Principles and Applications of NMR spectroscopy
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Module 1
Lecture No 2

So welcome back to this course so in the last lecture we saw that different properties of nuclei how it is determined whether a nucleus has a spin zero or not equal to zero and what are the different combination of atomic weight and atomic mass which helps in determining and I also showed you this periodic table where you can see that many of the nuclei can be studied by NMR either in the natural form or their isotope. So today we will look continue with that and look at what are the most common nuclei and how what is a how NMR spectroscopy is actually carried out.

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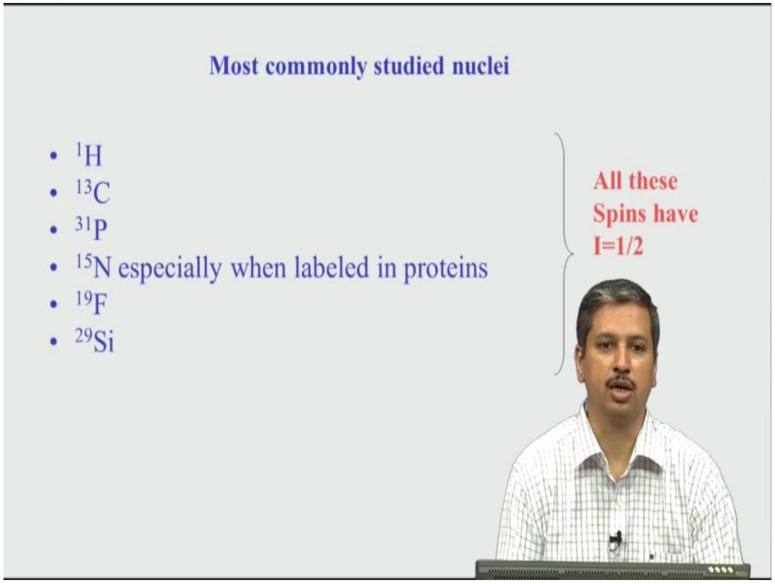

Most commonly studied nuclei

- ^{1}H
- ^{13}C
- ^{31}P
- ^{15}N especially when labeled in proteins
- ^{19}F
- ^{29}Si

All these Spins have I=1/2

So if you look at this slide this is the most common nuclei that we study is listed here, so typically of course 90 percent of the NMR is carried out on protons and the next most popular nuclei is carbon 13 nucleus, and third is phosphorous 31 uhh, N15 is also very popular nucleus if we are especially when we are looking at biomolecules, fluorine 19 is also a very popular especially in the drug industry in the pharmaceutical drugs, many of the drugs have fluorine and fluorine is also very close to proton in terms of sensitivity and which we will see and silicon is also useful for materials.

So these are basically the most popular nuclei and the interesting thing is all of them have spin I equal to half. So you can for spins which are half integers, so I equal to half they are very easy to study and very the basic phenomenon are can be easily understood and explained. So we will focus rest of the course on these particular nuclei and so let us see how NMR spectroscopy works.

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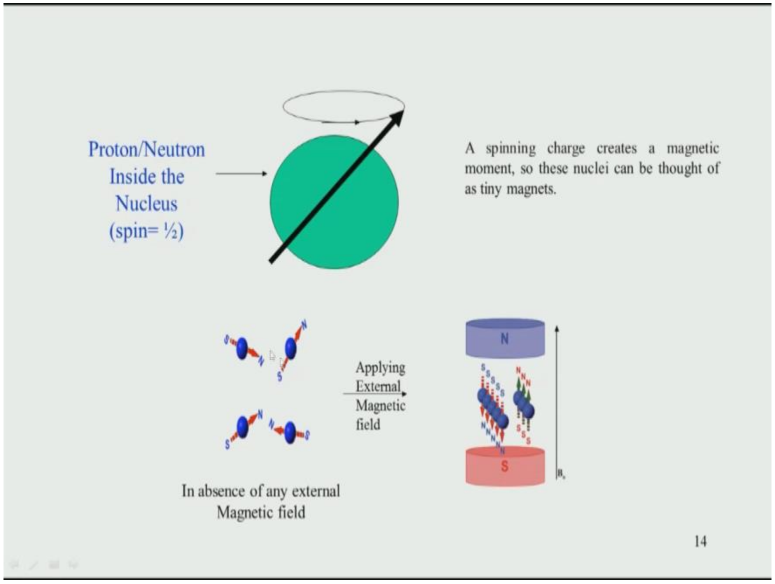

Proton/Neutron
Inside the
Nucleus
(spin= ½)

A spinning charge creates a magnetic moment, so these nuclei can be thought of as tiny magnets.

Applying External Magnetic field

In absence of any external Magnetic field

So the main thing in NMR as the word stands nuclear magnetic resonance so we have to let us go step by step and look at what is so we have looked at the first part of this terminology nucleus. So we saw that nucleus is what is important the spin of the nuclei.

So the next thing is magnetism, so let us look at magnetic field. So if you take a sample so this is a schematic drawing here of a spin which is shown in this form. So as I said spin is actually in abstract quantity but we still associates with it the properties of a motion that is spin. So this is a spinning nucleus and now imagine that you have a lot of spins in the sample, so let us take imagine for example a glass of water. A water has lot of molecules of H2O and each H2O has hydrogens which are the nucleus which we are going to look at.

So this many nuclei together in a sample are oriented randomly in absence of a magnetic field that is in a natural standard conditions. However if you apply a magnetic field this nucleus now what happens is they are they are having a spin and they have a charge, so remember the total nuclear charge is positive because of protons so it is a notal nucleus is charged positively and at the same time it has a spin associated with it. So this combination of charge and spin renders it as a magnetic property.

