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Interpreting electron–nuclear–magnetic field interactions from a hamiltonian expressed in tensorial notation

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Abstract

The general experimental hamiltonian expressed in tensorial notation is assessed in a way to ensure that the outcomes from such a hamiltonian reflect correctly the electron–nuclear–magnetic field interactions and yields the appropriate parameters. Without such knowledge the use of hamiltonians in tensorial notation to analyse magnetic resonance spectra may lead to questionable or even meaningless results reflected in several publications over the years. Furthermore, the errors that may occur in handling mixed hamiltonians compound the problem.

Keywords: Electron–nuclear–magnetic field interactions

1. Introduction

The fundamental expression used for extracting electron–nuclear–magnetic field interactions from experiments is given by an experimental hamiltonian expressed in terms of these interactions specified by unknown parameters that quantifies these interactions. For example

$$H = \mu_{\mathrm{B}}\mathbf{B}\cdot\mathbf{g}\cdot\mathbf{S}+\mathbf{S}\cdot\mathbf{D}\cdot\mathbf{S}+\mathbf{I}\cdot\mathbf{A}\cdot\mathbf{S}+\mathbf{I}\cdot\mathbf{P}\cdot\mathbf{I}-\mu_{\mathrm{N}}\mathbf{B}\cdot\mathbf{g}_{\mathrm{N}}\cdot\mathbf{S} \tag{1}$$

In (1) the first term describes the electron-applied magnetic field interaction, the second term an electron–electron interaction, the third term an electron–nuclear interaction, the fourth term the nuclear electronic quadrupole interaction and the final term the nuclear–applied magnetic field interaction. The matrices **g**, **D**, **A**, **P** and $\mathbf{g}_{\mathrm{N}}$ each may involve, in general, up to nine unknown interaction parameters. In spherical tensor notation (1) may be expressed as

$$\begin{aligned} H = \mu_{\mathrm{B}}\sum_j\left\{\sum_{m=-j}^{j}B_{jm}^{1,1,0}\Im_{jm}(\mathbf{B},\mathbf{S})\right\} &+ \sum_j\left\{\sum_{m=-j}^{j}B_{jm}^{0,2,0}\Im_{jm}(\mathbf{S},\mathbf{S})\right\} + \sum_j\left\{\sum_{m=-j}^{j}B_{jm}^{0,1,1}\Im_{jm}(\mathbf{I},\mathbf{S})\right\} \\ &+ \sum_j\left\{\sum_{m=-j}^{j}B_{jm}^{0,0,2}\Im_{jm}(\mathbf{I},\mathbf{I})\right\} - \mu_{\mathrm{N}} \times \sum_j\left\{\sum_{m=-j}^{j}B_{jm}^{1,0,1}\Im_{jm}(\mathbf{B},\mathbf{I})\right\} \end{aligned} \tag{2}$$

Equation (1) is the fundamental approach adopted in extracting meaningful parameters that describe interactions such as electron–nuclear–magnetic field interactions. These parameters may then be used in determining an insight into electronic and nuclear structures. This approach is critical in handling a wide range of problems in chemical physics, especially in magnetic resonance spectroscopy, and has

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been used successfully for decades in gaining an insight into complex systems.

In (2) **B** is a unit applied magnetic field vector with components B_x, B_y and B_z along which the magnetic field is directed. We have written the coefficient of the operator in (2) in the form given in other publications, namely, in the form $B_{j,m}^{j_B,j_S,j_I}$ and, as we shall see below, one of j_B, j_S, j_I will always be zero since we shall consider only two-vector tesseral operators. (When we are considering a tensorial B-value for a set of j and m values and the j_B, j_S and j_I values are unimportant we shall abbreviate $B_{jm}^{j_B,j_S,j_I} = B_{jm}$. Care needs to be exercised in distinguishing between the applied magnetic field vectors and the tensorial B-values.). We shall see also that this does not seriously compromise the generality of the hamiltonian. We choose j as an even number.

Unfortunately from several publications, over at least the last decade, the relationship between (1) and (2) is not fully understood. Equation (2) cannot be used alone to determine the various parameters that describe the electronic, nuclear and magnetic field interactions and this paper aims to show why.

