

Understanding NMR Pulse Sequences. Part 1. Understanding Magnetic Excitation with the Semi-classical Vector Model

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Abstract: Most NMR users, despite needing to understand the theoretical basis of NMR, do not have much knowledge on that area. This work is the first part of a series of description and concept introduction on the description and understanding, in a simple way, some details on NMR pulse sequences using the very simple NMR vector model (semi-classic model). Specifically, this work tries to show the concordance between the very popular vector model and the quantum mechanical results in relation to with the exciting process in NMR. The presented proposal could lead to several discussions and disagreements on this topic.

Introduction

All the NMR users need to understand how the different NMR pulse sequences work in order to make the necessary experimental adjustments, to interpret correctly the spectral results and to choose the most appropriate pulse sequence to obtain the desired information. The most complete description of NMR is accomplished using density matrix theory,¹ which is a complex methodology that requires a deep knowledge on quantum mechanics to use it. The simpler but also efficient spin product formalism² is much easily used to understand NMR experiments but, being directly derived from the density matrix theory, needs a significant knowledge of quantum mechanics in order to understand how it works and how to interpret its results. The alternative for NMR users that are not sufficiently familiar with quantum mechanics is the semi-classical vector formalism.³ In this series of reviews we will discuss different aspects of this vector formalism, with emphasis on its application to understand how NMR

works and to explain the functioning of some pulse sequences and its limitations. This first part of the series is focused on an apparently simple but very complex part of NMR: the generation of detectable transverse magnetization. In order to accomplish this is necessary to review several very basic NMR concepts and to maintain certain parallelism with the quantum mechanical methods.

The fundamental basis of NMR

The first topic that needs to be explained is that the vectors used in the semi-classical vector formalism come from the classical representation of the magnetic moment $\vec{\mu}$ of the nuclei. We know that only the nuclei that possess a magnetic moment different from zero are detected using NMR, as their magnetic moment is subjected to different energy levels when they are in the presence of a magnetic field B_0 . The nuclear magnetic moment energy levels are defined by the quantum mechanical solution of the equation that describes the angular momentum of an atomic

nucleus (\vec{L}) inside a magnetic field. The description of the process to determine those energy levels is discussed in the literature.⁴ A simple description of this phenomenon is that the number of energy states for a single nucleus (E_{number}) is determined by its spin number I according to Equation 1.

$$E_{number} = 2I + 1 \quad \text{Eq. 1}$$

According to Equation 1, a nucleus with spin $1/2$, like ^1H or ^{13}C , will have two energy levels, while a nucleus with spin 1, such as ^2H , will have three energy levels.

The question now is what is nuclear spin? The complete answer for this is quite complex, as nuclear spin is a quantum property that has no equivalent in classical physics. For now, we can simply say that nuclear spin is a movement property of the atomic nucleus that originates its magnetic moment, and that it can be predicted using the nuclear shell theory, which is very nicely described in the book of Bonagamba and Freitas.⁵ The nuclear spin I corresponds to a quantum number that surges naturally from the solution of the equation that describes the angular momentum of a nucleus and varies as shown in Equation 2. The nucleus with the highest nuclear spin is ^{93}Nb ($I = 9/2$).

$$I = \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, \dots, \frac{9}{2} \quad \text{Eq. 2}$$

The solution of the equation that describes the angular momentum of a nucleus also introduces the magnetic quantum number m_I , which is closely related to I , as shown in Equation 3.

$$m_I = -I, -I + 1, -I + 2, \dots, +I \quad \text{Eq. 3}$$

In fact, the number of states of the system is determined by m_I . For example, if a nucleus has spin $1/2$ it possesses two m_I values; $m_I = +1/2$ and $-1/2$, according to Equation 3, meaning that it has two energy levels. The relation of m_I with the energy of the system indicates that this quantum number is somehow determined by the orientation of the magnetic moment vector $\vec{\mu}$, while I is related to the magnitude of $\vec{\mu}$. This means that $\vec{\mu}$ has two orientations allowed by the quantum mechanics results.⁴ If we chose the z axis as the reference coordinate, the two allowed directions for $\vec{\mu}$ are the α orientation, where $\vec{\mu}$ is 54.7° from the z direction ($\vec{\mu}_\alpha$), and the β orientation, where $\vec{\mu}$ is 125.3° from z ($\vec{\mu}_\beta$).⁴ This can be easily seen in Figure 1.

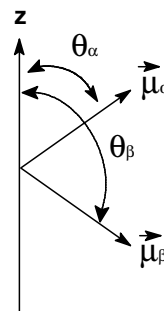


Figure 1. Orientation of the magnetic moment of a spin $1/2$ nucleus

The orientation of the magnetic moment $\vec{\mu}$ can be described by its projection on the z axis, as shown in Figure 2. It can be seen that $\vec{\mu}_\alpha$ leads to a projection $\vec{\mu}_{z\alpha}$, which is directed along the $+z$ direction. The projection

of $\vec{\mu}_\beta$ ($\vec{\mu}_{z\beta}$) is aligned in the opposite direction.

