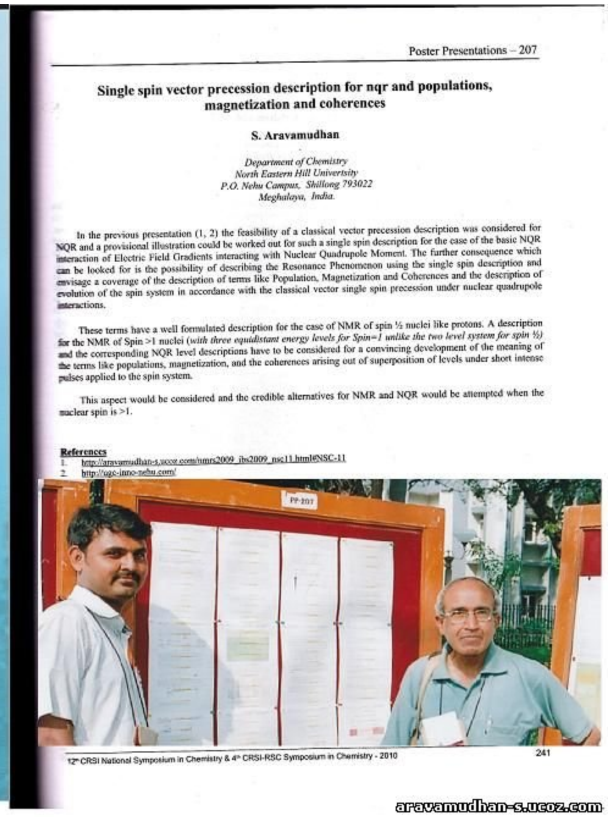
SINGLE SPIN VECTOR PRECESSION DESCRIPTION……: *Magnetic Resonance*



Poster Presentations – 207

Single spin vector precession description for nqr and populations, magnetization and coherences

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In the previous presentation (1, 2) the feasibility of a classical vector precession description was considered for NQR and a provisional illustration could be worked out for such a single spin description for the case of the basic NQR interaction of Electric Field Gradients interacting with Nuclear Quadrupole Moment. The further consequence which can be looked for is the possibility of describing the Resonance Phenomenon using the single spin description and envisage a coverage of the description of terms like Population, Magnetization and Coherences and the description of evolution of the spin system in accordance with the classical vector single spin precession under nuclear quadrupole interactions.

These terms have a well formulated description for the case of NMR of spin ½ nuclei like protons. A description for the NMR of Spin >1 nuclei (*with three equidistant energy levels for Spin=1 unlike the two level system for spin ½*) and the corresponding NQR level descriptions have to be considered for a convincing development of the meaning of the terms like populations, magnetization, and the coherences arising out of superposition of levels under short intense pulses applied to the spin system.

This aspect would be considered and the credible alternatives for NMR and NQR would be attempted when the nuclear spin is >1.

References
1. http://aravamudhan-s.ucoz.com/nmrs2009_ibs2009_nsc11.html#NSC-11
2. http://ugc-inno-nehu.com/

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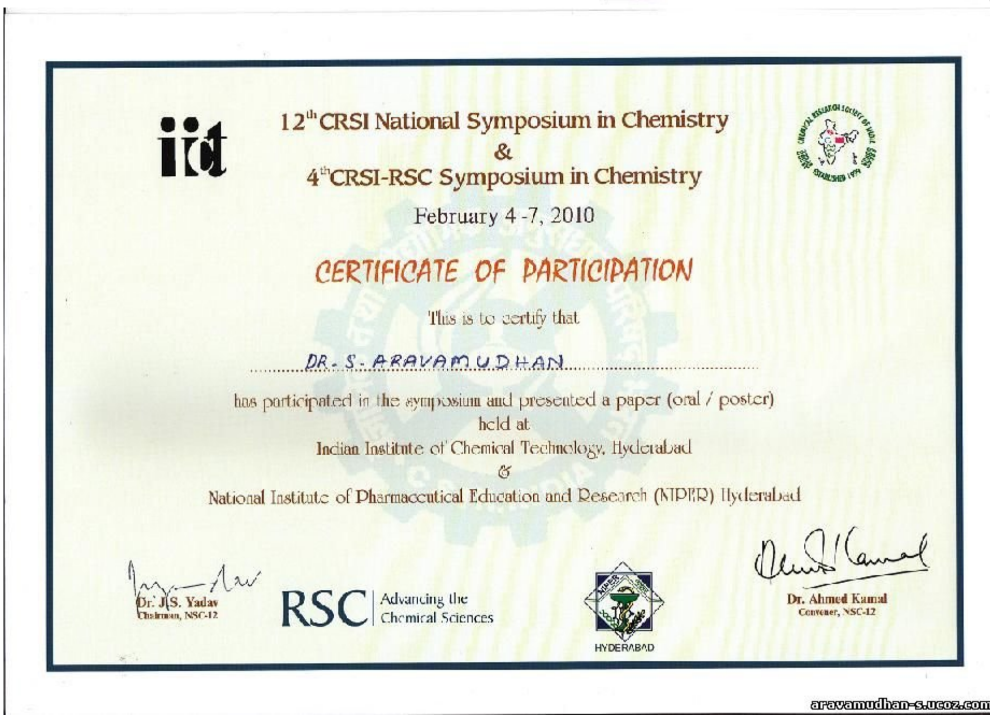

