energy of the nth level E sub n to sub E n plus delta E n and that delta E n is given by the standard perturbation theory which is the first order is n delta H n. Then there is the second order plus n not equal to n prime. These are things you have done in a quantum mechanics, if you have not done this is basically the formula mod square divided by E n minus E n prime.

Note that the n comes E n minus E n prime in the denominator that is the standard use of. So, if you look at it is delta H between n and n prime states and denominator is E n minus E n prime. If E n for example, is your ground state then E n prime is greater than E n and this term becomes negative. So, that is the way one works in quantum mechanics so, that is your delta n. This is the second order perturbation result, I do not need any order beyond that because I have to calculate the susceptibility and which is the second derivative.

So, that is that term I mean this is basically that term which is, remember these two is calculated, this is calculated this is calculated in first order then second order, but this one is already in second order in H. So, even the first order perturbation will give you the second order term. So, you do not need to go beyond this because the next order will be even higher; so, H to the power 4 order; so, you do not need that.

So, this is done in first order term, the last term this contribution is only calculated up to first order, this contribution is calculated to first and second order. So, that is the game one plays out here, but it is just not calculation that is important, its condensed matter physics, it is an experimental subject and you need to know the numbers.

So, if you have to understand what these contributions are typically their values and in what situation you do what. So, let me just explain what I mean. So, let us just take this term this n L L plus S that this term is let me calculate for you the order of magnitude of this terms.

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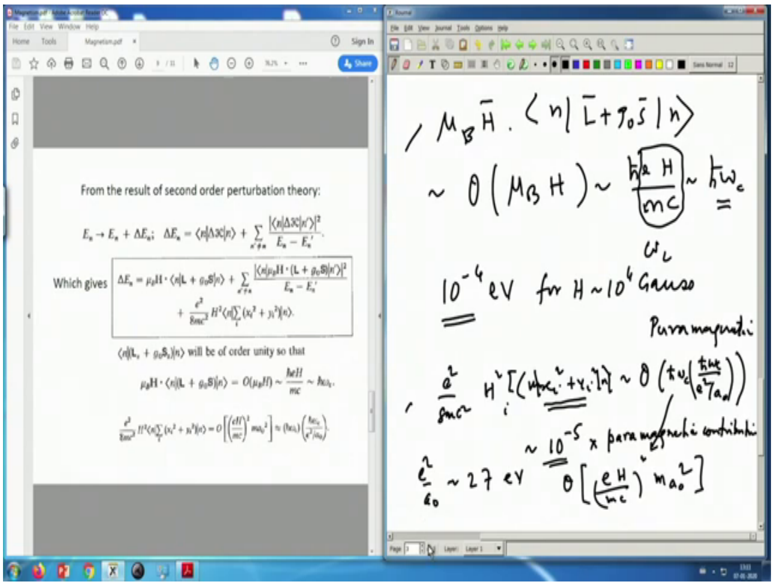

So, mu B H n L plus g 0 S n prime. So, this is the first term, this one coming from the. So, these two terms are called the paramagnetic and the diamagnetic term, we will come back to why it is called diamagnetic. The third term is called the diamagnetic term and the first term is the paramagnetic contribution. But it is just at the moment it is just a name, let us just go ahead and do it and see what it is.

So, let us just calculate this first order term, at least its order of magnitude you should know. This is the term that we are after now and its magnitude if you calculate is of the order of mu B H, the magnetic field which is h cross e H by m c, let us forget the 2. This is the order of magnitude calculation so, let us just do it and this you can carry, this remember your cyclotron frequency expression e h by m c.

So, this is the cyclotron frequency omega c and this we remember we mentioned earlier in the quantum Hall effect context that these even at 15 tesla or so, this will be like 10 degree Kelvin. So, this is an extremely small number when you are dealing with electrons and that number is about typically is about 10 minus 4 eV for a field for H of the order 10 to the power 4 Gauss.

Now, look at it this field is fairly large, but the contribution that it gives is this 10 minus 4 eV which is as I said in the beginning it is a very small number compared to other energy scale in a solid. So, the other main energy scale is of course, two scales are there; one is the Fermi level and the other is temperature.

Of course, there are these phonon scales and all that, but in electronic properties if you look at only the electrons, then there are these two other scales which is the Fermi energy and the temperature. And, if you look at this is in terms of temperatures this is about few degree. And so that means, your room temperature and your Fermi level of course, is at very high energies 30,000, 40,000 degree Kelvin. If you convert it to temperature then you have a room temperature which is 300 degree Kelvin and now you have this magnetic scale which is about a few degrees.

So, that is the scale that one has to remember for magnetic interactions. So, there is this hierarchy of scales in a solid, in a for electronic energies; let us just look at the other energy scale that. So, this is the one which is the paramagnetic is called the paramagnetic contribution. The other one is the let us look at the last one, the second one will be of course, down from the first one by this denominator.