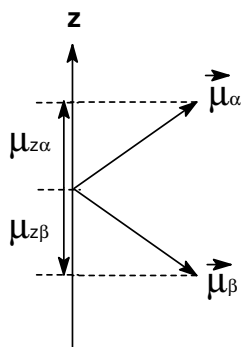


Figure 2. Projections of the nuclear magnetic moment.

From the quantum mechanical treatment of NMR the energy of those states is given by Equation 4,⁴ where γ is the magnetogiric ratio and m_l is the magnetic quantum number.

$$E = \gamma \hbar m_l B_o \quad \text{Eq. 4}$$

For nuclei with $I=1/2$ the values for m_l are $+1/2$ and $-1/2$ for the α and β states, respectively. Accordingly, the energy difference between both spin $1/2$ states is given by Equation 5, as Δm_l for the permitted transitions in NMR for any nuclei corresponds to ± 1 (see Figure 3).

$$\Delta E = |\gamma \hbar B_o| \quad \text{Eq. 5}$$

In the presence of a magnetic field, the energies of the different states (E_α and E_β) of a nucleus are degenerate ($E_\alpha = E_\beta$), since in those conditions the energy associated to the nuclear magnetic moment does not depend on its orientation. However, when a nucleus with spin $1/2$ is set inside a

magnetic field \vec{B}_o oriented along the z axis, the α state, which z -projection is parallel to \vec{B}_o , has a lower energy than the β state, which is antiparallel to \vec{B}_o .

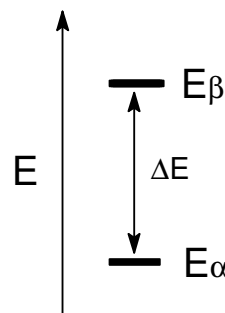


Figure 3. Energy levels for a spin $1/2$ nucleus.

If we use the Plank condition, $\Delta E = h\nu$, we can convert Equation 5 into the fundamental NMR equation, Equation 6.

$$\nu = \frac{\gamma}{2\pi} B_o \quad \text{Eq. 6}$$

We know that Equation 5 describes de behavior of atomic nuclei without electrons inside a magnetic field. The presence of the electros causes several effects on the frequency. Those effects are separated into diamagnetic, paramagnetic, anisotropic and intermolecular (like solvent) effects, which are included inside the shielding tensor σ . The shielding tensor σ is responsible for the very important chemical shift effect. The inclusion of those effects in Equation 6 yields the more general Equation 7.

$$\nu = \frac{\gamma}{2\pi} B_o (1 - \sigma) \quad \text{Eq. 7}$$

In principle, Equation 7 describes the NMR frequencies for a nucleus in a molecule, but it does not consider the coupling of the magnetic moment of that nucleus with the other magnetic nuclei present in the molecule. There are two main ways of coupling between magnetic nuclei, the spin-spin coupling, which occurs via the electrons of the bonds separating the nuclei, and the dipolar coupling, which corresponds to the direct interaction between the magnetic moments of the nuclei. In this first review we will consider only the spin-spin coupling effect. The equation that includes the spin-spin coupling effects between two nuclei **A** and **X** is derived from the quantum mechanical description of NMR and corresponds, for first order spin-spin coupling, to Equations 8 and 9.⁴

$$\nu_A = \frac{\gamma}{2\pi} B_o(1 - \sigma_A) \pm j_{AX} m_{IA} m_{IX} \quad \text{Eq. 8}$$

$$\nu_X = \frac{\gamma}{2\pi} B_o(1 - \sigma_X) \pm j_{AX} m_{IA} m_{IX} \quad \text{Eq. 9}$$

If the nuclei **A** and **X** have spin $\frac{1}{2}$ the resonance frequencies for both nuclei are given by Equations 10 to 13.

$$\nu_{A1} = \nu_A + \frac{j_{AX}}{4} \quad \text{Eq. 10}$$

$$\nu_{A2} = \nu_A - \frac{j_{AX}}{4} \quad \text{Eq. 11}$$

$$\nu_{X1} = \nu_X + \frac{j_{AX}}{4} \quad \text{Eq. 12}$$

$$\nu_{X2} = \nu_X - \frac{j_{AX}}{4} \quad \text{Eq. 13}$$

We know that putting together the values obtained from Equations 10 to 13 we obtain the NMR spectrum shown in Figure 4.