2. Theory

To illustrate the process of comparing the two experimental hamitonians, given by (1) and (2), we shall select the first three terms the **g**, **D** and **A** matrices as diagonal noting that $D_{xx} + D_{yy} + D_{zz} = 0$.

The experimental hamiltonians (1) and (2), can then be written as

$$H = \mu_B g_{xx} B_x S_x + \mu_B g_{yy} B_y S_y + \mu_B g_{zz} B_z S_z + D_{xx} S_x^2 + D_{yy} S_y^2 + D_{zz} S_z^2 + A_{xx} I_x S_x + A_{yy} I_y S_y + A_{zz} I_z S_z \quad (3)$$

$$H = \mu_B B_{00}^{1,1,0} \Im_{00}(\mathbf{B}S) + \mu_B B_{20}^{1,1,0} \Im_{20}(\mathbf{B}S) + \mu_B B_{22}^{1,1,0} \Im_{22}(\mathbf{B}S) + B_{20}^{0,2,0} \Im_{20}(S) + B_{22}^{0,2,0} \Im_{22}(S) + B_{00}^{0,1,1} \Im_{00}(\mathbf{I}S) + B_{20}^{0,1,1} \Im_{20}(\mathbf{I}S) + B_{22}^{0,1,1} \Im_{22}(\mathbf{I}S) \quad (4)$$

Equating (3) and (4) we derive the result that

$$\begin{aligned} B_{00}^{1,1,0} &= -\tfrac{1}{\sqrt{3}}\{g_{xx} + g_{yy} + g_{zz}\} \\ B_{20}^{1,1,0} &= \tfrac{\sqrt{2}}{\sqrt{3}}\left\{-\frac{1}{2}(g_{xx} + g_{yy}) + g_{zz}\right\} \\ B_{22}^{1,1,0} &= \tfrac{1}{\sqrt{2}}\{g_{xx} - g_{yy}\} \\ B_{20}^{0,2,0} &= \tfrac{\sqrt{3}}{\sqrt{2}} D_{zz} \\ B_{22}^{0,2,0} &= \tfrac{1}{\sqrt{2}}\{D_{xx} - D_{yy}\} \\ B_{00}^{0,1,1} &= -\tfrac{1}{\sqrt{3}}(A_{xx} + A_{yy} + A_{zz}) \\ B_{20}^{0,1,1} &= \tfrac{\sqrt{2}}{\sqrt{3}}\left(A_{zz} - \tfrac{1}{2}(A_{xx} + A_{yy})\right) \\ B_{22}^{0,1,1} &= \tfrac{1}{\sqrt{2}}(A_{xx} - A_{yy}) \end{aligned} \quad (5)$$

In other words using (1) we obtain the g, D and A-values. Using (2) we obtain the B-values where from (5) the g, D and A-values may be determined. Hence in this case the two hamiltonians may be described as equivalent. This is well known—see for example [1]. However, it is a specific example and must not be assumed to apply to more complex cases involving higher order terms.

Next, we shall consider a higher order hyperfine term IS^3. In general, if the electron-bearing nucleus has the nuclear spin then, from [2], we may express the hamiltonian as

$$H = C_{xx} I_x S_x^3 + C_{yy} I_y S_y^3 + C_{zz} I_z S_z^3 \quad (6)$$

In tensorial notation we need to consider the hamiltonian in the form

$$H = B_{00}^{0,1,1} \Im_{00}(\mathbf{I}S) + B_{20}^{0,1,1} \Im_{20}(\mathbf{I}S) + B_{22}^{0,1,1} \Im_{22}(\mathbf{I}S) + B_{20}^{0,3,1} \Im_{20}(\mathbf{I}S) + B_{22}^{0,3,1} \Im_{22}(\mathbf{I}S) + B_{40}^{0,3,1} \Im_{40}(\mathbf{I}S) + B_{42}^{0,3,1} \Im_{42}(\mathbf{I}S) + B_{44}^{0,3,1} \Im_{44}(\mathbf{I}S) \quad (7)$$

