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The Analysis of Spin Spin Interaction and Nuclear Magnetic Resonance of a Two, Three and Four Spin System

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Abstract

In nuclear magnetic resonance we obtain that$[H,F_Z] = 0$ and thus the Hamiltonian H and $F_Z$have a common set of orthonormalized eigenfunctions that require the use of Clebsch-Gordan coefficients used in the present paper. We have calculated such Clebsch-Gordan coefficients with the value $j_1 x j_2$ =1/2x1/2 and we have 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 the three-spin system are studied. On the four-spin system we give the generalities of such a system.

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Introduction

We proceed, in the present paper, to the application of the theory exposed in (1,4) for the analysis of spin interaction under nuclear magnetic resonance using the Clebsch-Gordan coefficients. We evidence the manner in which this theory is applied to the estimation of the eigenfunctions. If a system of nuclei is subjected to an external magnetic field, these nuclear magnets will be alligned to be parallel to the external field. These nuclear magnets absorb energy for the external magnetic field and they will oscillate at a given frequency (that is the region of radio frequency) and this oscillation will give rise to the so called nuclear magnetic resonance spectra (abbreviated as NMR spectra).These spectra are normally studied for different particle oscillation, we have, in fact, the so called A^2 spin system, or the AB and AX system for the case of two spin systems, still we have the ABX system for three spin and systems with four spin particles. If we have a three-spin system in nuclear magnetic resonance, each spin system is coupled to the other two, and the spectrum evidences three doublets of doublets, one centered at the shift of each of the three spins with the presence of these multiplets depending on the relative sizes of the couplings. The three spins can be in the up or down spin state, so we have a total of $2^n = 8$ that is the number of possible combinations corresponding to 8 energy levels. The energies are given by: $E_{m1m2m3} = m_1 v_{01} + m_2 v_{02} + m_3 v_{0,3} + m_1 m_2 J_{12} + m_1 m_3 J_{13} + m_2 m_3 J_{23}$ 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 our paper is in the (2.7) of our previous work (1,4) that is :

$$[H, F_z] = 0 \tag{1}$$

being

$$F_z = \sum_{j=1}^{N} F_{z,j} \tag{2}$$

The (1.1) between these two operators suggest that, being commutative, have a common complete set of orthonormalized eigenfunctions in common and the coefficients in the expansion are the Clebsch- Gordan coefficients given, generally speaking, by the following formula(1,4):

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

$$[(j_1+m_1)!\,(j_1-m_1)!\,(j_2+m_2)!\,(j_2-m_2)!\,(J+M)!\,(J-M)!]^{\frac{1}{2}} *$$

$$\Sigma_n (-)^n \frac{1}{n!(j_1+j_2+J-n)!(j_1-m_1-n)!(J-j_2+m_1+n)!(J-j_1-m_2-n)!} \tag{3}$$

Let us analyze such systems separately.

The Two Spin System

The eigenfunctions are the tensor space of the two spin basic functions of the spin system. We have calculated the Clebsch- Gordan coefficient $< j_1 j_2 \ m_1 \ m_2 \ /JM >$of a nuclear magnetic resonance system, AB or AX, with given the value. The coefficients are C_1,C_2,C_3 and C_4 and they have the following values (1,4):

$$C_1 = 1$$

$$C_2 = \sqrt{1/2} \ , \ \sqrt{1/2}$$

$$C_3 = \sqrt{1/2} \ , \ -\sqrt{1/2}$$

$$C_4 = -1 \tag{4}$$

We obtain now the eigenfunctions of the four possible spin states of the two spin system that are the following (1,2,3,4) :

$$\varphi_1 = \binom{1}{0}\binom{1}{0}, \qquad \varphi_2 = \frac{1}{\sqrt{2}}\binom{1}{0}\binom{0}{1} + \frac{1}{\sqrt{2}}\binom{0}{1}\binom{1}{0},$$

$$\varphi_3 = \frac{1}{\sqrt{2}}\binom{1}{0}\binom{0}{1} - \frac{1}{\sqrt{2}}\binom{0}{1}\binom{1}{0}, \ \varphi_4 = -\binom{0}{1}\binom{0}{1} \tag{5}$$

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

Incidentally we mention that one spin system is constituted by two energy levels and the energy of such levels are (1,2,3,4):

$$E_1 = +\frac{1}{2}\nu_{01} \quad \text{and } E_2 = -\frac{1}{2}\nu_{02} \tag{6}$$

where ν_{oj} is the Larmor frequency. Certain transitions are allowed and the selection rule where the transitions takes place, in NMR ,is given by the selection rule that takes into account only transitions in which we have that the quantum number m changes of one. The spectrum results in a single line at the Larmor frequency.

