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Total angular momentum of water molecule and its interaction with a constant magnetic field

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The water molecule has many biological functions and is one of the most abundant molecules in the human body. Then, in order to carry out a study of the molecule in physical and chemical phenomena, the model used depends on the phenomenon. For some cases, it is necessary to consider the electronic distribution, while in other cases, it is necessary to consider the protons of the hydrogen atoms, for example, to explain the physics in magnetic resonance imaging. In this work, the water molecule model considered is conformed by three particles: The two nuclei of the hydrogen atom and the oxygen atom negatively double charged and unstructured. The spatial wave function and the interaction of the angular momentum of protons with a constant magnetic field has been studied in a previous work. The present work is a completion, in order to have the complete wave function of this model, considering the spin of the protons, where the energy is degenerated ($B = 0$). Finally, the interaction of the spin of the nuclei of hydrogen atoms with a magnetic field is studied, representing the case of magnetic resonance imaging, where it is obtained a break in the degeneration of the energy levels, which are in the order of radiofrequency.

Keywords: Water molecule; total angular momentum; energy levels; quantum mechanics; magnetic resonance imaging.

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1. Introduction

The water molecule is an important material to simulate cells of human body parts, for example, to calculate cross sections of the radiolysis of water [1]. Then, it is important to have a model of it. The model used can be simplified when considering the phenomena to be studied. The water molecule model studies have not consider all the components of the water molecule (protons, neutrons and electrons), in some cases it considers the protons alone [2, 3] and in others the electronic configuration [4, 5]. Taking the case of radiolysis of water, the studies are carrie out in simulations, and these simulations are performed with chemical experimental parameters [5, 6] using some toolkits [7]. However, there is few work with theoretical modeling and generally it goes back many years [8, 9].

1.1. Three-body model of the water molecule

As mentioned above, there are several models to represent the water molecule, most of them are represented by the electronic configuration. For some phenomena, these models are not very useful, such as magnetic resonance imaging (MRI). It is a powerful technique to obtain three dimensional images of the structure and composition of human body parts [10–12], 80% of human body tissues consist of water molecules [13]. The main assumption used in the MRI is to consider the protons of the hydrogen atoms in the water molecule [14–16], it is because the resonance frequency of protons occurs at radio frequency. The basic principle of the MRI thechnique consists that when a human body is placed in a constant magnetic field, some proton spins of the hydrogen atom in the water molecules become aligned whereas some others become anti-aligned with respect to the direction of the magnetic field. When a radio frequency (RF) is turned on, it produces an effect on the direction of the spin, which is reversed: parallel becomes anti-parallel and vice versa. This state is called the excited spin state. Finally, when the RF is turned off and the proton spins return to the ground state, they release the excess energy in the form of electro-magnetic radiation (RF), which is detected by the radio frequency coils (RFC) components of the MRI technology [17] and thus obtain the image. Considering the above, it is necessary to have a water molecule model whose important particles are the protons of the hydrogen atoms. A model that emphasizes highlighting the protons in hydrogen atoms within water molecules coniders three particles: the two protons from the hydrogen nuclei and the oxygen atom (doubly charged negative and unstructured). Classically, this model is represented by a triangle. It is well known that the distance between the protons and the oxygen is constant ($d_o = 95.60$ pm), as well as, the distance between protons (d_p =151.05 pm), due to the electrostatic interaction [4, 18]. In a previous work [19] it was possible to obtain the wave function and the energy of this system, analytically. Where it was found the spatial state function of the water molecule and the energy, which is degenerated. The spatial function, is given by

$$\psi_{l_1,m_1;l_2,m_2}(\theta_1,\phi_1;\theta_2,\phi_2) = Y_{l_1 m_1}(\theta_1,\phi_1) \times Y_{l_2,m_2}(\theta_2,\phi_2), \qquad (1)$$

where Y_{l_i,m_i} are the spherical harmonics. l_i and m_i are the orbital quantum number and magnetization quantum number, respectively, for each proton, denotated by $i = 1, 2$. When the water molecule is placed in a constant magnetc field, the degeneration partially persists for the quantum orbital numbers l_1 and l_2 and it breaks for the quantum magnetic numbers m_1 and m_2.

In this work, a complete study of [19] is carried out using the water model previously mentioned to calculate the total wave function, which corresponds to the total angular momentum ($\hat{J} = \hat{L} + \hat{S}$) and the analysis is performed when the water molecule is placed in a constant magnetic field. This molecule model can be thought as a hydrogen atom (with the exception that the potential does not depend on the radial part, since it is a constant), then, there is an analogy to the anomalous Zeeman effect. Then, it is calcuated the fine structure through the relativistic correction and the spin-orbit interaction for the water molecule. The work is organized as follows: In Sec. 2, the states of the total angular momentum are shown In Sec. 3, it is introduced a constant magnetic field to obtain the fine structure for the water molecule model and it is found the total energy. Finally, in Sec. 4, the results are discussed and conclusions are presented.