12th CRSI National Symposium in Chemistry
&
4th CRSI-RSC Symposium in Chemistry
February 4 -7, 2010

CERTIFICATE OF PARTICIPATION

This is to certify that

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Even though the spin couplings are a matter of routine consideration for chemists, how exactly the coupled state can be vectorially depicted and what re the various dispositions of the coupling spins is not well visualized by the users. However, the physics of the subject of spin couplings can be convincingly handled with the techniques of mathematical physics. However trying to evolve a visualization for NQR in terms of classical spin vector descriptions requires a detailed depiction of spin-spin coupling, as it is illustrated in this presentation

SINGLE SPIN VECTOR PRECESSION DESCRIPTION FOR NQR AND POPULATIONS, MAGNETIZATION AND COHERENCES

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Meghalaya INDIA

In the previous presentation (1, 2) the feasibility of a classical vector precession description was considered for NQR and a provisional illustration could be worked out for such a single spin description for the case of the basic NQR interaction of Electric Field Gradients interacting with Nuclear Quadrupole Moment. The further consequence which can be looked for is the possibility of describing the Resonance Phenomenon using the single spin description and envisage a coverage of the description of terms like Population, Magnetization and Coherences and the description of evolution of the spin system in accordance with the classical vector single spin precession under nuclear quadrupole interactions.

These terms have a well formulated description for the case of NMR of spin ½ nuclei like protons. A description for the NMR of Spin >1 nuclei (*with three equidistant energy levels for Spin=1 unlike the two level system for spin ½)* and the corresponding NQR level descriptions have to be considered for a convincing development of the meaning of the terms like populations, magnetization, and the coherences arising out of superposition of levels under short intense pulses applied to the spin system.

This aspect would be considered and the credible alternatives for NMR and NQR would be attempted when the nuclear spin is >1

Reference:

1. http://aravamudhan-s.ucoz.com/nmrs2009_ibs2009_nsc11.html#NSC-11
2. http://ugc-inno-nehu.com/

The Poster Site of NSC11 is viewable at URL:
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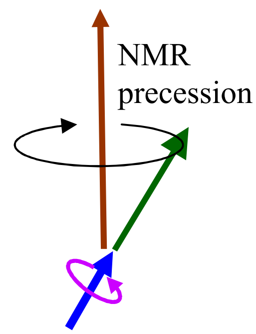
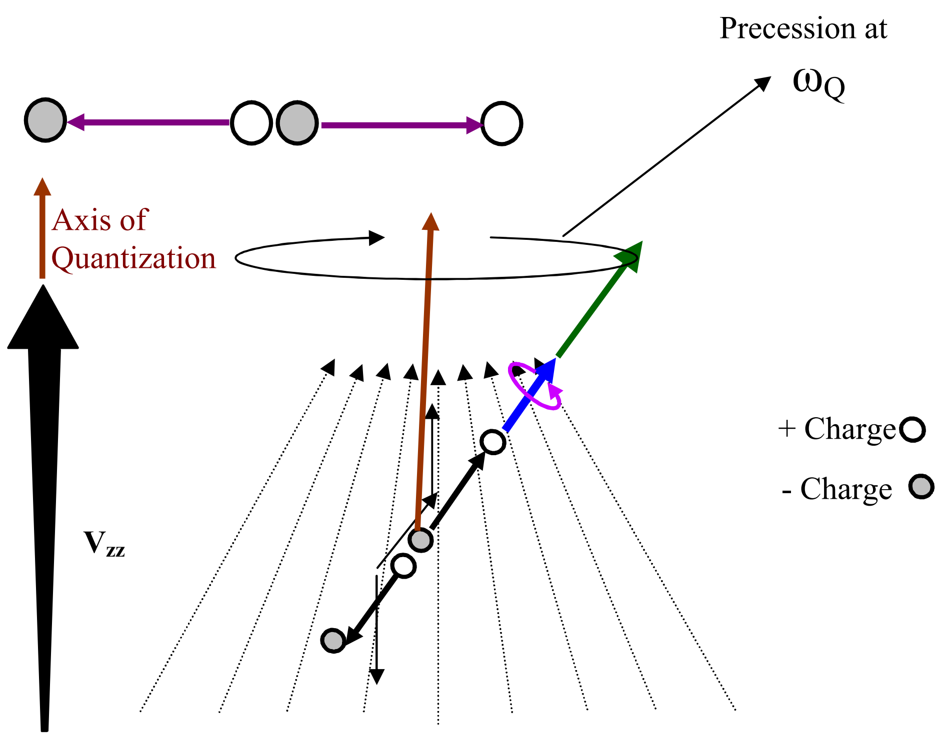
The Display SHEET-11 depicts a classical vector description for the precession of SPIN due to the Interaction of Nuclear Quadrupole Moment with the Electric Field Gradient.