So it becomes now it has a magnetic dipole associated with every nucleus. So every nucleus which has a charge and spin is now a magnet, a small magnet. So we can associate with a magnet what is called magnet dipole like similar to the magnets which you see in day to day life we call it north pole and south pole. So we associate a dipole moment magnetic dipole moment with every nucleus.

So you can see that if you take a collection of spins they are basically a set of magnets in the sample. So now these tiny magnets are very tiny because nucleus is very small. These tiny magnets when they are put in a magnetic field now they will start what is called as aligning with the this the magnetic field. So there is what is some of the spins will be parallel parallely aligned with the magnetic field where the north pole is facing the south and south pole is north facing the north pole and anti-parallel means opposite align spins.

And why is this happening? This is happening because there is an energy of there is an interaction of these spins with the magnetic field and this what we will be looking at in throughout this course is a interaction of this nuclei that is nucleus which is a magnet with the magnetic field which is a central which is a most important idea or the concept in nuclear magnetic resonance.

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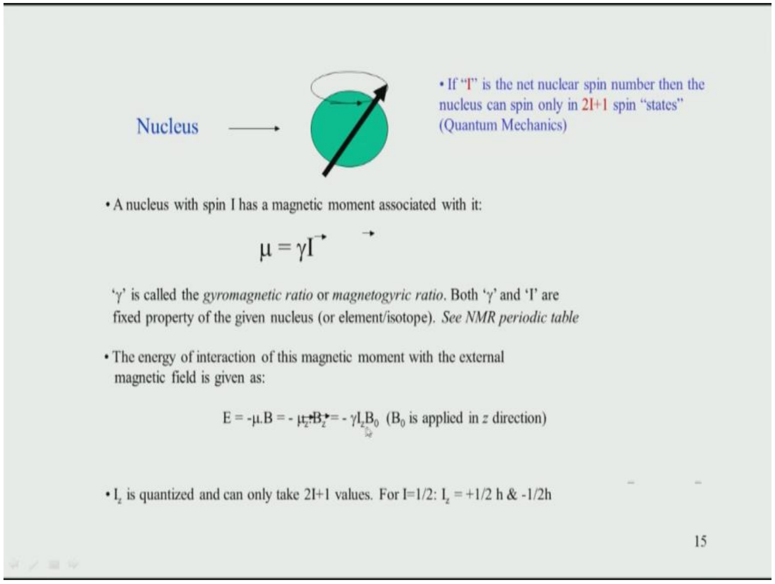

- If "I" is the net nuclear spin number then the nucleus can spin only in 2I+1 spin "states" (Quantum Mechanics)

- A nucleus with spin I has a magnetic moment associated with it:

$$\mu = \gamma \vec{I}$$

'γ' is called the *gyromagnetic ratio* or *magnetogyric ratio*. Both 'γ' and 'I' are fixed property of the given nucleus (or element/isotope). *See NMR periodic table*

- The energy of interaction of this magnetic moment with the external magnetic field is given as:

$$E = -\mu.B = -\mu_z B_z = -\gamma I_z B_0 \quad (B_0 \text{ is applied in } z \text{ direction})$$

- I_z is quantized and can only take 2I+1 values. For I=1/2: $I_z = +1/2\,\hbar$ & $-1/2\hbar$

So if you look at now a nucleus now which has now a magnetic dipole moment just now which I mentioned because of its charge and spin and that magnetic dipole moment is denoted like this. It is equal to gamma into I. Gamma is basically a constant for a particular type of nucleus. It is known as gyromagnetic magnetic ratio. Very important this one ratio which is very important parameter which is used in useful for understanding NMR.

So we will so this is the gamma and the next value next term here is called nuclear spin angular momentum that is called I, angular momentum is I. So now this myu is a vector quantity because it has a direction and similarly I is a vector quantity because it has a direction. So therefore I can now split this myu into three components, that is Ix, Iy and Iz and we look at that now. So this myu that is the magnetic dipole which is shown here I mean schematically this interacts with the magnetic field.

So when we apply a magnetic field this magnetic dipole moment interacts with the external magnetic field and this energy this interaction is given like this by this formula where E is equal to - myu dot, this is a dot product with a magnetic field. So as I said we can now spilt this into three components, myu x, myu y, myu z and this can be bx, by, bz but assuming that I apply a magnetic field in the z direction in what happens is the x and y components are gone and therefore only the z component of myu remains.

And therefore this is simplified and it becomes - myu z bz. Now - myu z is basically now if you look at this term here it is myu z. Myu is nothing but gamma into iz, so that is what is written here it is gamma into iz into b0. So this b0 is called as a magnetic field. So this is our external magnetic field which we have applied and typically we say that it is applied along z direction and therefore the total final energy of interaction becomes equal to - gamma iz b0.

So this is the about the important concept. Now according to quantum mechanics that if you have a spin I it has a possibility of two I + one spin states. Now what is a spin state? Spin state is basically what I was referring to as energy levels in the previous class. We look at different energy levels we showed that there is what is called there is what is called a ground state and a exciting state. Similarly the energy levels this angular momentum which is denoted like by I is also we say is quantize and it has different levels and that is there are two I + one level.

For example, suppose I is equal to half which is a case for protons for hydrogen and then if you multiply two into half + one it becomes two. So that means a hydrogen atom or hydrogen nucleus has now which is a proton has now two spin states that is two spin states and that is given by either the + half or the - half. So this is what we will put here. That means this Iz has two possible values the Iz can either be + half or - half for a spin which is total spin is when I equal to half.