If we equate these equations we obtain a unique solution for the eight B-values, namely,

$$\begin{aligned} B_{00}^{0,1,1} &= (C_{xx} + C_{yy} + C_{zz}) \frac{\{1 - 3S(S+1)\}}{5\sqrt{3}} \\ B_{20}^{0,1,1} &= \left(\frac{1}{2}(C_{xx} + C_{yy}) - C_{zz}\right) \frac{\sqrt{2}\{1 - 3S(S+1)\}}{5\sqrt{3}} \\ B_{22}^{0,1,1} &= (C_{yy} - C_{xx}) \frac{\{1 - 3S(S+1)\}}{5\sqrt{2}} \\ B_{20}^{0,3,1} &= \left(\frac{1}{2}(C_{xx} + C_{yy}) - C_{zz}\right) \frac{\sqrt{6}}{\sqrt{35}} \\ B_{22}^{0,3,1} &= (C_{yy} - C_{xx}) \frac{3}{\sqrt{70}} \\ B_{40}^{0,3,1} &= \left(\frac{3}{2}(C_{xx} + C_{yy}) + 4C_{zz}\right) \frac{1}{\sqrt{70}} \\ B_{42}^{0,3,1} &= (C_{yy} - C_{xx}) \frac{1}{\sqrt{14}} \\ B_{44}^{0,3,1} &= (C_{xx} + C_{yy}) \frac{1}{2\sqrt{2}} \end{aligned} \quad (8)$$

The outcome shows that (6) is not described as only a third rank tensor by the $B_{2m}^{0,3,1}$ and $B_{4m}^{0,3,1}$ terms ($m = 0$, 2 and 4) only. We also have $B_{00}^{0,1,1}$ and $B_{2m}^{0,1,1}$ ($m = 0$ and 2). The unique solution yields the sum of a first rank tensor and a third rank tensor. It also follows that in this case we cannot determine the C-values from the B-values. To use (7) to obtain the C-values the B-values must be chosen as defined in (8).

Furthermore, (8) may be used to determine the general rotation of the x, y and z-vectors. As an example, if we rotate the vectors such that $x \to z \to y \to x$ then the B-values change by $C_{xx} \to C_{zz}$, $C_{yy} \to C_{xx}$ and $C_{zz} \to C_{yy}$. It then follows that the new B-values, B', may be expressed as

$$\begin{aligned} B'_{00} &= B_{00} \\ B'_{20} &= -\frac{1}{2}B_{20} - \frac{\sqrt{3}}{2}B_{22} \\ B'_{22} &= \frac{\sqrt{3}}{2}B_{20} - \frac{1}{2}B_{22} \\ B'_{40} &= \frac{3}{8}B_{40} + \frac{\sqrt{5}}{4}B_{42} + \frac{\sqrt{35}}{8}B_{44} \\ B'_{42} &= -\frac{\sqrt{5}}{4}B_{40} - \frac{1}{2}B_{42} + \frac{\sqrt{7}}{4}B_{44} \\ B'_{44} &= \frac{\sqrt{35}}{8}B_{40} - \frac{\sqrt{7}}{4}B_{42} + \frac{1}{8}B_{44} \end{aligned} \tag{9}$$

These relationships may be determined in another way by rotation of the B-values as given in [3,4] confirming the form of (8).

We examine next the case when the experimental hamiltonian may be described as

$$\begin{aligned} H = {} & \mu_B\{g_{xx}B_xS_x + g_{yy}B_yS_y + g_{zz}B_zS_z\} \\ & + \{A_{xx}I_xS_x + A_{yy}I_yS_y + A_{zz}I_zS_z\} \\ & + \frac{D_{zz}}{2}\{3S_z^2 - S(S+1)\} \\ & + \mu_B\left\{G_{xx}B_xS_x^3 + G_{yy}B_yS_y^3 + G_{zz}B_zS_z^3\right\} \\ & + \left\{C_{xx}I_xS_x^3 + C_{yy}I_yS_y^3 + C_{zz}I_zS_z^3\right\} \end{aligned} \tag{10}$$

In (10) we have added the higher order terms BS^3 and IS^3. Equation (10) may be expressed in the following tensorial notation.