SINGLE SPIN VECTOR PRECESSION DESCRIPTION……: *Magnetic Resonance*

GIVEN THE POSSIBILITY TO DESCRIBE THE NUCLEAR QUADRUPOLE RESONANCE USING A SINGLE SPIN VECTOR PRECESSION APPROACH, THE NEXT STEP IS TO PROVIDE A SUBSTANTIABLE DESCRIPTION OF THE RELEVANT QUANTITIES **:** FOR, DESCRIBING PULSED TRANSIENT MAGNETIC RESONANCE EXPERIMENTS. HENCE, MAGNETIZATION IN TERMS OF POPULATION AND COHERENCE UNDER PERTURBATION BY R.F. PULSE ARE TO BE VISUALIZED IN ACCORDANCE WITH THE CLASSICAL VECTOR PRECESSION DESCRIPTION. EVEN FOR THE CASE OF N.M.R. THE NON-CLASSICAL QUNTITIES LIKE COHERENCES CANNOT BE EASILY ENVISAGED USING THE CLASSICAL VECTOR APPROCHES. AND, OBVIOUSLY, N.Q.R. PHENOMENON WOULD BE EVEN MORE ELUSIVE.

AN EFFORT WOULD BE MADE TO RECONCILE WITH THE CLASSICAL VECTOR APPROACH, FOR THE DESCRIPTIONS OF ALL SUCH RELEVANT QUANTITIES FOR TRANSIENT MAGNETIC RESONANCE PHENOMENON TO BE ABLE TO FURTHER GAIN CONFIDENCE TO DESCRIBE THE N.Q.R. PHENOMENON.

MOST OF WHAT IS DESCRIBED HEREIN ARE MOSTLY SUGGESTIVE AND WOULD BE SUBJECTED MODIFICATIONS AS THE ADVANCED EXPERIMENTAL SITUATIONS WOULD WARRANT.

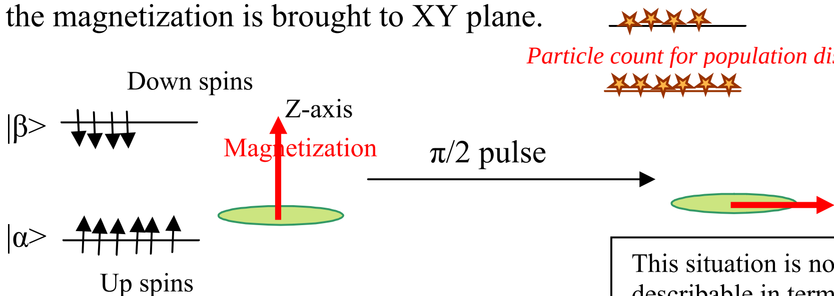
THUS THIS IS INTENDED TO BE USEFUL SUPPLEMENT (for Chemists) TO WHAT IS ALREADY AVAILABLE IN THE STANDARD BOOKS ON MAGNETIC RESONANCE AS ENLISTED IN THE CITED REFERENCES.

Reference: "SPIN DYNAMICS" , Basics of Nuclear Magnetic Resonance, Malcom Levitt, John Wiley & Sons Pvt. Ltd., Year 2001 paper back volume, Page: 278 ; *Section 10.2.5 : Relationships between Populations and Coherences.*

SINGLE QUANTUM COHERNCE IS CONSIDERED IN THIS PRESENTATION

SINGLE SPIN VECTOR PRECESSION DESCRIPTION……: ***Magnetic Resonance***

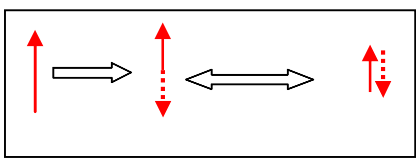
For a two level system: Number of fraction of total number of spins occupying a particular level (stationary state) is the population. Thus below 4/10 =0.4 is the population of |β> State and 0.6 is for the |α> state (Not exactly a Bolzmann distribution). These are discrete Eigen states well defined. The difference in the population is responsible for the Magnetization in thermal equilibrium. When a 90º pulse is applied, the magnetization is brought to XY plane.



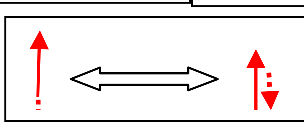
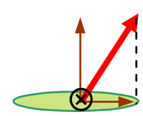
This situation is not describable in terms of the Energy levels and spin orientations

The spins are said to be in a state of coherent superposition. This is a non-stationary state and emits radiation. Thus F.I.D results.