So this is basically a now if you look at this formula again if I put the value Iz equal to half it becomes - gamma half h cross into b0 where h cross is what is shown here. And if it is + - half and this becomes - gamma into - half into b0 h cross that becomes +.

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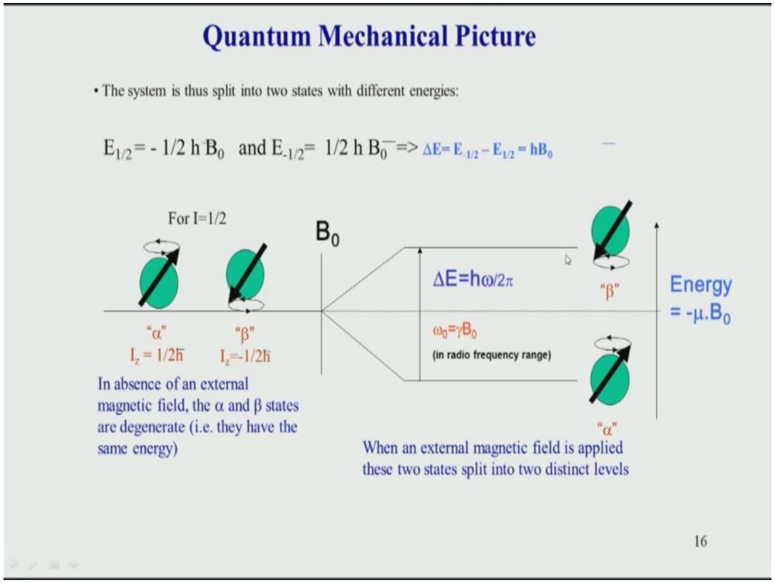

Quantum Mechanical Picture

- The system is thus split into two states with different energies:

$E_{1/2} = -1/2\ h\ B_0$ and $E_{-1/2} = 1/2\ h\ B_0 \Rightarrow \Delta E = E_{-1/2} - E_{1/2} = hB_0$

In absence of an external magnetic field, the α and β states are degenerate (i.e. they have the same energy)

When an external magnetic field is applied these two states split into two distinct levels

So in other words we can see that now this energy of interaction has two values depending on whether your the spin Iz is either + half or - half. So by - half it becomes positive if you refer to the previous formula and if you look at - half + half that is it becomes - value. So therefore what is happened that we have now created two energy levels because of this interaction of this nucleus with the magnetic field we have ended up with now two spin states or two energy levels, one energy level corresponds to the lower energy value which is when the spin is in + half state that is + half that is called alpha state and when Iz is - half the total energy is positive as shown here and that is the upper that is excited state and that is called as beta state.

So what has happened now? Basically when we apply a magnetic field which we call as b0 and put a sample in that magnetic field the all the nuclei in the sample now are now exposed now are split into two energy levels now that energy one ground state energy level and an excited state energy level. And the ground state energy level is called as alpha and the excited state is called as beta. So this is what we talked about now in the nuclear magnetic resonance technology we have looked at nucleus, we have looked at magnet.

Now the next term is resonance, so what happens next? So what happens next is essentially you supply an energy which will so take the molecules from the ground state and take them to the exciting state. So this energy has to be exactly equal to the gap between the two energy levels., Then only the molecules will observe and this is the basic idea of spectroscopy which we looked at in the previous class.

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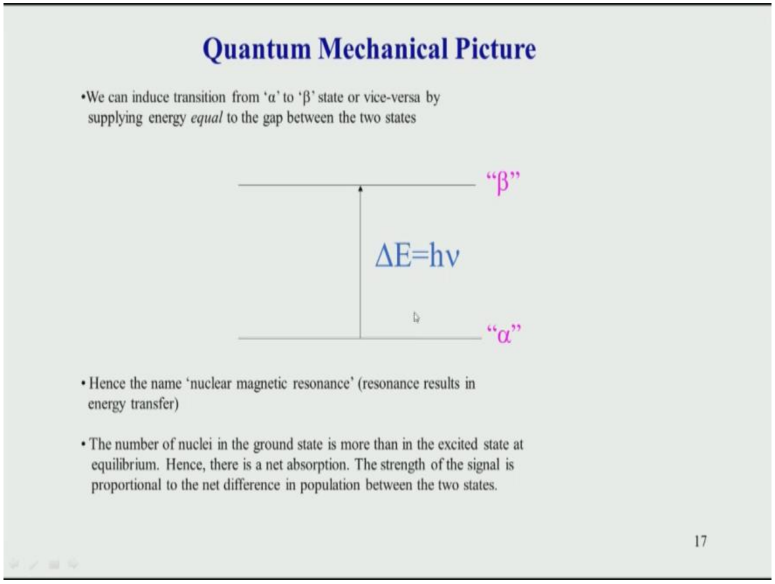

Quantum Mechanical Picture

- We can induce transition from ‘α’ to ‘β’ state or vice-versa by supplying energy *equal* to the gap between the two states

“β”

$\Delta E = h\nu$

“α”

- Hence the name ‘nuclear magnetic resonance’ (resonance results in energy transfer)
- The number of nuclei in the ground state is more than in the excited state at equilibrium. Hence, there is a net absorption. The strength of the signal is proportional to the net difference in population between the two states.

So what happens is if I apply an energy which matches this energy level gap, this is called resonance. In resonance basically the molecules which are now in alpha the ground level alpha state they get excited and they absorb the energy and they go to the beta state.

