Review Article *Open Access*

Journal of Modern Classical Physics
& Quantum Neuroscience

ISSN: 3068-4196

The Use of Clebsch Gordan Coefficients in Analysis of Spin- Spin Interaction under Nuclear Magnetic Resonance

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Citation: Elio Conte (2025) The Use of Clebsch Gordan Coefficients in Analysis of Spin- Spin Interaction under Nuclear Magnetic Resonance. J.of Mod Phy & Quant Neuroscience 1(2), 01-04.
WMJ/JPQN-103

Abstract

In nuclear magnetic resonance we have that [H, Fz] = 0 and thus H and Fz have a common set of orthonormalized eigenfunctions that employ the use of Clebsch-_Gordan coefficients that we use in the present paper. We have calculated the Clebsch_Gordan coefficients with the value j_1xj_2 *=1/2x1/2 and we estimated the energy levels and the transition energies of this system under the nuclear magnetic resonance. The generalities of the* A^2*, AB; AX, and three spin system are studied.*

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Submitted: 05.05.2025 **Accepted:** 14.05.2025 **Published:** 22.05.2025

Keywords: Nuclear Magnetic Resonance (NMR), Spin- Spin Interaction, Energy States in NMR, Coupling Constants in NMR, Clebsch-Gordan Coefficients

Introduction

Since our publication, inexplicably, after 53 years, the ref.1 has not received the attention it deserved [1]. We proceed, in the present paper, to the application of this theory to the analysis of spin-spin interaction and nuclear magnetic resonance systems using the Clebsch-Gordan coefficients to show how this theory, free from approximations in the calculation of the eigenfunctions, should be applied. If an external magnetic field is applied to a system of nuclei with definite magnetic moments, the nuclear magnets will be lined up parallel to the external field. In particular, under suitable conditions, these nuclear magnets absorb energy for the external magnetic field oscillating at a frequency in the r.f. region and this absorption will give rise to the so called nuclear magnetic resonance spectra (abbreviated as NMR spectra). These spectra are normally studied for the single particle oscillation, for the ,so called, A^2 system, or for the AB and AX system , and for the ABX system. In brief, when the spins are strongly coupled or weakly coupled, they can be characterized by certain limitations. For example, weakly coupled spin systems are called AX, AMX, AMPX. Whereas, the strongly coupled spins are identified as AB, ABC, ABCD. The A^2 system is a spin system where the groups of nuclei are magnetically equivalent. They are labeled, in general, as AnBn, and, in particular, as the A^2 system.

They have just two energy levels for a single spin, and it can be labelled with either the m value of the labels α and β. From quantum mechanics we can show that the energies of these two levels, E_α and E_β, are: $E_\alpha = +1\ 2\ v_{01}$ and $E_\beta = -1\ 2 v_{02}$ where v_{0j} with j=1,2 is the Larmor frequency of spin 1. The Larmor frequency depends on a quantity known as the gyromagnetic ratio, γ, the chemical shift δ, and the strength of this negative Larmor frequency and the applied magnetic field, B_0. The frequency is given from:

$$v_{01} = -1\ 2\pi\ \gamma_1(1+\delta_1)B_0$$

where again we have used the subscript 1 to distinguish the nucleus. The gyromagnetic ratio is characteristic of a particular kind of nucleus, such as proton. The spectrum of two coupled spins consists of two doublets, each split by the same amount, one centered at the chemical shift of the first spin and one at the shift of the second. The splitting of the doublets is the scalar coupling, J_{12}, measured in Hz; these indices evidence the spins that are involved. If we write the shifts of the two spins as δ_1 and δ_2, we give the corresponding Larmor frequencies, $v_{01}$and ν_{02} as:

$$v_{01} = -1\ 2\pi\ \gamma_1(1+\delta_1)\ B_0 \text{ and } \nu_{02} = -1\ 2\pi\ \gamma_2(1+\delta_2)B_0.$$