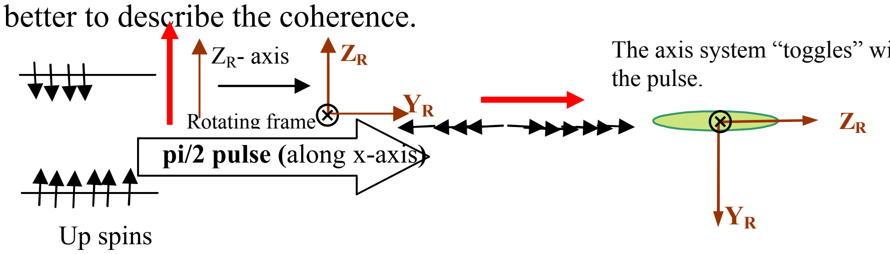
Thus a pi/2 pulse establishes a coherence is non classical and Vector description could become a presumptuous description holding out a validity for the Classical Vector description. However, just to prove this point of view an effort would be made in this presentation to describe with a Vector diagrammatic approach.
The time dependent rf perturbation results in the precessing magnetization vector in the xy plane. This coherence may be viewed from the spin orientation point of view as follows.
Approach 1: Typically the coherent superposition is the state $1/\sqrt{2}$ [|α>+|β>]
Thus this state can be described as the "spin up" getting a component of "spin down".



For the equal weights: of up-spin and down-spin states. True for pi/2 pulse

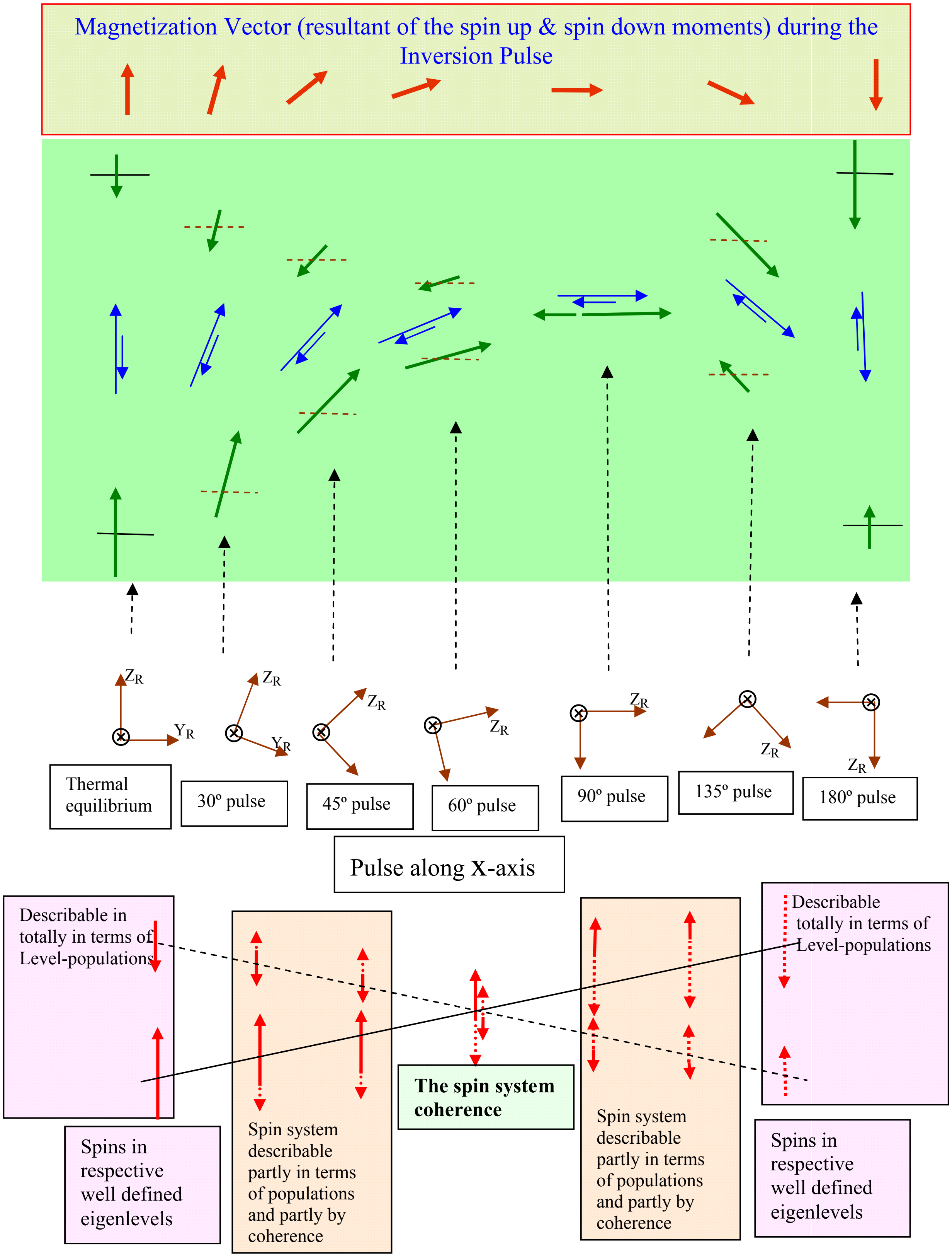
Then for pi/4 pulse,  could be useful 

The Z-component must be describable as population and the XY component as the coherence. In terms of individual spins, labeling the occupation in terms of full spins is not possible as all spins must be under the influence of the pulse. Hence following strategy could be better to describe the coherence.