$$\begin{aligned} H = {} & \mu_B B_{00}^{1,1,0}\Im_{00}(\mathbf{B}, \mathbf{S}) + \mu_B B_{20}^{1,1,0}\Im_{20}(\mathbf{B}, \mathbf{S}) \\ & + B_{20}^{0,2,0}\Im_{20}(\mathbf{S}) + B_{00}^{0,1,1}\Im_{00}(\mathbf{I}, \mathbf{S}) + B_{20}^{0,1,1}\Im_{20}(\mathbf{I}, \mathbf{S}) \\ & + \mu_B B_{20}^{1,3,0}\Im_{20}(\mathbf{B}, \mathbf{S}) + \mu_B B_{40}^{1,3,0}\Im_{40}(\mathbf{B}, \mathbf{S}) \\ & + \mu_B B_{44}^{1,3,0}\Im_{44}(\mathbf{B}, \mathbf{S}) + B_{20}^{0,3,1}\Im_{20}(\mathbf{B}, \mathbf{S}) \\ & + B_{40}^{0,3,1}\Im_{40}(\mathbf{I}, \mathbf{S}) + B_{44}^{0,3,1}\Im_{44}(\mathbf{I}, \mathbf{S}) \end{aligned} \tag{11}$$

For (10) and (11) to be equivalent we must set

$$\begin{aligned} B_{00}^{1,1,0} &= -\frac{1}{\sqrt{3}}\{g_{xx} + g_{yy} + g_{zz}\} \\ & \quad + (G_{xx} + G_{yy} + G_{zz})\frac{\{1 - 3S(S+1)\}}{5\sqrt{3}} \\ B_{20}^{1,1,0} &= \frac{\sqrt{2}}{\sqrt{3}}\left\{-\frac{1}{2}(g_{xx} + g_{yy}) + g_{zz}\right\} \\ & \quad + \left(\frac{1}{2}(G_{xx} + G_{yy}) - G_{zz}\right)\frac{\sqrt{2}\{1 - 3S(S+1)\}}{5\sqrt{3}} \\ B_{22}^{1,1,0} &= \frac{1}{\sqrt{2}}\{g_{xx} - g_{yy}\} + (G_{yy} - G_{xx})\frac{\{1 - 3S(S+1)\}}{5\sqrt{2}} \\ B_{20}^{0,2,0} &= \frac{\sqrt{3}}{\sqrt{2}}D_{zz} \\ B_{22}^{0,2,0} &= \frac{1}{\sqrt{2}}\{D_{xx} - D_{yy}\} \\ B_{00}^{0,1,1} &= -\frac{1}{\sqrt{3}}(A_{xx} + A_{yy} + A_{zz}) \\ & \quad + (C_{xx} + C_{yy} + C_{zz})\frac{\{1 - 3S(S+1)\}}{5\sqrt{3}} \\ B_{20}^{0,1,1} &= \frac{\sqrt{2}}{\sqrt{3}}\left(A_{zz} - \frac{1}{2}(A_{xx} + A_{yy})\right) \\ & \quad + \left(\frac{1}{2}(C_{xx} + C_{yy}) - C_{zz}\right)\frac{\sqrt{2}\{1 - 3S(S+1)\}}{5\sqrt{3}} \\ B_{22}^{0,1,1} &= \frac{1}{\sqrt{2}}(A_{xx} - A_{yy}) + (C_{yy} - C_{xx})\frac{\{1 - 3S(S+1)\}}{5\sqrt{2}} \end{aligned} \tag{12a}$$

$$\begin{aligned} B_{20}^{1,3,0} &= \left(\frac{1}{2}(G_{xx} + G_{yy}) - G_{zz}\right)\frac{\sqrt{6}}{\sqrt{35}} \\ B_{22}^{1,3,0} &= (G_{yy} - G_{xx})\frac{3}{\sqrt{70}} \\ B_{40}^{1,3,0} &= \left(\frac{3}{2}(G_{xx} + G_{yy}) + 4G_{zz}\right)\frac{1}{\sqrt{70}} \\ B_{42}^{1,3,0} &= (G_{yy} - G_{xx})\frac{1}{\sqrt{14}} \\ B_{44}^{1,3,0} &= (G_{xx} + G_{yy})\frac{1}{2\sqrt{2}} \\ B_{20}^{0,3,1} &= \left(\frac{1}{2}(C_{xx} + C_{yy}) - C_{zz}\right)\frac{\sqrt{6}}{\sqrt{35}} \\ B_{22}^{0,3,1} &= (C_{yy} - C_{xx})\frac{3}{\sqrt{70}} \\ B_{40}^{0,3,1} &= \left(\frac{3}{2}(C_{xx} + C_{yy}) + 4C_{zz}\right)\frac{1}{\sqrt{70}} \\ B_{42}^{0,3,1} &= (C_{yy} - C_{xx})\frac{1}{\sqrt{14}} \\ B_{44}^{0,3,1} &= (C_{xx} + C_{yy})\frac{1}{2\sqrt{2}} \end{aligned} \tag{12b}$$