So this is basically the idea of resonance the concept of resonance which comes in the terminology of nuclear magnetic resonance. So you see we have completed this the three terms nuclear magnetic resonance. So basic idea of NMR is now can be said as follows you take a sample which has of containing molecules in which the atoms have non-zero the nucleus have non-zero spin, take the sample in a magnetic field, the magnetic field let us say is applied along z direction the molecules now have get distributed into two populations into two states alpha and beta because of their interaction with the magnetic field and now you take the molecules which are in the ground state and excite them to energy by applying an energy which is equal to the difference in energy level that is deltaE.

And then take them to the excited state and that is called resonance. So this is basically the whole idea of nuclear magnetic resonance, hence the name which NMR comes from, okay. And the strength of the signal which is absorbed is now proportional to the difference. So what happens in NMR is that you have lot of molecules in the ground state and you have some molecules also in the excited state. So when we assign a radiation which is equal to deltaE the molecules will go from here to the exited state. At the same time the molecules will come from beta to ground state.

This is called stimulated excitation and stimulated emission. So therefore the total net how much energy is observed will depend on the difference in the population of how many molecules are here - how many molecules are here, if they are equal then there is no net excitation and the signal will be zero. That means no NMR radiation will be energy will be absorbed, but if the difference is not zero suppose you have more in alpha state and less in the beta there will be more signals more molecules absorbing then more molecules coming down.

So therefore there is a net positive absorption of the energy and that is what we do rely on NMR. That means we all depends on the net difference the word difference is very important here the net difference in the population between the two states. So this population difference is a very important term and this is applicable in general in across all spectroscopy wherever we talk about energy quantization, we talk about population because molecules are not always exactly equal to here and here there will be always a difference and that difference comes from a very famous law known as the Boltzmann law.

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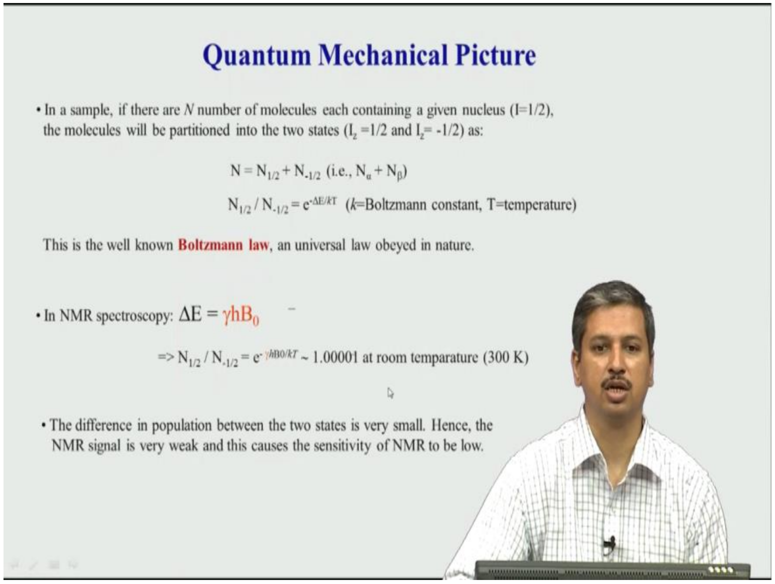

Quantum Mechanical Picture

- In a sample, if there are *N* number of molecules each containing a given nucleus (I=1/2), the molecules will be partitioned into the two states (I_z =1/2 and I_z= -1/2) as:

$$N = N_{1/2} + N_{-1/2} \text{ (i.e., } N_\alpha + N_\beta)$$

$$N_{1/2} / N_{-1/2} = e^{-\Delta E/kT} \quad (k\text{=Boltzmann constant, T=temperature})$$

This is the well known **Boltzmann law**, an universal law obeyed in nature.

- In NMR spectroscopy: $\Delta E = \gamma h B_0$

$$\Rightarrow N_{1/2} / N_{-1/2} = e^{-\gamma h B0/kT} \sim 1.00001 \text{ at room temparature (300 K)}$$

- The difference in population between the two states is very small. Hence, the NMR signal is very weak and this causes the sensitivity of NMR to be low.

So we will look at this Boltzmann law now, so what Boltzmann law says is that there is always a more energy more population in the ground state that is when the spin is - half that is the alpha state compared to the upper state. That means in the room equilibrium scenario standard conditions you will always have more molecules which are sitting in the ground state then in the excited state. And this ratio of the population is given by this formula N N by N half by N - half equal to this e raised to - delta e over kt.

So this is a very **very** famous Boltzmann law we universally abide in nature so where k is a Boltzmann constant and t equal to the temperature. So let us look slightly go deeper into this concept now. So what it means is suppose I take a given value of b0, so typically in NMR as you will see in the coming slides we have what is called a tesla, so b0 the unit of magnetic field is tesla. And based on these values if you put in these values which we will see in more detail later, but for now if you put in these values which is typically use in NMR it turns out that the ratio is just slightly above 1.

So what it means is that very the alpha and beta states are almost equally populated though not exactly equal they are almost equally. So the difference between the ground state and the excited state is very small. Now if the difference is small remember according to the previous slide the absorption of energy is also small. So the difference if it is more, the absorption is more. So in other words what we are looking at is the sensitivity. How many what is the total amount of radiation or light absorbed by this molecules all depends on this difference and in NMR the difference is very small.

And that is one of the reason we say that NMR spectroscopy is very weak low sensitive technique compared to UV, IR or other spectroscopy techniques the reason being that the difference in population between the ground and the excited state is less in NMR compared to other techniques.