Figure 4. Spectrum of a coupled system formed by nuclei **A** and **X** with spin $\frac{1}{2}$

Spectra with first order coupling such as the one shown in Figure 4 are easily predicted using Equation 14, where **n** is the number of nuclei coupled to the observed nucleus and **l** is the nuclear spin of those nuclei, to predict the multiplicity of the signal for each nucleus and the Pascal triangle to obtain the relative intensity for each line.⁶

$$\text{Multiplicity} = 2nl + 1 \quad \text{Eq. 14}$$

Magnetic moment precession and spin excitation

As mentioned before, the magnetic moment of a spin $\frac{1}{2}$ nucleus inside a magnetic field has only two possible orientations, the lowest energy one, which projection along the Z direction is parallel to the magnetic field, α , and the highest energy one, which projection is antiparallel to \mathbf{B}_0 , β . Lets consider the behavior of a α magnetic moment. The tendency of \mathbf{B}_0 is to align the magnetic moment to the Z direction, but Quantum Mechanics only allows for the exchange of the angles formed by the Z axis and μ_α (θ_α) to θ_β . The alignment of the magnetic moment with the Z axis ($\theta = 0$) is not allowed by the Quantum Mechanics. Because of that, μ_α will only do precession around the +Z axis at the Larmor frequency of the nucleus, as shown in Equation 7. The precession of the magnetic moment is shown in Figure 5. A similar effect happens with a nucleus which magnetic moment is β , with the only difference that its precession is on the opposite direction (see Figure 5).

In order to make the system absorb energy, it is necessary to change μ_α to μ_β , and that can be accomplished only using a second magnetic field \mathbf{B}_1 . Evidently, this new magnetic field must be applied on the XY plane in order to promote the μ_α to μ_β transition.

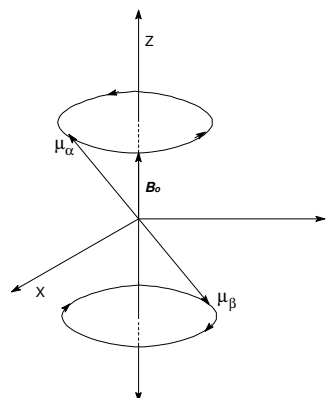


Figure 5. Precession of the magnetic moments around \mathbf{B}_0 .

The effect of \mathbf{B}_1 is not so simple to understand because of the precession of the magnetic moments around \mathbf{B}_0 and the simultaneous promotion of μ_β to μ_α as well as other effects. The rotation of the magnetic moments requires that \mathbf{B}_1 be precessing at the Larmor Frequency in order to have a cumulative effect on the magnetic moments. In fact, if \mathbf{B}_1 has a precession frequency different from the Larmor frequency its effect on the magnetic moment will be null, as shown in Figure 6.

In order to change the state of the magnetic moment from α to β , it is necessary to change the magnetic moment angle from θ_α to θ_β . In Figure 6 is shown the effect of a static \mathbf{B}_1 aligned with the X axis on the magnetic moment in two opposite positions. In Figure 6A the effect of \mathbf{B}_1 is to reduce the angle θ_α , while in Figure 6B is to increase θ_α .

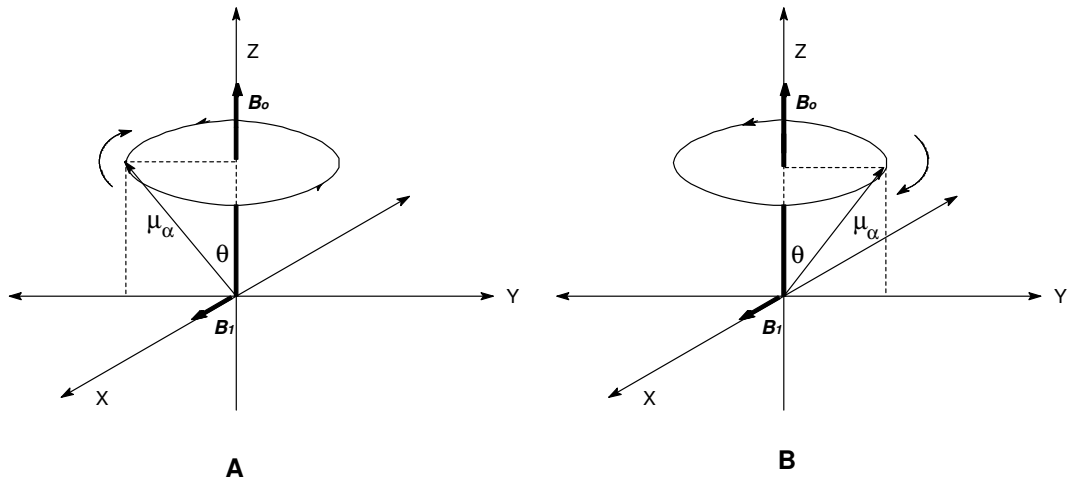


Figure 6. Effect of a static \mathbf{B}_1 set along the X axis on μ_α when the XY projection of the magnetic moment is aligned with the $-Y$ axis (A) and the $+Y$ axis (B).

Therefore, because \mathbf{B}_1 is static, it has no effect on the angle of the precessing magnetic moment. This is a special case of \mathbf{B}_1 precessing with a frequency different from the Larmor frequency. In order to have a continuous and cumulative effect on the

magnetic moment \mathbf{B}_1 must be in precession at the Larmor frequency, thus maintaining constant its position relative to the XY projection of the magnetic moment, as shown is Figure 7.