In summary, we have shown that we may express the higher order term IS^3 electron–nuclear term and the BS^3 magnetic–electron term in the hamiltonian as two distinct rank tensors of different orders.Furthermore we have determined the B-values for both tensors.Any relationship between the two different rank tensors is strictly associated with the definition of electron–nuclear interactions.Furthermore, it should not be assumed that a hamiltonian with higher order terms above fourth order expressed in tensorial notation might be described by a hamiltonian in the form of the electron–nuclear–magnetic field interactions.In addition, it is clear that to use a hamiltonian in tensorial notation to treat the B-values as arbitrary variables would, in general, lead to little knowledge, if any, of the interaction origins of the B-values.The way to handle the tensorial notation hamiltonian would be to define the B-values in term of the interaction parameters.By varying the B-values through the appropriate interaction parameters would be the way to use the hamiltonian in the tensorial notation.Once again this reinforces the requirement to establish the relationship between the two hamiltonians.Also, it should be noted that from our example we are able to determine readily the corresponding B-values for the BI^3 and I^3S cases.Furthermore, although we have illustrated the approach for the case when the interaction matrices are diagonal it is straightforward to handle the non-diagonal case when, for example, $g_{\alpha\beta} = g_{\beta\alpha}, D_{\alpha\beta} = D_{\beta\alpha}$ and $A_{\alpha\beta} = A_{\beta\alpha}$.

To complete the higher terms up to fourth order we need to consider the J^2 and J^4 terms where $J = S$ or I.

To illustrate the results we refer to [5] where the appropriate hamiltonian for a d^5 ion in a weak crystal field of tetragonal symmetry was expressed in terms of four parameters a, D, F and G namely,

$$\begin{aligned} H = {} & D\left\{S_z^2 - \frac{1}{3}S(S+1)\right\} \\ & + \frac{a}{120}\left[\left\{35S_z^4 + 25S_z^2 - 30S(S+1)S_z^2 - 6S(S+1)\right.\right. \\ & \left.\left. + 3S^2(S+1)^2\right\} + \frac{5}{2}\left\{S_+^4 + S_-^4\right\}\right] \\ & + \frac{F}{180}\left\{35S_z^4 + 25S_z^2 - 30S(S+1)S_z^2 - 6S(S+1)\right. \\ & \left. + 3S^2(S+1)^2\right\} + G\{S_+^4 + S_-^4\} \end{aligned} \tag{13}$$

Analytical expressions for a, D, F and G were derived [5] in terms of the electronic structure of the d^5 ion.$D = 3\ D_{zz}/2$ and $D_{xx} = D_{yy} = -D/3$. In tensorial notation this may be written as

$$\begin{aligned} H = {} & B_{20}^{0,2,0}\mathfrak{T}_{20}^{0,2,0}(\mathbf{S}) + B_{40}^{0,4,0}\mathfrak{T}_{40}^{0,4,0}(\mathbf{S}) + B_{44}^{0,4,0}\mathfrak{T}_{44}^{0,4,0}(\mathbf{S}) \\ = {} & \frac{\sqrt{2}}{\sqrt{3}}D\mathfrak{T}_{20}^{0,2,0}(\mathbf{S}) + \frac{\sqrt{7}}{\sqrt{10}}\left\{\frac{a}{6} + \frac{F}{9}\right\}\mathfrak{T}_{40}^{0,4,0}(\mathbf{S}) \\ & + \sqrt{2}\left\{\frac{a}{12} + 4G\right\}\mathfrak{T}_{44}^{0,4,0}(\mathbf{S}) \end{aligned} \tag{14}$$

Hence, up to and including fourth order higher order terms we are able to obtain equivalent hamiltonians. However, a relationship cannot be assumed. For example, considering the case for I^5S by expressing the hamiltonian in tensorial notation as a sum of first, third and fifth rank tensors we are unable to find an equivalent hamiltonian representing the I^5S higher order terms and the hamiltonian in tensorial notation. This means that the B-values in this case have no relationships with the electron–nuclear–magnetic field interaction parameters.