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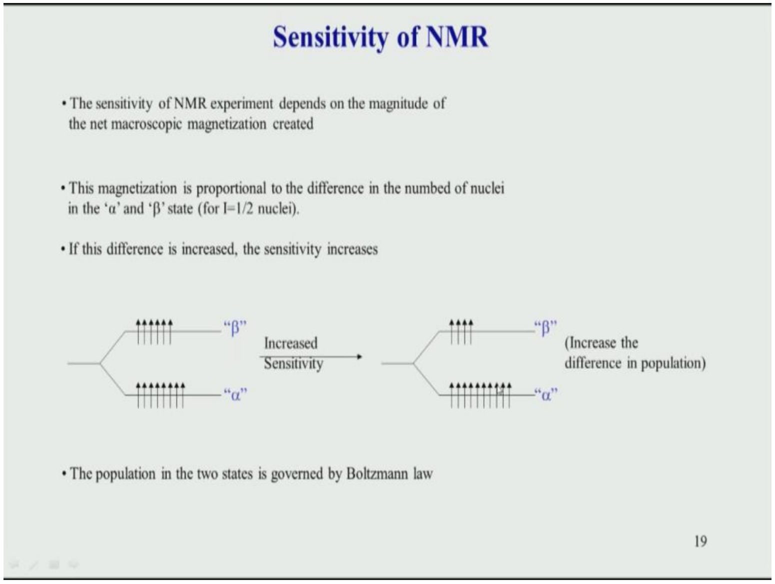

Sensitivity of NMR

- The sensitivity of NMR experiment depends on the magnitude of the net macroscopic magnetization created
- This magnetization is proportional to the difference in the numbed of nuclei in the ‘α’ and ‘β’ state (for I=1/2 nuclei).
- If this difference is increased, the sensitivity increases

- The population in the two states is governed by Boltzmann law

So now let us go further into this Boltzmann population difference so as I said the sensitivity means we will look at sensitivity in again in later on. But sensitivity as I said is depends on how many molecules absorbed the energy and that depends on the difference in the population.So if I want to increase sensitivity I should increase the population difference. That means I should have more molecules sitting on the ground state than in the excited state.

So this difference is what matters. If you see here in this picture you have almost all the spins are equally populated. I mean these two states are equally populated, the small difference is there. However, if you see in this picture we have increased the difference in the population so I have more molecules sitting in the ground state than exciting state.

So this is what is always try as people try about in NMR. How do we increase this difference? Because finally this is what matters when we record a spectroscopy spectrum is how much is the difference and that difference comes from various factors and as I said one of the thing if you roll back to the Boltzmann law the difference comes from this factor here.

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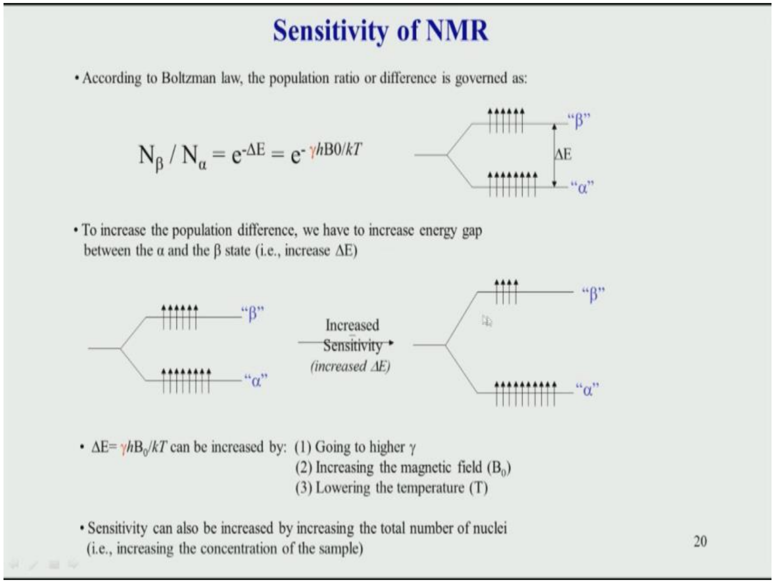

Sensitivity of NMR

- According to Boltzman law, the population ratio or difference is governed as:

$$N_\beta / N_\alpha = e^{-\Delta E} = e^{-\gamma h B0/kT}$$

- To increase the population difference, we have to increase energy gap between the α and the β state (i.e., increase ΔE)

- $\Delta E = \gamma h B_0/kT$ can be increased by: (1) Going to higher γ
  (2) Increasing the magnetic field (B_0)
  (3) Lowering the temperature (T)

- Sensitivity can also be increased by increasing the total number of nuclei (i.e., increasing the concentration of the sample)

So if I increase the b0 this b0 value that is the magnetic field I can increase the difference because if you look at this mathematical formula if I increase deltaE e raised to - delta e will go down which means that the less number of nucleus will be here and compared to N alpha. So what we are trying to do here? We are trying to increase this N alpha compared to N beta, so relative ratio and that is governed by this famous Boltzmann formula equation.

So here you can see I can either increase gamma this is a constant H I cannot vary, I can change b0 make it very high value increase the value or I can decrease the temperature, right? And so this k is constant. So H and k is constant so if I decrease the temperature also I can get this (())(17:01). So these are the three basic parameters which basically determine the (())(17:06) this is what is shown here that if I want to increase the difference in population, that means I want to increase the sensitivity I have to basically rely on three parameters either I go to either I go to higher gamma value or I can increase the magnetic field or I can lower the temperature.