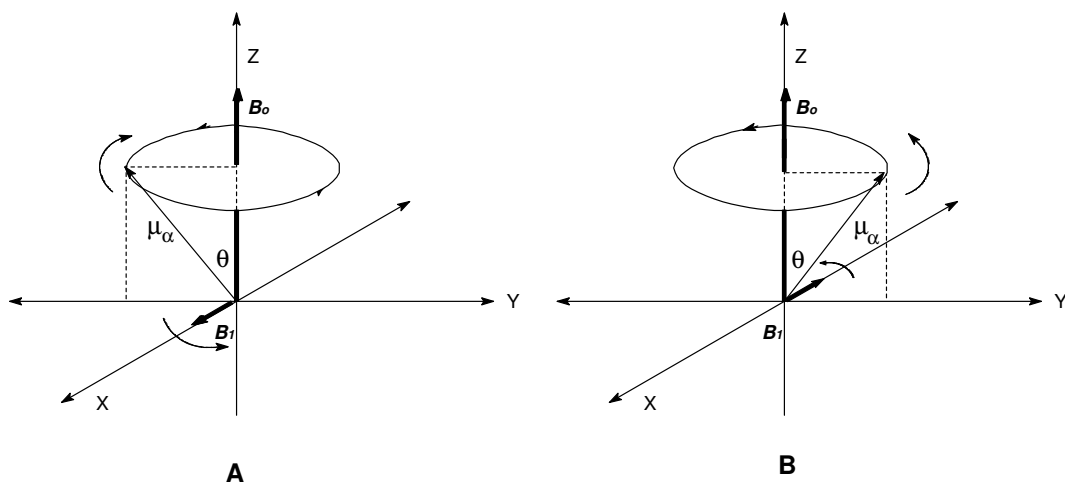


Figure 7. Effect of \mathbf{B}_1 rotating at the Larmor frequency on μ_α when the XY projection of the magnetic moment is aligned with the $-Y$ axis (A) and the $+Y$ axis (B).

The results from quantum mechanics are clear regarding the fact that only the two angles θ_α and θ_β are allowed for the system, therefore, the effect of a rotating \mathbf{B}_1 will be to change θ_α to θ_β or vice versa.

Fortunately the electromagnetic radiation contains an oscillating magnetic field, which is the result of two magnetic fields that rotate with the same frequency but in opposite direction, as shown in Figure 8. The magnetic field that rotates in the same direction as the magnetic moment at the Larmor frequency, corresponds

to \mathbf{B}_1 . As explained before, the magnetic field that rotates in the opposite direction has no effect on μ .

The frequency of the rotating magnetic fields \mathbf{B}_1 and $-\mathbf{B}_1$ is simply determined by the frequency of the electromagnetic radiation used. In the case of NMR with the magnetic fields used (up to 21.15 Tesla) the Larmor frequencies necessary for the excitation of all the different nuclei are inside the range of the radiofrequency (usually from 20 to 900 MHz).

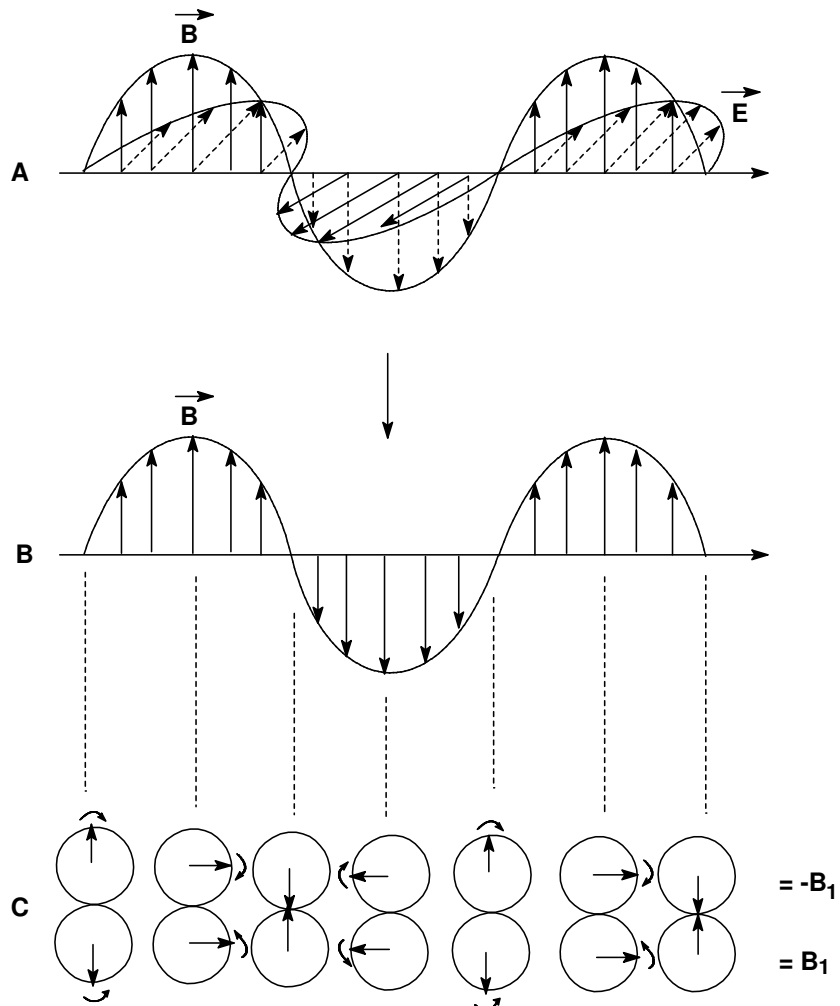


Figure 8. A-Magnetic and electric oscillating fields that compose the electromagnetic radiation. B-Oscillating magnetic field from the electromagnetic radiation. C-Rotating magnetic fields \mathbf{B}_1 and $-\mathbf{B}_1$.