3. Conclusions

In general, we have shown that in using tensorial notation in interpreting magnetic resonance spectra it is essential that the relationship between the B-values and the specific interactions under investigation be known. If not then if the B-values are fitted to experimental spectral data it must be understood that they cannot be used in any meaningful way to explain the spectra from specifically defined interactions such as electron–electron, electron–nuclear, nuclear–nuclear, and the corresponding electron and nuclear applied magnetic field interactions.

Another area that needs to be addressed is that in the literature we find cases where a mixed hamiltonian involving terms expressed in the form of (1) with higher-order terms expressed in spherical tensor notation in the form of (2)—see for example [6–8].

If a mixed hamiltonian, as shown below, was used where the first five terms in (11) were replaced by the first seven terms in (10), specific terms have been omitted.

$$\begin{aligned} H = {} & \mu_B\{g_{xx}B_xS_x + g_{yy}B_yS_y + g_{zz}B_zS_z\} \\ & + \{A_{xx}I_xS_x + A_{yy}I_yS_y + A_{zz}I_zS_z\} \\ & + \frac{D_{zz}}{2}\{3S_z^2 - S(S+1)\} + \mu_B B_{20}^{1,3,0}\mathfrak{T}_{20}(\mathbf{B},\mathbf{S}) \\ & + \mu_B B_{40}^{1,3,0}\mathfrak{T}_{40}(\mathbf{B},\mathbf{S}) + \mu_B B_{44}^{1,3,0}\mathfrak{T}_{44}(\mathbf{B},\mathbf{S}) \\ & + B_{20}^{0,3,1}\mathfrak{T}_{20}(\mathbf{B},\mathbf{S}) + B_{40}^{0,3,1}\mathfrak{T}_{40}(\mathbf{I},\mathbf{S}) \\ & + B_{44}^{0,3,1}\mathfrak{T}_{44}(\mathbf{I},\mathbf{S}) \end{aligned} \tag{15}$$

It follows, for instance that we must modify the g and A-values, to obtain the correct results, namely,

$$\begin{aligned} & g_{xx} \to g_{xx} - \frac{G_{xx}}{5}\{1 - 3S(S+1)\} \\ & g_{yy} \to g_{yy} - \frac{G_{yy}}{5}\{1 - 3S(S+1)\} \\ & g_{zz} \to g_{zz} - \frac{G_{zz}}{5}\{1 - 3S(S+1)\} \\ & A_{xx} \to A_{xx} - \frac{C_{xx}}{5}\{1 - 3S(S+1)\} \\ & A_{yy} \to A_{yy} - \frac{C_{yy}}{5}\{1 - 3S(S+1)\} \\ & A_{zz} \to A_{zz} - \frac{C_{zz}}{5}\{1 - 3S(S+1)\} \end{aligned} \tag{16}$$

This illustrates that in this case the g-values and the hyperfine interaction constants determined from using hamiltonian (15) would be incorrect.

In summary, we have shown specifically for the inclusion of the higher order terms of up to and including fourth order that great care needs to be used in extracting meaningful data from a hamiltonian expressed in tensorial notation. This work flags that prior to extending a hamiltonian to any higher order terms it is imperative to explore, for each one, not only the appropriate electron–nuclear–magnetic field interactions but to derive the relationship, if one exists, between the two hamiltonians so that they are equivalent. Furthermore, in the case where the *B*-values can be express in terms of the electron–nuclear–magnetic field parameters we have illustrated how to use the hamiltonian in tensorial notation to explore an EPR spectrum, for example, to yield meaningful results in terms of the hamiltonian give in the form of (1).

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