So based on these different parameters the population ratios will keep changing and essentially what NMR spectroscopist strive is to go by the best possible parameters optimal parameters in this. So for example gamma highest gamma in the whole of NMR is proton and the whole of the periodic table which I showed you your highest is gamma. So obviously gamma is a most sensitive nucleus or atom which can be studied (())(17:50) magnetic field is something which is in our control. We can increase a magnetic field, so if you go to higher and higher magnetic field you can actually increase the sensitivity and we will see later this how important this is and it also contributes to the resolution of the spectrum.

And of course lowering the temperature is another parameter which is also under our control. So we can lower the temperature, but again in solution you cannot do much because in solution the lowest you can go is zero degrees because below that the sample will freeze depending on the boiling freezing point of the solvent. But typically when you take a water sample you cannot do much because the below zero degree the sample freezes.

So therefore, temperature although is a very important parameter is not so much of importance as much as the magnetic field and gamma is considered. So therefore this is how we increase the sensitivity of NMR spectroscopy. Now the whole this is what is called quantum mechanical picture so we are looking from quantum mechanics point of view.

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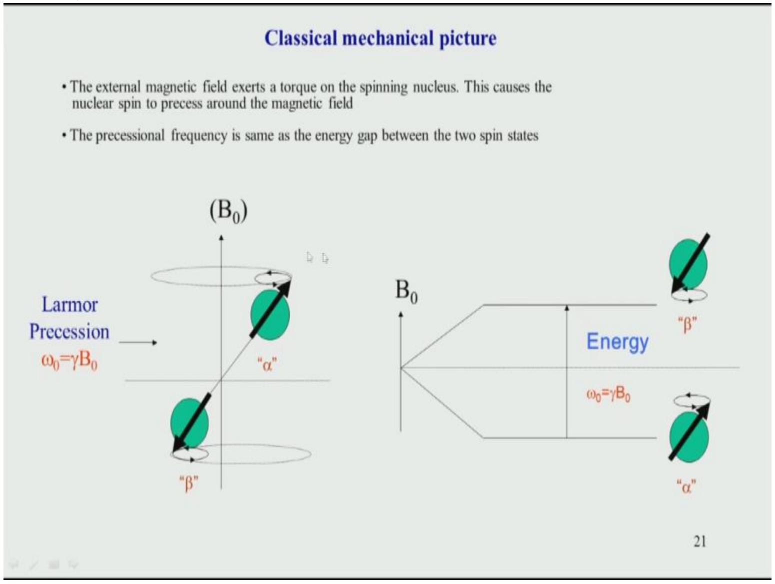

Classical mechanical picture

- The external magnetic field exerts a torque on the spinning nucleus. This causes the nuclear spin to precess around the magnetic field
- The precessional frequency is same as the energy gap between the two spin states

You can also look at NMR from a classical point of view. So what is so there are two different ways to understand NMR. So these are again one of the unique technique spectroscopy technique which can be understood both from classical (())(19:03) as well as quantum mechanics. Typically all spectroscopy techniques are understood from quantum mechanics point of view but here we will also show how we can actually understand from a classical picture.

So in a classical model you can visualize like this, you imagine that there is a nucleus which is now which is spinning around its axis, so this is a nucleus shown. Now there are two possibilities it is having alpha state and a beta state which is shown here. Now what happens is when you apply a magnetic field which is shown here b0 the spins now start to precess means move around revolve around this magnetic field.

This is called a famous Larmor precession, this is derived can be derived and is derived in many of the text books which we will not able to go in detail the derivation but the idea is that the spin now starts moving around the magnetic field is like similar something similar to earth going around the sun. So this is what is called precession and this precessional frequency is actually given by omega equal to gamma b0. So this is the derivation which can be seen found in many books.

So this is what is the central idea is that the precessional frequency of the spin around the external magnetic field is given by gamma b0. Now, if you look at the quantum mechanical picture, this is what we have been looking at in the last few slides. Then, we talked about the energy levels and here also if you see the difference in energy levels deltaE is given by this, the energy of difference is given by omega the frequency this is the frequency at which the molecules absorb the radiation from ground state to excited state and that difference deltaE is equal to H myu and that is related the frequency of excitation is now given by this omega zero equal to gamma b0.

So you see there is an exact match between the two which is expected because we are looking at the same system from two different prospective, but what is interesting is that whatever you understand whatever we can see from NMR quantum mechanics point of view can also be understood from a classical point of view.So many of the times you will see that we will be using this classical picture model this picture what you are seeing here on the screen this is what we will be using to explain many of the NMR phenomenon, but remember the main thing is also what is can be explained based on this picture.

So we will be essentially going back and forth between these two pictures just in case whenever depending on the requirement.

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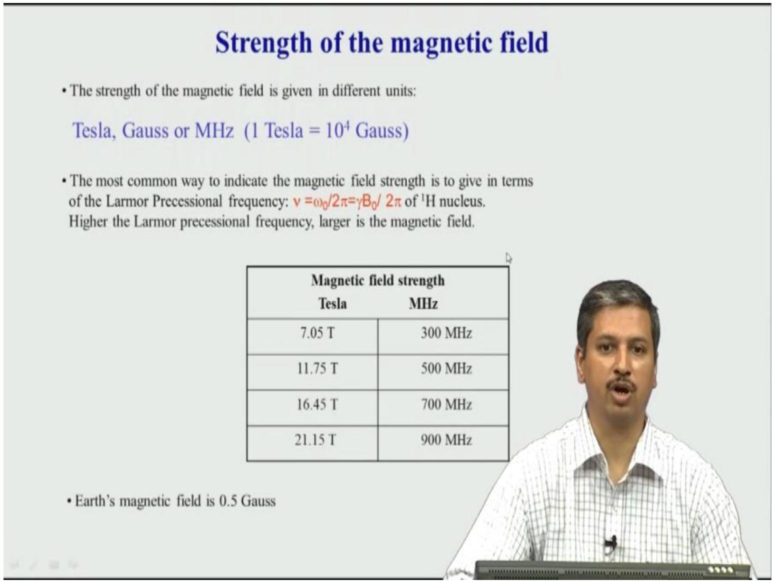

