NMR of a 'bare' proton :-

A 'bare' nucleus is, of course, an ideality

Nuclei are parts of atoms and molecules. It is mainly considered that NMR of bare proton. From quantum mechanics, it is evident that energy of interaction of nuclear magneton having nuclear magnetic moment μ with an external magnetic field B_z, applied in z-direction is given by

$$E = -\mu B_z \quad \text{——} ①$$

substituting the value $\vec{\mu}$ from eq. ② as given

$$\vec{\mu} = g_N \mu_N \vec{I} \quad \text{——} ②$$

The nuclear spin I is quantized in the presence of magnetic field and the energy of nuclear field is defined by its component m_I. Hence we may write,

$$E_{m,I} = -g_N \mu_N B_z m_I \quad \text{——} ③$$

Now let us consider a bare proton ^1H with $I = 1/2$ so that $m_I = \pm 1/2$. Thus for $m_I = 1/2$ for energy..

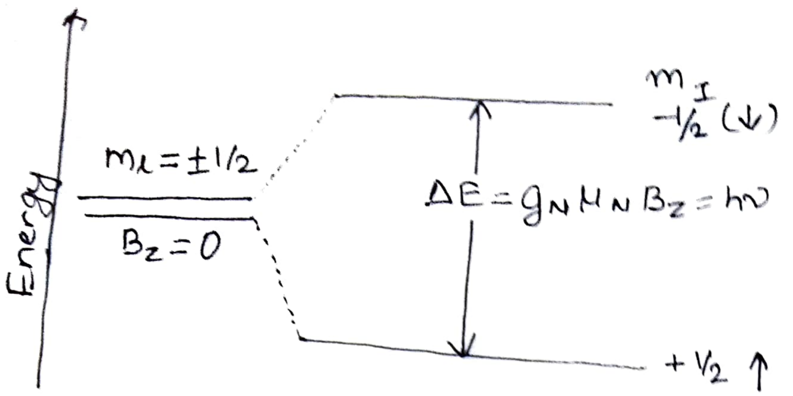
$$E_{1/2} = -\frac{1}{2} g_N \mu_N B_z \quad \text{——} ④$$

And for $m_I = -1/2$, the energy

$$E_{-1/2} = \frac{1}{2} g_N \mu_N B_z \quad \text{——} ⑤$$

In the absence of external magnetic field, the two components of proton spin have same energy i.e. they are degenerate.

In the presence of magnetic field, the components have



Splitting of nuclear energy levels of a bare proton in a magnetic field when the magnetic field is kept constant and frequency is varied.

the same energy (i.e. they are degenerate). However, in the presence of magnetic field, the components have different energies given by eq. ④ and ⑤.

This is expressed by saying that the magnetic field lifts or removes the degeneracy of the spin components. This is called Zeeman's splitting of energy level. This energy difference is given by

$$\Delta E = E_{-1/2} - E_{1/2} = g_N \mu_N B_z$$ — ⑥

This is explained in diagram above.

To induce the transition between the two energy levels $E_{-1/2}$ and $E_{1/2}$ i.e. to flip the nuclear spin from the upward direction (↑) to the downward direction (↓), there must be application of oscillating radiofrequency field perpendicular to the direction of B_z. The nuclear spin flips, provided the energy $h\nu$ of the radiofrequency field perpendicular to the energy levels $E_{-1/2}$ and $E_{1/2}$, ~~i.e. in order to let the~~

of radiofrequency is exactly equal to ΔE i.e.

$$\Delta E = g_N \mu_N B_z = h\nu \quad \text{—— ⑦}$$

This is called Bohr frequency condition.

Thus, the NMR frequency of a bare proton (or a bare nucleus with $I = 1/2$) is given by

$$\nu = \frac{\Delta E}{h} = \frac{g_N \mu_N B_z}{h} \quad \text{—— ⑧}$$

g_N may be positive or negative depending upon condition but ν must be positive. Hence, only the absolute value of g_N should be used in calculating ν.

Acc. to eq. ⑧, $\nu \propto B_z$

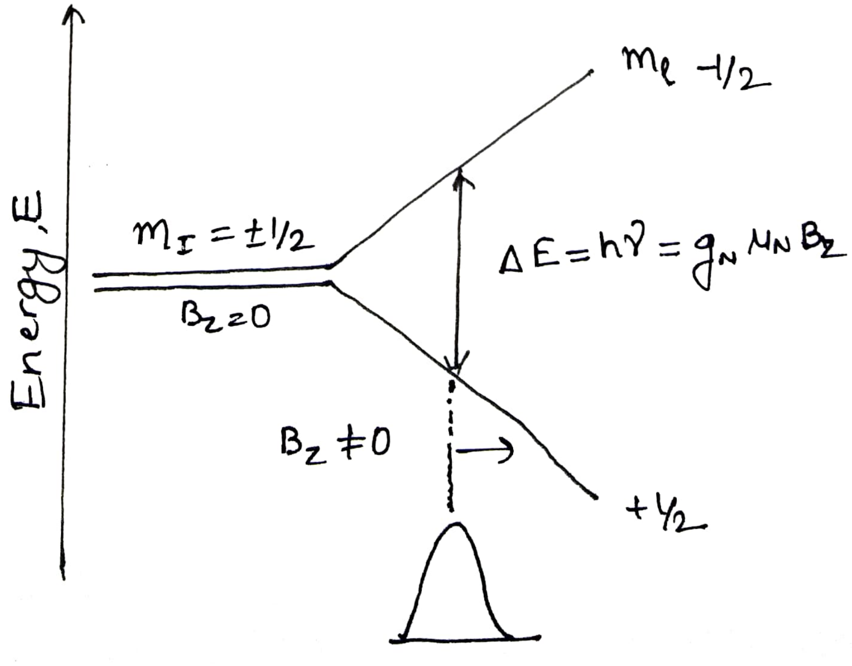
Hence the NMR spectra can be recorded into two ways –

(i) keeping the ~~fre~~ magnetic field B_z is fixed and varying the frequency ν as shown in (prev. dig

(ii) keeping ν fixed and varying B_z.

The (ii) is the prefered method of NMR spectroscopy.

↳



Q: Calculate the NMR frequency (in MHz) of the proton (${}^{1}H$) in a magnetic field of intensity 1.4092 tesla given that $g_N = 5.585$ and $\mu_N = 5.05 \times 10^{-27}\ JT^{-1}$.

$$\nu = \frac{g_N \mu_N B}{h}$$

$$= \frac{(5.585) \times (5.05 \times 10^{-27})(1.4902T)}{6.626 \times 10^{-34}\ Js}$$

$$= 60 \times 10^{6}\ s^{-1} = 60 \times 10^{6}\ Hz = 60\ MHz.$$

Nuclei ${}^{16}_{6}C$ and ${}^{12}_{6}C$ have no spin $(I=0)$ so that they have no magnetic moment; they are called non-magnetic nuclei.

Non-magnetic nuclei do not show NMR spectra because. their magnetic moment being zero, their energy level do not exist. Thus if an organic molecule contains Hydrogen, carbon and oxygen