The axis system "toggles" with the of the pulse.

SINGLE SPIN VECTOR PRECESSION DESCRIPTION……: *Magnetic Resonance*



The **N.Q.R** is a consequence of the energy levels created by the interaction of the Nuclear Quadrupole Moment **(N.Q.M.)** with the Electric Field Gradient **(E.F.G.)** in the system. The Spin ½ nuclei do not possess **NQM**, and two coupled spin ½ nuclear system is usually treated as a composit spin 1 system. It is only the spins which have spin =1 or >1 which can have **NQM**. The **NMR** of such composit spin 1 system would be compared with the single spin 1 system in order to envisage the **description** of the phenomena in terms of *classical vectors* and the **definitions** in terms of *quantum mechanical terms*.

1. The composit (two spin ½) spin 1 system can be considered in the singlet and triplet manifolds. A classical vector description of the coupled system is considered.

2. A single nuclear spin 1 system can be considered for the NMR experiments under high magnetic fields, and for the NQR in the zero external field limits.

Two uncoupled proton spins each spin =1/2

$\mathbf{I_1}$ & $\mathbf{I_2}$ are spin ½ nuclei.

Total maximum spin component along quantization axis would be $I_z = 1 = I_{1z} + I_{2z}$

If this two-system has to be described as a single composite system with Spin quantum Number = 1 (a coupled, two spin ½, system) , then, not only should the max $I_z = 1$, but also $\mathbf{I = I_1 + I_2 = 1}$

Then $|\mathbf{I}| = \sqrt{|\mathbf{I}^2|} = \sqrt{|\mathbf{I \cdot I}|} = \sqrt{|(\mathbf{I_1+I_2}) \cdot (\mathbf{I_1+I_2})|}$

$(\mathbf{I_1+I_2}) \cdot (\mathbf{I_1+I_2}) = \mathbf{I_1 \cdot I_1 + I_1 \cdot I_2 + I_2 \cdot I_1 + I_2 \cdot I_2}$ **and with** $\mathbf{I_1 \cdot I_2 = I_2 \cdot I_1}$ **;**

$\mathbf{I^2 = I_1^2 + I_2^2 + 2\, I_1 \cdot I_2}$

For the situation when the two spins ($\mathbf{I_1 = I_2 = 1/2}$) are not coupled, then

$\mathbf{I^2 = I_1^2 + I_2^2}$ **. Hence the equality $\mathbf{I = I_1 + I_2 = 1}$ is not tenable.**

The two uncoupled spin ½ nuclei still are describable as in doublet state, and not in triplet or singlet.

For the coupled spin quantum number I = 1, which is a triplet state, should have the I-1 state describable which is I=0, the singlet state.

This in elegant quantum mechanical Terms is described as the coupled system has their wave functions as eigenfunctions of the $\mathbf{I^2}$ Operator, genuinely $\mathbf{I = I_1 + I_2}$ with the coupling possibilities of $\mathbf{I_1 - I_2}$ and $\mathbf{I_1 + I_2}$.

Uncoupled system as well as the coupled system of two spin ½ nuclei, both, can have the alignment of components along the quantization axis parallel or anti parallel, with $I_{1z} + I_{2z}$ or $I_{1z} - I_{2z}$.

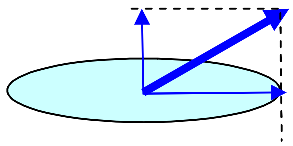
These situations can be given a pictorial vector diagrammatic description.

REFERENCE:

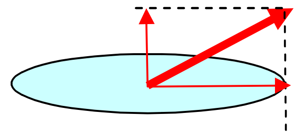
Atkin's "Physical Chemistry", Seventh Edition (year 2002), Peter Atkins and Julio de Paula, Page 395, Oxford University Press (First edition 1978).