In NMR spectroscopy, the A^2 system concerns a spin system where two protons (designated as "A") are magnetically equivalent and have the same chemical shift. The spectrum of two coupled spin is realized by two doublets. We have that each split is given by the same amount and we have a spectrum in which the first is centered at the chemical shifts of the first spin and the second is shifted at the second shift of the second spin. The coupling, J_{12} *in* H_Z, is the splitting of the doublets. For the two shifts, given as as δ_1 and δ_2, we have that (1,2,3,4):

$$\nu_{01} = \frac{1}{2\pi}\gamma_1(1+\delta_1)B_0 \tag{7}$$

$$\nu_{02} = \frac{1}{2\pi}\gamma_2(1+\delta_2)B_0 \tag{8}$$

The energies of the four possible levels are given by the following relations(1,2,3,4):

Number of States	Energy
1	$E=\frac{1}{2}\nu_{01} + \frac{1}{2}\nu_{02} + \frac{1}{4}J_{12}$
2	$E=\frac{1}{2}\nu_{01} - \frac{1}{2}\nu_{02} - \frac{1}{4}J_{12}$
3	$E=-\frac{1}{2}\nu_{01} + \frac{1}{2}\nu_{02} - \frac{1}{4}J_{12}$
4	$E=-\frac{1}{2}\nu_{01} - \frac{1}{2}\nu_{02} - \frac{1}{4}J_{12}$

(9)

The selection rule is $\Delta = \pm 1$ and the transitions are, respectively,

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

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

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

$$-\nu_{01} + \frac{1}{2}J_{12} \tag{10}$$

The Three Spin System

For the case of three spin systems (1,2,3,4): 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. The appearance of such multiplets depends on the size of the couplings. The eigenstates are given by the following spin-spin functions and coefficients:

$$j = \frac{3}{2}$$

$$\psi_1 = \beta_1\beta_2\beta_3$$

$$\psi_2 = \frac{\alpha_1\beta_2\beta_3 + \beta_1\alpha_2\beta_3 + \beta_1\beta_2\alpha_3}{\sqrt{3}}$$

$$\psi_3 = \frac{\beta_1\alpha_2\alpha_3 + \alpha_1\beta_2\alpha_3 + \alpha_1\alpha_2\beta_3}{\sqrt{3}}$$

$$\psi_4 = \alpha_1\alpha_2\alpha_3$$

$$j = \frac{1}{2}$$

$$\psi_5 = \frac{\alpha_1\beta_2\beta_3 + \beta_1\alpha_2\beta_3 - 2\beta_1\beta_2\alpha_3}{\sqrt{6}}$$

$$\psi_6 = \frac{-\beta_1\alpha_2\alpha_3 + 2\alpha_1\alpha_2\beta_3 - \alpha_1\beta_2\alpha_3}{\sqrt{6}}$$

$$j = \frac{1}{2}$$

$$\psi_7 = \frac{\alpha_1\beta_2\beta_3 - \beta_1\alpha_2\beta_3}{\sqrt{2}}$$

$$\psi_8 = \frac{\alpha_1\beta_2\alpha_3 - \beta_1\alpha_2\alpha_3}{\sqrt{2}} \tag{11}$$

The energies states of the NMR spectrum are given by the general formula (1,2,3,4):

$$E = m_1\nu_{01} + m_2\nu_{02} + m_3\nu_{03} + m_1 m_2 J_{12} + m_1 m_3 J_{13} + m_2 m_3 J_{23}. \tag{12}$$

M is given as M= $m_1 + m_2 + m_3$ and the value of state transitions are given as it follows(1,2,3,4):

Number	M	energetic transitions
1	3/2	$E=1/2(\nu_{01} + \nu_{02} + \nu_{03}) + 1/4(J_{12} + J_{13} + J_{23})$
2	1/2	$E=1/2(\nu_{01} - \nu_{02} + \nu_{03}) + 1/4(-J_{12} + J_{13} - J_{23})$
3	1/2	$E=1/2(-(\nu_{01} + \nu_{02} + \nu_{03}) - 1/4(-J_{12} - J_{13} + J_{23})$
4	-1/2	$E=1/2(-(\nu_{01} - \nu_{02} + \nu_{03}) + 1/4(+J_{12} - J_{13} - J_{23})$
5	1/2	$E=1/2(\nu_{01} + \nu_{02} - \nu_{03}) + 1/4(J_{12} - J_{13} - J_{23})$
6	-1/2	$E=1/2(\nu_{01} - \nu_{02} - \nu_{03}) + 1/4(-J_{12} - J_{13} + J_{23})$
7	-1/2	$E= 1/2(-\nu_{01} + \nu_{02} - \nu_{03}) + 1/4(-J_{12} + J_{13} - J_{23})$
8	-3/2	$E=1/2(-\nu_{01} - \nu_{02} - \nu_{03}) + 1/4(+J_{12} + J_{13} + J_{23})$

The Four Spin System

A four spin-1/2 system in NMR exhibit a spectrum that is more complex than a simple or doublet: the NMR spectrum will evidence a number of peaks that originate from the combination of different spin of the four nuclei and their interaction (spin-spin couplings).The patterns and intensities of transitions will depend on the relative chemical shifts and coupling constants between the spins. The system of four spin-1/2 particles, has 2^4=16 possible eigenstates of the total spin. These states are usually divided into a singlet state, three triplet states, and a quintet state (S=2, five states). These states can be constructed combining the spins of the individual particles using the technique of the Clebsch-Gordan coefficients or the Kronecker product.

Conclusions

We have that (1,4) $[H,F_Z] = 0$ and therefore the Hamiltonian H and F_Z have a common set of orthonormalized eigenfunctions that require the use of Clebsch-Gordan coefficients used in the present paper. We calculated the Clebsch-Gordan coefficients with the value $j_1 x j_2$ =1/2x1/2 and, using the relative quantum eigenfunctions, we have estimated the energy levels and the transition energies of the system under the nuclear magnetic resonance. After we have studied the generalities (2,3,4) of the A^2, AB; AX, and three spin system reporting the relative well- Known NMR spectroscopy. The generalities of the four-spin system are given.

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