This is system is called homonuclear if the two nuclei are of the same type, such a proton, in this case the two gyromagnetic ratios are equal. The system is called heteronuclear if the two nuclei are of different types. After we have the three-spin system. If we have a three-spin system in nuclear magnetic resonance, each spin system is coupled to the other two, and the spectrum consists of three doublets of doublets, one centered at the shift of each of the three spins. Obviously, the presence of these multiples will depend on the relative sizes of the couplings. The three spins can be in the α or β spin state, so there are a total of 8 possible combinations corresponding to 8 energy levels. The energies are given by: $E_{m1m2m3} = m_1 v_{01} + m_2 \nu_{02} + m_3 \nu_{0,3} + m_1 m_2\ J_{12} + m_1 m_3\ J_{13} + m_2 m_3\ J_{23}$ where m_i is the value of the quantum number m for the ith spin and J is the coupling constant of the spin of the system.

The Methodological Procedure and Results

The central point of this our paper is in the (2.7) of our previous work (1) that is :

$$[H, F_z] = 0 \qquad (1.1)$$

being

$$F_z = \sum_{j=1}^{N} F_{z,\mathrm{j}} \qquad (1.2)$$

The relation between these two operators indicates that, being commutative, have a common complete set of orthonormalized eigenfunctions in common and their coefficients in the expansion are the Clebsch. - Gordan coefficients given by the following formula

$$C(j_1 j_2 m_1 m_2|JM) = \delta_{M,m_1+m_2}\left[\frac{(2J+1)(j_2-j_1+J)!\,(j_1-j_2+J)!\,(j_1+j_2-J)!}{(j_1+j_2+J+1)!}\right]^{\frac{1}{2}}$$

The eigenfunctions are the tensor space of the two spin basic functions of our spin system as constructed by n resonance spin system such that we have 2^n energy states. We have calculated the Clebsch- Gordan coefficient $< j_1 j_2\ m_1\ /JM >$of a nuclear magnetic resonance system, AB or AX, with the value $j_1 x j_2$ that are reported in Table 1.

Table 1: Clebsch-Gordan Coefficients of a Nuclear Magnetic Resonance Spin System, AB or AX.

	J	1	1	0	1
	M	+1	0	0	-1
m_1	m_2				
+1/2	+1/2	1			
+1/2	-1/2		$\sqrt{1/2}$	$\sqrt{1/2}$	
-1/2	+1/2		$\sqrt{1/2}$	$-\sqrt{1/2}$	
-1/2	-1/2				1

On the basis of this calculation, we obtain the eigenfunctions of the four possible spin states that are the following for a two-spin system on the basis of Tab.1:

$$\varphi_{1=}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}, \qquad \varphi_2=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}+\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix},$$

$$\varphi_3=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}-\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}, \ \varphi_4=-\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} \quad (1.4)$$

We have now all the elements for the estimation of one or two spin nuclear magnetic resonance spectra. One spin system.

We have two energy levels for one spin system. The energy of such energy level is the following

$$E_1=+\frac{1}{2}\nu_{01} \quad \text{and } E_2=-\frac{1}{2}\nu_{02} \qquad (1.5)$$

where ν_{0j} is the Larmor frequency. Only certain transitions are allowed and they are contained in the selection rules about which the transitions take place. In NMR the selection rule considers only transitions in which the quantum number m change of one. It is allowed in quantum mechanical framework and the spectrum results in a single line at the Larmor frequency.

Two Spin Systems

In NMR spectroscopy, the A^2 system relates a spin system where two protons (designated as "A") are magnetically equivalent and have the same chemical shift. A third proton (designated as "X") has a different chemical shift.

The spectrum of two coupled spin is constituted by two doublets. We have that each split is by the same amount and we have a spectrum in which one is centered at the chemical shifts of the first spin and the second is shifted at the second shift of the second spin. The scalar coupling $J_{12}\, in\ Hz$, is the splitting of the doublets. Given the two shifts, as ð$_1$ and ð$_2$, we have that

$$\nu_{01}=\frac{1}{2\pi}\gamma_1(1+ð_1)B_0 \qquad (1.6)$$

$$\nu_{02}=\frac{1}{2\pi}\gamma_2(1+ð_2)B_0 \qquad (1.7)$$

The energies of the four possible levels are given by the following relations, on the basis of the results of Table1:

Number	Spin states	Energy
1	$\varphi=\alpha_1\alpha_2$	E=$\frac{1}{2}\nu_{01}+\frac{1}{2}\nu_{02}+\frac{1}{4}J_{12}$
2	$\varphi=\alpha_1\beta_2+\beta_1\alpha_2$	E=$\frac{1}{2}\nu_{01}-\frac{1}{2}\nu_{02}-\frac{1}{4}J_{12}$
3	$\varphi=\alpha_2\,\beta_1-\beta_2\,\alpha_1$	E=$-\frac{1}{2}\nu_{01}+\frac{1}{2}\nu_{02}-\frac{1}{4}J_{12}$
4	$\varphi=\beta_1\beta_2$	E=-$\frac{1}{2}\nu_{01}-\frac{1}{2}\nu_{02}-\frac{1}{4}J_{12}$

In this case for the selection rules, we have M=m_1+m_2 and the selection rule is $\Delta M=\pm1$. The possible values of the transitions are, respectively,

$$-\nu_{02}-\frac{1}{2}J_{12}\,,$$

$$-\nu_{02}+\frac{1}{2}J_{12}$$

$$-\nu_{01}-\frac{1}{2}J_{12}$$

$$-\nu_{01}+\frac{1}{2}J_{12} \qquad (1.9)$$

For the case of three spin systems the spectrum consists of three doublets of doublets with each spin centered at the each of the other three spins when each spin is coupled to the other two [2,3]. The appearance of such multiples depends on the size of the couplings. The energies of states are given by the general formula:

$E=m_1\nu_{01}+m_2\nu_{02}+m_3\nu_{03}+m_1m_2J_{12}+m_1m_3J_{13}+m_2m_3J_{23}$. (1.10)

M is given as M= $m_1+m_2+m_3$ and the value of states transitions are given as it follows:

Number	Spin States	M	Energetic Transitions
1	$\alpha_1\alpha_2\alpha_3$	3/2	E=1/2$(v_{01}+v_{02}+v_{03})+1/4(J_{12}+J_{13}+J_{23})$
2	$\alpha_1\beta_2\alpha_3$	1/2	E=1/2$(v_{01}-v_{02}+v_{03})$+ $1/4(-J_{12}+J_{13}-J_{23})$
3	$\beta_1\alpha_2\alpha_3$	1/2	E=1/2(-$(v_{01}+v_{02}+v_{03})-1/4(-J_{12}-J_{13}+J_{23})$
4	$\beta_1\beta_2\alpha_3$	-1/2	E=1/2(-$(v_{01}-v_{02}+v_{03})+1/4(+J_{12}-J_{13}-J_{23})$
5	$\alpha_1\alpha_2\beta_3$	1/2	E=1/2$(v_{01}+v_{02}-v_{03})+1/4(J_{12}-J_{13}-J_{23})$
6	$\alpha_1\beta_2\beta_3$	-1/2	E=1/2$(v_{01}-v_{02}-v_{03})+1/4(-J_{12}-J_{13}+J_{23})$
7	$\beta_1\alpha_2\beta_3$	-1/2	E= 1/2$(-v_{01}+v_{02}-v_{03})+1/4(-J_{12}+J_{13}-J_{23})$
8	$\beta_1\beta_2\beta_3$	-3/2	E=1/2$(-v_{01}-v_{02}-v_{03})+1/4(+J_{12}+J_{13}+J23)$

For the three spin system we have the same procedure employed in the two system. Clebsch Gordan coefficients and symmetrized eigenfunctions give immediately the energy states and the transition energies of this system with the same procedure that we have used in the previous case.

Conclusions

In nuclear magnetic resonance we have that (1) $[H, F_z]=0$ and thus H and F_z have a common set of orthonormalized eigenfunctions that employ the use of Clebsch-Gordan coefficients that we used in the present paper. We have calculated the Clebsch-Gordan coefficients with the value $j_1 x j_2$ =1/2x1/2 and, using the common symmetrized and ant symmetrized eigenfunctions, we have estimated the energy levels and the transition energies of this system under the nuclear magnetic resonance. After we have studied the generalities (2,3) of the A^2, AB; AX, and three spin system reporting the relative well- Known NMR spectroscopy.

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