Net Magnetization and Effect of B_1

It is well known that a sample of N spin $\frac{1}{2}$ atoms in equilibrium inside a magnetic field B_0 is distributed between the two magnetic moments states μ_α and μ_β . The populations of such energy levels are respectively N_α and N_β , where $N_\alpha + N_\beta = N$.

Clearly, when the magnetic field B_1 is applied, the populations of the μ_α and μ_β energy levels change, as the equilibrium is altered. If we know that the only transitions that are allowed by the influence of B_1 for each nucleus are μ_α

$\rightarrow \mu_\beta$ or $\mu_\beta \rightarrow \mu_\alpha$ how B_1 generates a magnetization on the XY plane that corresponds with M_0 ? For this we need first to determine what is M_0 .

If we go back to the equilibrium condition without the influence of B_1 , the system can be represented by Figure 9.

If we decompose a single magnetic moment into its projections on the XY plane and along the Z axis, we obtain Figure 10, where it can be seen that $\mu_z = \mu \cos\theta$.

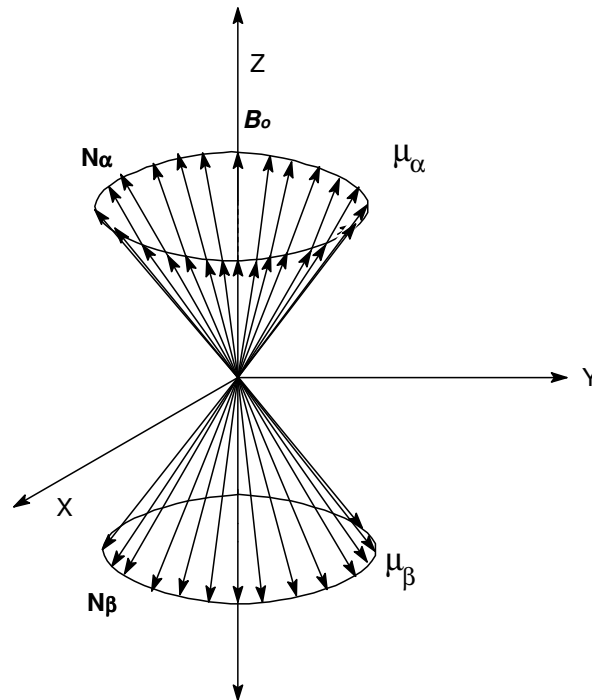


Figure 9. Distribution of N magnetic moments in equilibrium under the influence of an external magnetic field B_0 .

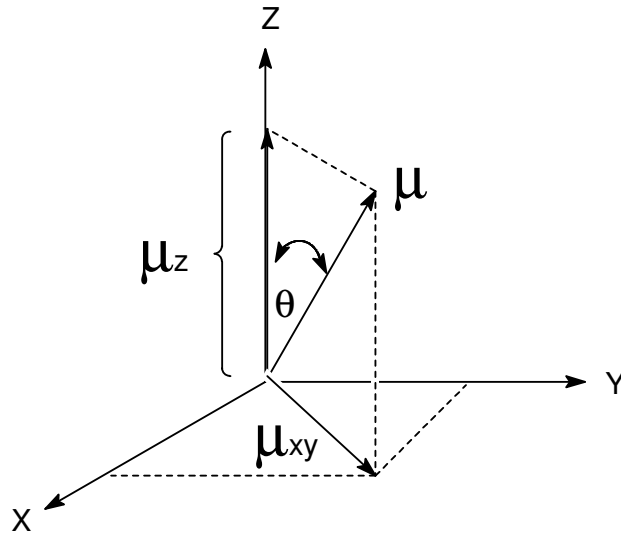


Figure 10. Decomposition of the magnetic moment μ into its projection μ_{xy} and μ_z

If we now decompose each magnetic moment μ from Figure 9 into its projections on the XY plane (μ_{xy}) and along the Z axis (μ_z), we obtain Figure 11. From Figure 11 it is easy to see that $M_{xy}=0$. On the other hand, according to the

results from Figure 9 we observe that $M_z = N_\alpha \mu_z$ and $M_{-z} = N_\beta \mu_{-z}$. Since $E_\alpha < E_\beta$ it is expected that $N_\alpha > N_\beta$, therefore, the net magnetization M_o corresponds to $M_z + M_{-z}$ and $M_o = N_\alpha \mu_z + N_\beta \mu_{-z}$.