Strength of the magnetic field

- The strength of the magnetic field is given in different units:

Tesla, Gauss or MHz (1 Tesla = 10^4 Gauss)

- The most common way to indicate the magnetic field strength is to give in terms of the Larmor Precessional frequency: $\nu = \omega_0/2\pi = \gamma B_0/2\pi$ of ^1H nucleus. Higher the Larmor precessional frequency, larger is the magnetic field.

Magnetic field strength	
Tesla	MHz
7.05 T	300 MHz
11.75 T	500 MHz
16.45 T	700 MHz
21.15 T	900 MHz

- Earth's magnetic field is 0.5 Gauss

So now, let us look at the classical picture in little more detail. So this is what I was shown in the previous slide that the frequency of precession the frequency at which the magnetic the nucleus precesses around magnetic field is given by this frequency omega myu equal to omega gamma b0 by 2 pi. Now here in the b0 so this what the units of b0 as I said is measured in units of tesla or it can be units of gauss. So if you see the myu is a frequency unit, right? It is a megahertz it is in hertz, whereas b0 is in the tesla.

So if you multiply this gamma which is you can see from a table a look up table if you multiply you will get this value of myu in the typical range of megahertz. And that is why if you see all the NMR systems wherever we have is typically we talk about in megahertz. So we say that we say we have a 300 megahertz spectrometer, we say we have a 500 megahertz spectrometer. So these numbers megahertz and these numbers 300, 500 they are all coming from this tesla. So essentially the magnetic field is what is determining the frequency.

So when you say when somebody says that I have a 500 megahertz NMR spectrometer in my laboratory, what he means to say is that he has a magnet which is 11.75 tesla. So the most the point here is that the spectroscopy the frequency depends on the magnetic field directly given by this formula and to this put it in perspective the earth's magnetic field is very small, it is 0.5 gauss.

Whereas if you look at this we are talking about in the 10 to the power 4 gauss in the typical laboratory magnetic field. So the magnetic field we use in NMR is really orders of magnitude very high (com) higher compared to what is earth’s magnetic field. So therefore we are using very strong magnetic field and their associated precautions which has to be taken practically that we will look at when we come to the hardware aspect.

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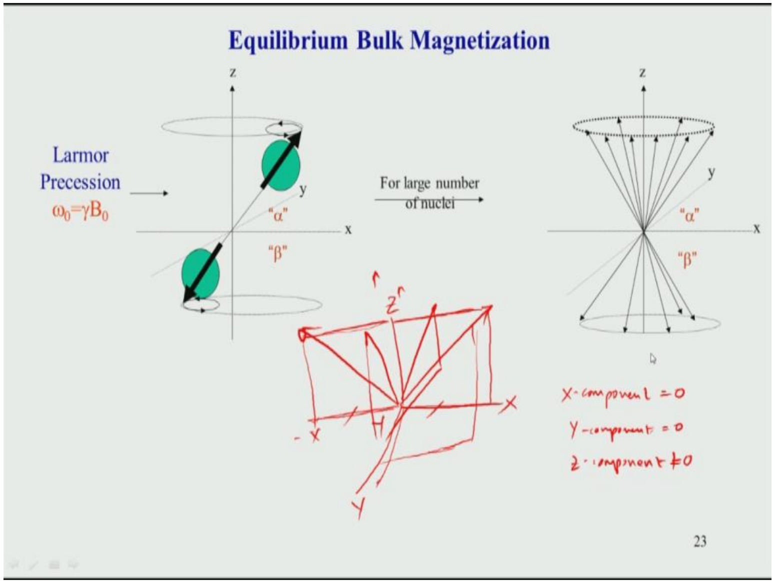

Equilibrium Bulk Magnetization

Larmor Precession $\omega_0 = \gamma B_0$

For large number of nuclei

X-component = 0
Y-component = 0
Z-component ≠ 0

So now coming to this classical picture just as I said we will be toggling between these two different pictures and it is sometimes very easy to understand NMR from a classical point of view and sometimes from quantum mechanics point of view. So let us now look at this classical picture model. So what this says is that imagine one nucleus which is like this which is having a spin like again the same analogy the analogy you can use is earth spinning around its axis and also it is revolving around the sun, so we can use that picture and keep that picture in mind.

So there is a nucleus which is now precessing around the magnetic field. Now this is about one nucleus one hydrogen atom. But remember in a sample we will never have one hydrogen atom, what you will be having is a collection or a number of hydrogen atoms.

For example, let us take you take a water sample you take a glass of water, the concentration of water is 55 molar which means there is 55 moles of water in 1 liter and one mole is 6 into the power 10 to the 6 into 10 to the power 23. So therefore you can see there are so many different I mean 10 to the power 23 atoms of hydrogen. So therefore if you look at all those hydrogen atoms together you will get a picture something like this which is shown on the right.