UNCOUPLED SPINS:

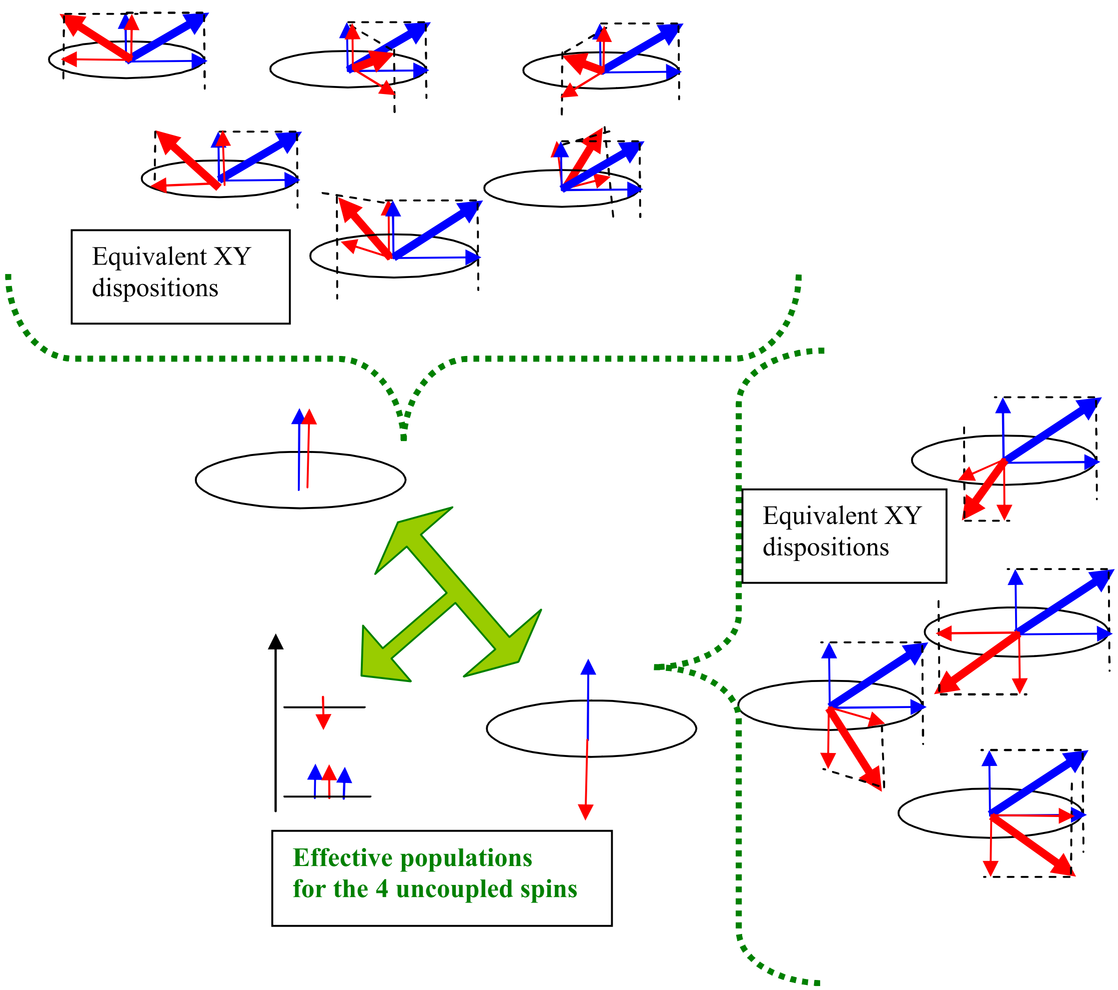
SPIN #1



SPIN #2



When the two uncoupled spins are represented together Vectorial representation, then the XY components of the two spins can be disposed in the XY plane in mutually independent directions and the consequence would be that no interactions are envisaged between the two XY components. Hence there would be no justification trying to vectorially add the two XY components, one of spin #1 and the other of spin #2



COUPLED SPINS (two spin ½):

SPIN COUPLING;
$I_1^2 + I_2^2 + 2\, I_1 . I_2$

I^2 for triplet state = (I(I+1)) = (1(1+1)) = 2
For singlet = 0(0+1) = 0

TRIPLET: Spin =1 SINGLET: Spin =0

TRIPLET: Spin =1
$M_z = +1$ $|\alpha_1\alpha_2>$

$I_1^2 = 3/4 \quad I_2^2 = 3/4 \quad I_1^2 + I_2^2 = 3/2$
$2 - 3/2 = 2\, I_1 . I_2$
$1/4 = I_{1z} I_{2z} + [I_{1x} I_{2x} + I_{1y} I_{2y}]$
$1/4 - 1/4 = 0 = [I_{1x} I_{2x} + I_{1y} I_{2y}]$

$\cos\theta = [I_{1x} I_{2x} + I_{1y} I_{2y}] / |I_{1xy}|\,|I_{2xy}| = 0$

$I = \sqrt{2}$
I_z $=1 = I_{1z} + I_{2z}$
$I_{1xy}^2 = (3/4 - 1/4) = I_{2xy}^2 = 1/2$
$I_{xy} = \sqrt{(I_{1xy}^2 + I_{2xy}^2)} = \sqrt{(1/2 + 1/2)} = 1$
I_{xy} $= \sqrt{(2-1)} = 1$