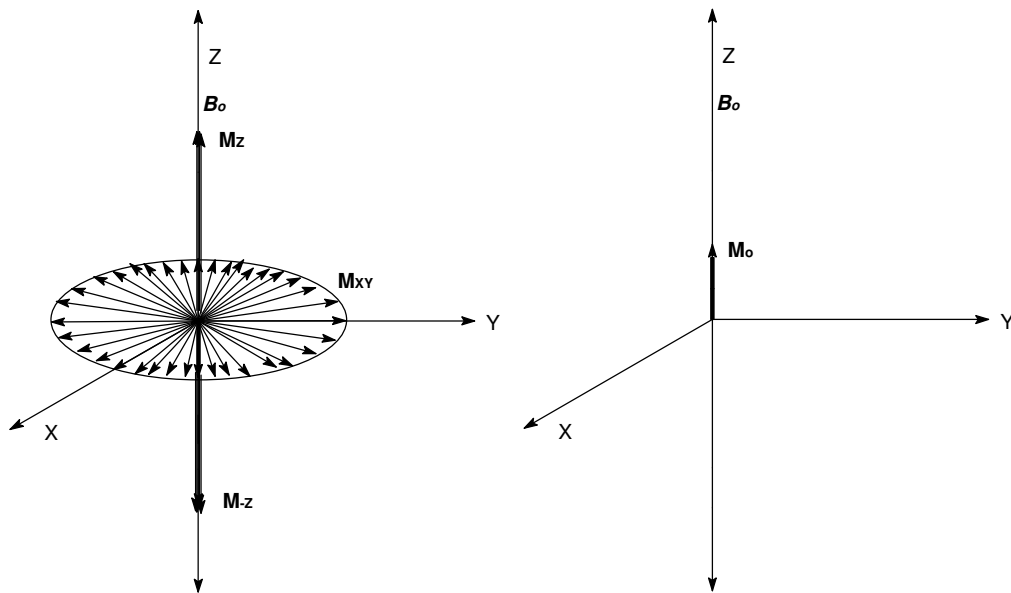


Figure 11. Addition of the projections of the magnetic moments of N spin $\frac{1}{2}$ nuclei inside an external magnetic field B_o .

We also know that $\mu_z = -\mu_z$, therefore $M_o = (N_\alpha - N_\beta) \mu_z$. Finally, from the quantum mechanical results⁴ $\mu_z = \gamma(\hbar/2\pi) m_l$ and since for this case $m_l = 1/2$ we can conclude that $\mu_z = \gamma(\hbar/4\pi)$ and therefore M_o is described by Equation 15:

$$M_o = (N_\alpha - N_\beta) \gamma(\hbar/4\pi) \quad \text{Eq. 15}$$

In order to determine $N_\alpha - N_\beta$ we can make use of the Boltzmann equation for the population distribution at thermal equilibrium for two energy levels, Equation 16.

$$\frac{N_\beta}{N_\alpha} = e^{-\frac{\Delta E}{kT}} \quad \text{Eq. 16}$$

In Equation 15 k corresponds to the Boltzmann constant ($1.380\,6504 \times 10^{-23} \text{ J K}^{-1}$) and T to the absolute equilibrium temperature of the system. We have already seen that for the NMR system $\Delta E = |\gamma \hbar B_o|$ (Equation 5), therefore Equation 16 becomes Equation 17.

$$\frac{N_\beta}{N_\alpha} = e^{-\frac{|\gamma \hbar B_o|}{kT}} \quad \text{Eq. 17}$$

According to the fact that ΔE for NMR is much smaller than the thermal energy (kT) we can approximate Equation 16 to Equation 18:

$$\frac{N_\beta}{N_\alpha} = 1 - \frac{\gamma \hbar B_o}{kT} \quad \text{or}$$

$$N_\beta = N_\alpha - N_\alpha \frac{\gamma \hbar B_o}{kT} \quad \text{Eq. 18}$$

Again, since ΔE for NMR is very small, almost zero, the population of both energy levels is about the same, that is $N_\alpha \approx N_\beta$ and since $N =$

$N_\alpha + N_\beta$ we can use the approximation $N_\alpha = 1/2 N$ and substitute the second N_α for that value in Equation 18, thus leading to Equation 19:

$$N_\alpha - N_\beta = \frac{N \gamma \hbar B_o}{2 kT} \quad \text{Eq. 19}$$

Finally, if we substitute Equation 19 into Equation 15 we obtain a numeric description of the net magnetization of the system in thermal equilibrium, as shown by Equation 20:

$$M_o = \frac{N \gamma^2 \hbar^2}{4 kT} B_o \quad \text{Eq. 20}$$

If we have a solution with a 100 μM sample of a compound that contains 20 hydrogen atoms per molecule for analysis using ^1H NMR in a 300 MHz (7.05 Tesla) spectrometer it means that we will have about 1.2×10^{21} protium atoms in the sample ($N = 1.2 \times 10^{21}$) and the net magnetization of that sample will correspond to $4.09 \times 10^{-35} \text{ J T}^{-1}$ (or A m^2). For this calculation there were used the values $\gamma_{\text{H}} = 26.75 \text{ rad s}^{-1} \text{ T}^{-1}$; $\hbar = 1.054 \times 10^{-34} \text{ rad J s}$; $k = 1.38 \times 10^{-23} \text{ J K}^{-1}$. If we consider that the magnetic moment of a free protium nucleus is $1.41 \times 10^{-26} \text{ J T}^{-1}$ and that all the 1.2×10^{21} nuclei have their magnetic moments aligned with B_o the net magnetization would be $1.69 \times 10^{-5} \text{ J T}^{-1}$, a value that is about 30 orders of magnitude greater than M_o . Therefore, the net magnetization in equilibrium is quite small, corresponding to $2.42 \times 10^{-28}\%$ of the magnetization generated by the simple sum of all the present nuclei. This is the explanation to the low sensitivity of NMR when compared to other spectroscopic techniques.

The question now is how to align this net magnetization M_o with the XY plane using B_1 .

For this we must know that \mathbf{B}_1 has two effects on the rotating magnetic moments of the sample. In order to better understand the vector involved in this part of the explanation it is important to introduce the well known concept of the rotating coordinate system, which is simply a coordinate system in which the X and Y axis rotate at the same frequency that \mathbf{B}_1 (which is the Larmor frequency of the nuclear magnetic moments). In such coordinate system \mathbf{B}_1 will be static, usually aligned along one of the rotation axis, X' for example. In the same way, the nuclei magnetic moments μ will also be static in the absence of \mathbf{B}_1 , as shown in Figure 12B. In the moment that \mathbf{B}_1 is introduced in the system along X', the torque effect of \mathbf{B}_1 on the magnetic moments will lead them to loose the homogeneous distribution around the precession cone, concentrating them at the right location in the cone relative to \mathbf{B}_1 (Figure 12C). This agglomeration of the magnetic moment in a single part of the cone is called a coherence, as shown in Figure 12D. It is interesting to notice that the magnetic moments that are inside the β cone also align to the right of \mathbf{B}_1 , thus being concentrated in a way that their projection on the $\mathbf{X}'\mathbf{Y}'$ plane is aligned opposite to the projection of the magnetic moments form the α cone, and the sum of both projections on $\mathbf{X}'\mathbf{Y}'$ plane originate \mathbf{M}_o (Figure 12E). The size of \mathbf{M}_{xy} is easily calculated knowing that the size of the residual vector (μ_{res}) is given by $(\mathbf{N}_\alpha - \mathbf{N}_\beta)(1.41 \times 10^{-26})$

and that $\mathbf{N}_\alpha - \mathbf{N}_\beta$ is given by Equation 19 and for the case in study corresponds to 2.92×10^5 . According to this we have that $\mu_{res} = 4.12 \times 10^{-21}$ J T⁻¹ and $\mathbf{M}_{xy} = \mu_{res} \cos(90-\theta) = 4.12 \times 10^{-21} \times 0.814$ J T⁻¹ = 3.35×10^{-21} J T⁻¹, which is a much greater value than \mathbf{M}_o (14 orders of magnitude greater) and therefore does not correspond to that value.

The second effect of \mathbf{B}_1 is to exchange the populations of the α and β energy states by changing the magnetic moment vector angle from θ_α to θ_β and vice versa. Since the system is absorbing energy lets suppose that \mathbf{N}_α is decreased to $\mathbf{N}_\alpha - n$ while \mathbf{N}_β is increased to $\mathbf{N}_\beta + n$ by the effect of \mathbf{B}_1 . Such effect would decrease the residual magnetic moment (μ_{res}) from Figure 12E to the value $\mu_{res}^* = \mu_{res} - 2n(1.41 \times 10^{-26})$ and \mathbf{M}_{xy} to $\mathbf{M}_{xy}^* = 0.814 [\mu_{res} - 2n(1.41 \times 10^{-26})]$. If we want to have $\mathbf{M}_{xy} = \mathbf{M}_o$ then we have to resolve the equation $4.09 \times 10^{-35} = 0.814[4.12 \times 10^{-21} - 2n(1.41 \times 10^{-26})]$, which affords $n = 1.46 \times 10^5$. This result indicates that when \mathbf{B}_1 is applied for a sufficient time to generate a $\mathbf{M}_{xy} = \mathbf{M}_o$ it increases the population of the β state of the system in about 7.3×10^5 nuclei. The time \mathbf{B}_1 is applied to obtain this condition is called t_{90} as it corresponds to the time that it is necessary to give a result that is equivalent to rotate \mathbf{M}_o , which originally aligned with the +Z axis, 90° to the -Y axis. The effect obtained according Figure 12 when \mathbf{B}_1 is on for t_{90} microseconds is usually represented in the NMR books as shown on Figure 13.