And so, we when the first one is present we do not even bother to look at the second one in the paramagnetic contribution. Now, let us look at the last one which is e square by 8 m c square H square into n x i square plus y i square. So, sum over i and this typically this suppose this one x i square plus y square is take for example, a hydrogenic at radius.

So, typically if you do that then what you will find is that it is of the order of h cross omega c into h cross omega c by e square by a naught, a naught is the hydrogen orbit hydrogen radius. And, this basically tells you is that this is an extremely small energy scale and this scale is about 10 minus 5 times the paramagnetic contribution ok. So, this is a exceedingly small compared to the previous one for the similar fields for example.

Typically, because you see the e square by a naught is typically about 13.6 into 2 about 27 eV. So, if you put these numbers the other way this is also equal to e H, this term is also equal to e H by m c square into m a 0 square ok, this is the same as this. So, either way if you calculate whichever way you like you can just calculate and you will find that this energy is about 10 minus 5 times the paramagnetic contribution.

So that means what? That means, if you have a system where you find paramagnetic contribution, if a magnetic system gives you paramagnetic contribution there is no point in calculating this term. This term is called the Larmor diamagnetism or Langevin diamagnetism, its discussed even from your BSc days.

And, even probably in schools, high schools you have heard of this Larmor or Langevin diamagnetism. So, that is of no significance that contribution is always there of course, remember in a magnetic system all these contributions are there. But what are you going to calculate? What is significant? You will only calculate this paramagnetic contribution if it exists and then there is nothing else that is required.

Of course, if you want to get to accuracies which demand you to go to far higher than these corrections to this then you need to calculate the diamagnetic part. But, otherwise you do not need to calculate the diamagnetic contribution if you have paramagnetic term non-zero. Because, that is about 10 to the 5 times more than the paramagnetic contribution. The other thing that we have done here is that we have actually taken ionic contributions separately and summed.

Remember this is these are all summed over i's, as if these ions are and their spins and magnetic moments are completely independent. They do not see each other, they do not talk to each other. So, that is an assumption that more or less holds in many materials where these ions are separate and they therefore, their magnetic interaction they do not have magnetic interactions between one the magnetic moment at one iron to the other. So, in that case you can basically sum over the contribution and then the total contribution is just their sum.

There will be cases where we will show later on this is not valid and in those cases of course, you have to go beyond this. But, still the magnetic moments and magnetic terms are just these and of course, then there will be terms which come from other factors, other interactions. So, we will discuss them later, but at the moment we are considering moments ions with moments both angular momentum and spin contribution.

And, these are some and they interact with the magnetic field and there may two major contribution. One is this the paramagnetic contribution another is the diamagnetic contribution and we know now how to calculate this. So, our task is to calculate these things for different ions and with different levels of fillings in the in their atomic shells. So, that is what we are going to do in the next class.

But, the message from today is that there are two contributions to the magnetic change in magnetic and change in energy due to magnetic field of a free electron. One comes from the momentum being shifted by e A by c and the other one comes from the magnetic field interacting with the spin. And, that p plus A by c term gives a contribution both to paramagnetism and it gives a contribution to diamagnetism.

So, it is the only contribution to diamagnetism and I will show you why it is called diamagnetism. I have already alluded to it because if you look at it this last term is proportional to H square and it turns out to be negative.

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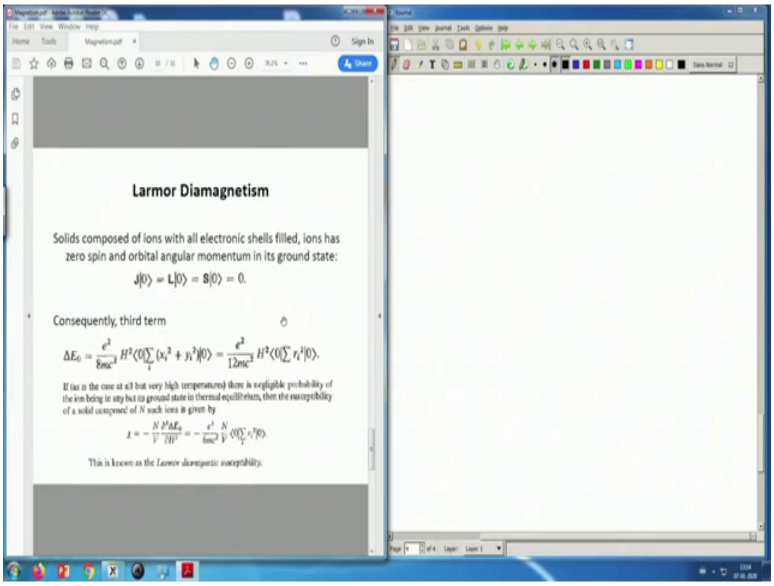

And, I will come back to it in my next class and that is why it is called the susceptibility is negative and it is called the Larmor susceptibility, diamagnetic susceptibility. So, these two contributions have to be calculated based on the atomic configurations inside the ion.