$M_z = -1$ $|\beta_1 \beta_2>$
$1/4 - 1/4 = 0 = [I_{1x} I_{2x} + I_{1y} I_{2y}] = 0$

$\cos\theta = [I_{1x} I_{2x} + I_{1y} I_{2y}] / |I_{1xy}|\,|I_{2xy}| = 0$

$I_{1xy}^2 = (3/4 - 1/4) = I_{2xy}^2 = 1/2$
$|I_{1xy}| = |I_{2xy}| = \sqrt{1/2}$
$|I_{1xy}||I_{2xy}| = 1/2$

$M_z = 0$ $1/\sqrt{2}\,[\,|\alpha_1 \beta_2> + |\beta_1 \alpha_2>]$ ----> $< I_{1z} I_{2z} > = 1/2\,[-1/4 - 1/4] = -1/4$

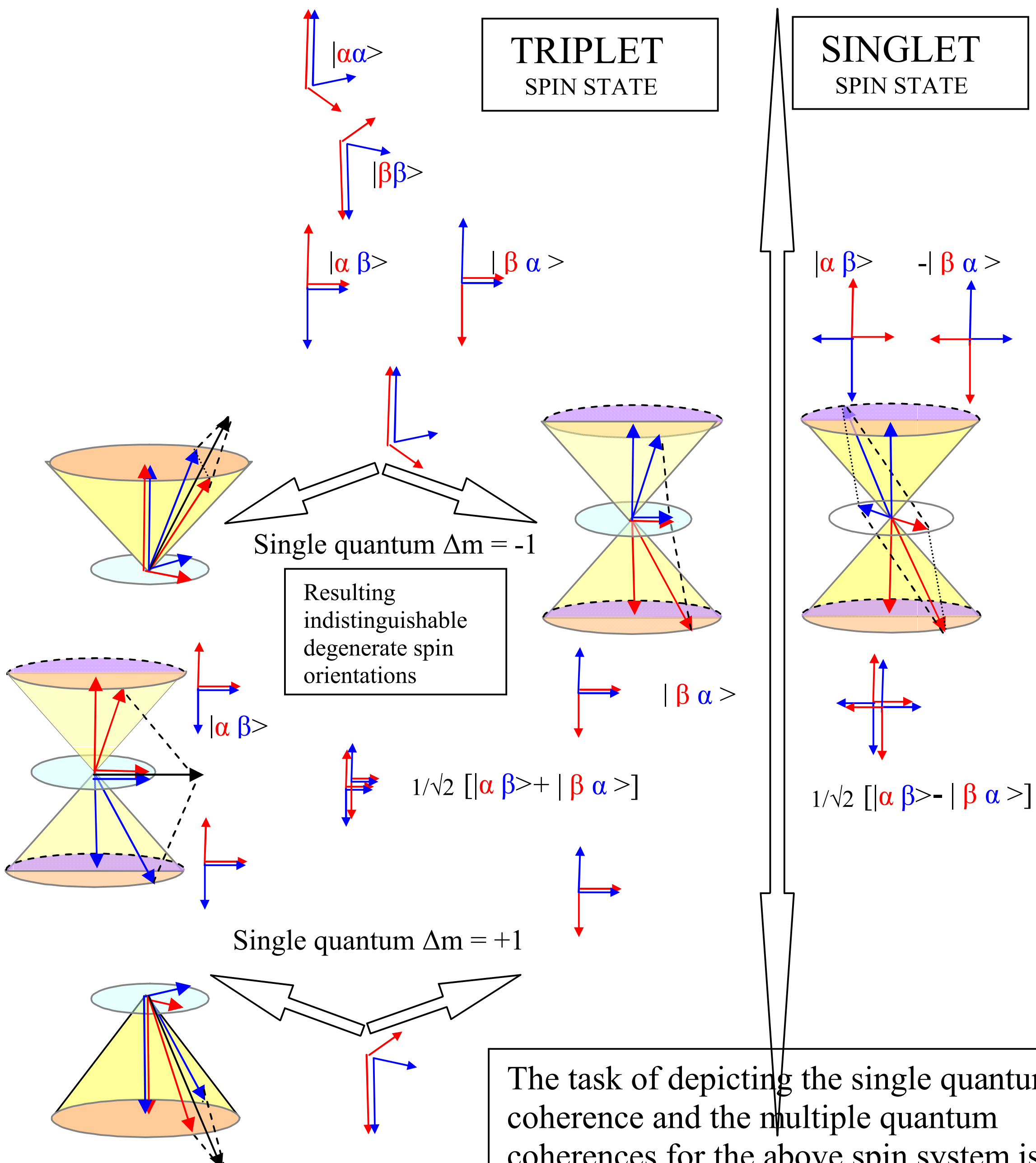
$1/4 + 1/4 = 1/2 = [I_{1x} I_{2x} + I_{1y} I_{2y}]$ **$\cos\theta = 1/2 / 1/2 = 1$**, $\theta = 0$