So here you see each nucleus I am showing as an arrow is shown as an arrow here, so each nucleus is an arrow so we can this is although there are only few arrows shown here, in reality imagine that you have 10 to the power 23 or 10 to the power 20 atoms nucleus which are all like this. So therefore you have now some of them pointing upwards this is those are the nucleus which are in the alpha state and remember there are also some in the ground (st) excited state that is beta state and they are lesser in number because of the Boltzmann principle which we saw and that is pointing downwards.

So now if you look at each of this vector arrows, what is happening here is that now this vector arrow if you look at in this frame. So let us now draw a picture of how this looks like, let us see this is z axis which is what is shown here, then you have an x axis and you have a vector something like this. Now this vector can be now have two components it will have a z component and x component at the same time there is also a y axis so it will have a y component, okay so this is a y component.

Now if you look at another vector which is in this direction for example, one of the other vector here now that will have a component along again - x and it will have along z this component and it will also have along y axis. So if you see this component this which is - x component is exactly cancelled by what is here, so this will cancel each other and there is no no vector no net component in the x axis. So we can say that x component is equal to zero. Similarly if you look at y component of some other pair of nuclei some pointing here, some pointing here again in the y axis they (())(26:32) each other and y component also becomes equal to zero.

But if you look at the z component what is along the z axis? This is this component which is drawn here, this is always pointing in this direction no matter you no matter what is you take it is always pointing in the z axis. Therefore, the z component is never equal to zero. Only the x and y cancel each other. So if you look at so this is the picture we have to keep in mind that whenever you have a net this one you will basically end up with net z component and all the x and y becomes equal to zero.

So this is a basic idea in a classical picture that all the x and y component cancel out you are left only with the z component and that is what matters. Now if you look at this phenomenon where x and y goes to zero is because all these arrows which is shown here they are pointing all in the random directions they are not together they are fanned out like a cone. So this is like a cone and all of them are fanned out means distributed all along this cone and therefore this thing become zero. This would not have happened if they have not been along in random directions.

So therefore we use the word random phase approximation. So random phase approximation is a term used in NMR to denote that the spins are all randomly located in a cone and they are not aligned with each other, so this is called random phase approximation and now what because of that only the z component adds up but all the x and y cancels. This is as far as alpha spins are concerned. Now if you look at the beta spin, the same scenario will happen.

In the beta spin same thing the z axis will add up in the - z but x and y will all cancel each other. So therefore you will end up with - z value and here you end up with + z value. So now the + z value whatever is here will start subtracting from the - z value which is here.

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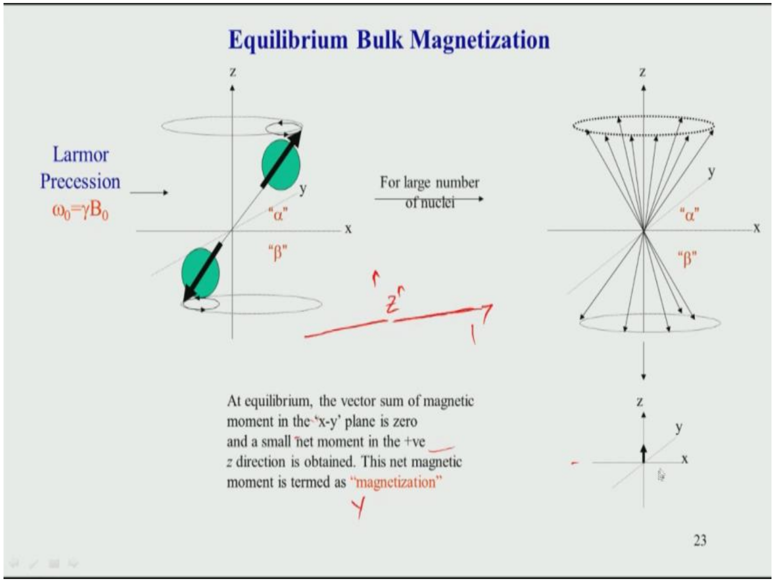

Equilibrium Bulk Magnetization

At equilibrium, the vector sum of magnetic moment in the 'x-y' plane is zero and a small net moment in the +ve z direction is obtained. This net magnetic moment is termed as "magnetization"

So therefore you end up with finally what is known as a net spin vector. So we will look at the final picture which emerges because of this consideration what is happening now if you see here at in the generally so that means the positive z values will actually cancel with the negative z values and that will result in a net vector which is now pointing in this z axis. So this is our final magnetization, this has come because the positive z values which came up from here from the alpha spins cancelled with whatever was in the beta, but these are not equal because remember according to the Boltzmann law there is more population more molecules in this side compared to more molecules in that side and therefore there will not be always exact cancellation of the z value and the z value will be positive because more spins are up on the up side than downside and this vector what you see here is called the net magnetization.

This is the popular word which we will use in NMR and this is a positive direction z axis this is where we apply the magnetic field. So whatever NMR is done is now carried out with this particular magnetization. So all NMR spectroscopy techniques what we will see is all based on looking at this net. So before we look at this what the thing you should keep in mind is suppose that alpha molecules the number of molecules alpha state are let us say equal to molecules in the beta state, then what will happen? What will happen is these two z values will cancel exactly and it will become zero.

So when the magnetic vector this is zero it means alpha state and beta state are equally populated. But when alpha state is more populated than beta, then this will be positive. If beta state is more populated then alpha, then this will become negative. So therefore this magnetization vector all depends on what is the population between in the alpha state and the beta state. And that is what is the whole idea of NMR you manipulate you manipulate the population by applying some radio frequency energy and based on that manipulation the molecules the magnetization vector will either be positive, zero or negative or it come in any other direction. So we will see now in the next class how this magnetic vector is manipulated and how NMR data is recorded.