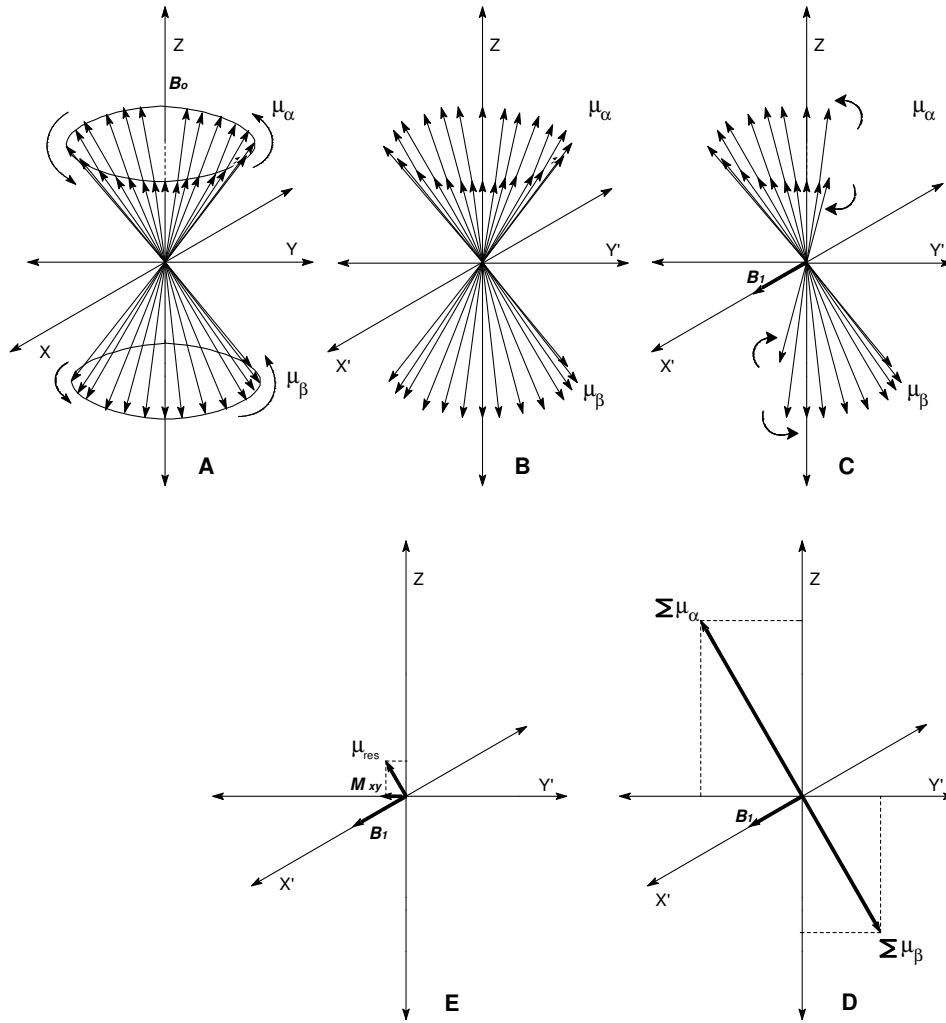


Figure 12. Effect of B_1 on the nuclei magnetic moments generating a coherence, which projection on the $X'Y'$ plane corresponds to M_0 .

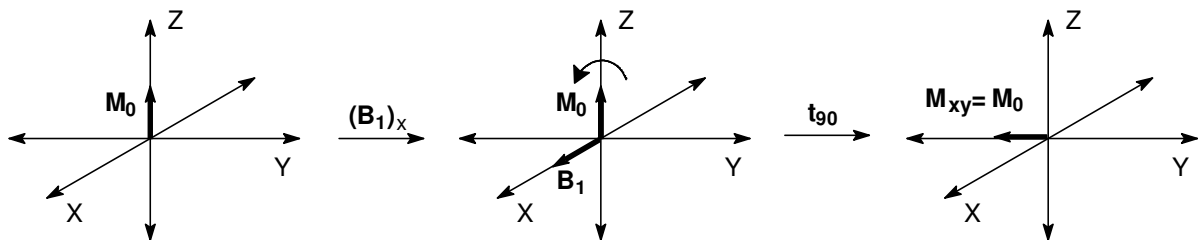


Figure 13. Classical representation of a 90° pulse.

Evidently, this method can be used to explain how to obtain other excitation angles like t_{180} or t_{45} simply by calculating the size of the final

M_{xy} magnetization and determining n in each case.

Conclusion

The semi-classical vector model, with the presented coherence concept, is appropriate to explain how to carry out excitation in NMR, but this methodology is ignored by most NMR books, which discuss the effect of \mathbf{B}_1 without considering the rules of quantum mechanics. The model shown here might be criticized on the basis of the fact that introducing another magnetic field (\mathbf{B}_1 in this case), which is in resonance with the Larmor frequency of the spins changes the nature of the system under consideration, but this argument is not complete to explain the effect of \mathbf{B}_1 , being necessary to use the concept of magnetic coherence to accomplish this.

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