SINGLET: Spin =0
For Singlet I = 0 $I^2 = I(I+1) = 0(0+1) = 0$
$M_z = 0$ 1/sqrt(2) $[\,|\alpha_1 \beta_2> - |\beta_1 \alpha_2>\,]$

$I^2 = 0 = 3/4 + 3/4 + 2\, I_1 . I_2$
$-3/4 = I_{1z} I_{2z} + [I_{1x} I_{2x} + I_{1y} I_{2y}]$
$-3/4 = -1/4 + [I_{1x} I_{2x} + I_{1y} I_{2y}]$
$\cos\theta = [I_{1x} I_{2x} + I_{1y} I_{2y}] / |I_{1xy}||I_{2xy}| = (-1/2)/(1/2) = -1$ $\theta = 180$

SINGLE SPIN VECTOR PRECESSION DESCRIPTION……: *Magnetic Resonance*

Representing the Coupled pair of spins requires the disposition of the Transverse component also to be depicted



The task of depicting the single quantum coherence and the multiple quantum coherences for the above spin system is beyond the scope of this presentation

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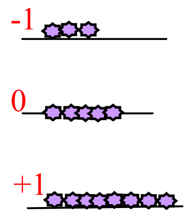
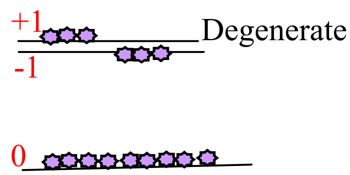
Spin-1 Nuclei NMR and NQR



Depicting the population: by the number of particles.



NMR

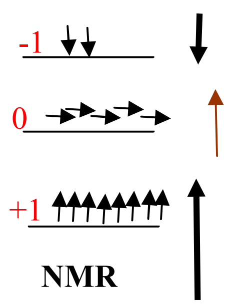
At External High-Magnetic-Field

Spin orientations determine the energy of the particles and the order of the energy levels. Depicting the particle distributions with the spin orientations results in the detailed visualization as in the figures below:

NQR

In External Electric **Field – gradients;** at **Zero-**External-Magnetic-Field

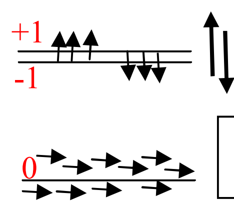
Reference Direction for the Quantized Spin Orientations



NMR

Net Magnetization

Spins in the **XY** plane should be subjected to random phase criteria at thermal equilibrium and hence would not contribute to NET magnetization.



NQR

No Net Magnetization

1. No need to consider singlet and triplet manifolds as it arises in the case of two spin ½-composit soin-1 system.
2. Comparing the spin ½ orientations in the two eigenlevels and the spin-1 orientations above, a description of Δm=±1 transitions, the resonance frequencies and the spin flip angle for the transitions being only pi/2 and not pi as in the spin ½ system require additional features to visualize and substantiate the NQR precession description in the classical vector approach.

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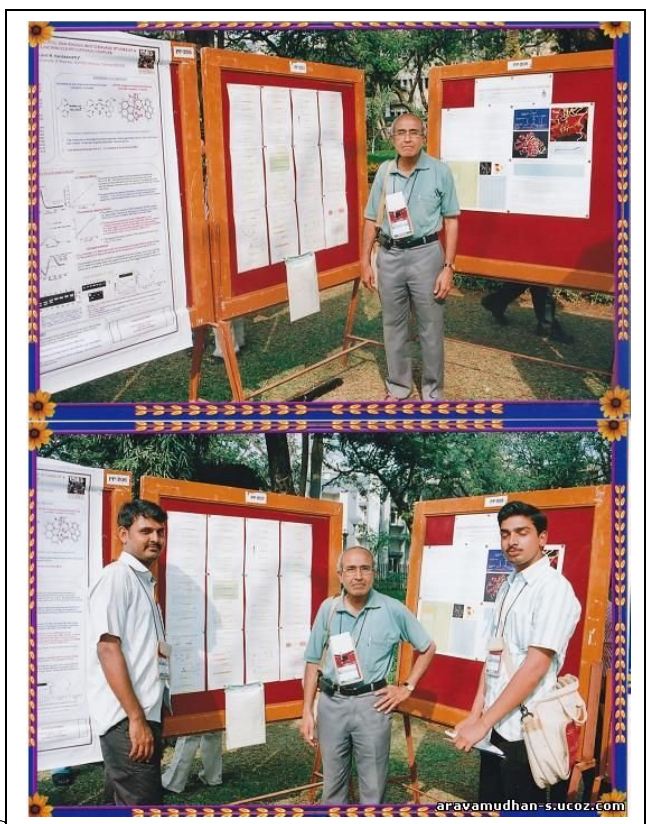
SINGLE SPIN VECTOR PRECESSION DESCRIPTION……: ***Magnetic Resonance***



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