2. Total angular momentum of water molecule

To obtain the total angular momentum, it is used the formalism of sum of angular momentum. This water molecule model considers the two orbital angular momentums (l_1 and l_2) and two spin values ($s_1 = s_2 = 1/2$), corresponding to each proton (denotated by i =1, 2). The sum of an orbital angular momentum and 1/2-spin, it is well known. The case $l_i = 0$ implies that there is no angular momentum and the total angular momentum is purely spin angular momentum. For the case of $l_i > 0$, the resulting angular momentum j_i, only has two possibilities $j_i = l_i \pm 1/2$. Then, the states are giving by:

$$\begin{aligned} |j_i; m_i >_{l_i} &= \left|l_i \pm \frac{1}{2}; m_i\right\rangle_{l_i} \\ &= \sqrt{\frac{l_i \mp m_i + \frac{1}{2}}{2l_i + 1}}\left|l_i, \frac{1}{2}; m_i + \frac{1}{2}, -\frac{1}{2}\right\rangle \\ &\pm \sqrt{\frac{l_i \pm m_i + \frac{1}{2}}{2l_i + 1}}\left|l_i, \frac{1}{2}; m_i - \frac{1}{2}, \frac{1}{2}\right\rangle, \end{aligned} \tag{2}$$

where, $m_i = -j_i, -j_i + 1 ..., j_i - 1, j_i$ and $|l_i, \frac{1}{2}; m_i \pm \frac{1}{2}, \mp\frac{1}{2} >= |l_i; m_i \pm \frac{1}{2} > |\frac{1}{2}; \mp\frac{1}{2} >$ is the tensor product of the spatial part (first bra) and the spin part (second bra), where,

$$\left|\frac{1}{2}; \frac{1}{2}\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \left|\frac{1}{2}; -\frac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{3}$$

Equation (2) can be rewriten by the wave function:

$$\begin{aligned} \Phi_{j_i = l_i \pm \frac{1}{2}, m_i}(\theta_i, \phi_i) &= \frac{1}{\sqrt{2l_i + 1}} \\ &\times \begin{pmatrix} \pm\sqrt{l_i \pm m_i + \frac{1}{2}}\, Y_{l_i, m_i - \frac{1}{2}}(\theta_i, \phi_i) \\ \sqrt{l_i \mp m_i - \frac{1}{2}}\, Y_{l_i, m_i + \frac{1}{2}}(\theta_i, \phi_i) \end{pmatrix}, \end{aligned} \tag{4}$$

where the $Y_{l_i, m_i \pm \frac{1}{2}}(\theta_i, \phi_i)$ are the spatial functions (spherical harmonics Eq. (1)) for the water molecule [19].
The final calculation is to obtain the sum of the two angular momentums j_1 and j_2 for each proton, giving by four possible combinations:

1. $j_1 = l_1 - 1/2$ and $j_2 = l_2 - 1/2$
2. $j_1 = l_1 - 1/2$ and $j_2 = l_2 + 1/2$
3. $j_1 = l_1 + 1/2$ and $j_2 = l_2 - 1/2$
4. $j_1 = l_1 + 1/2$ and $j_2 = l_2 + 1/2$

Then, it is known that the total angular momentum is obtained by

$$\begin{aligned} |j; m >^{(l_1, l_2)}_{(j_1, j_2)} &= \sum_{m_1}\sum_{m_2} {}_{l_1, l_2} < j_1, j_2; m_1, m_2 | j; m > \\ &\times |j_1, j_2; m_1, m_2 >_{l_1, l_2}, \end{aligned} \tag{5}$$

where $|j_1, j_2; m_1, m_2 >_{l_1, l_2} = |j_1; m_1 >_{l_1} \otimes |j_2; m_2 >_{l_2}$ and $< j_1, j_2; m_1, m_2 | j; m >$ are the Clebsh-Gordan coefficients.

Then, the wave function is giving by

$$\begin{aligned} &\Psi_{l_1, l_2; m_1, m_2; \frac{1}{2}, \pm\frac{1}{2}}(\theta_1, \phi_1, \theta_2, \phi_2) \\ &= \Phi_{l_1 \pm \frac{1}{2}, m_1}(\theta_1, \phi_1)\Phi_{l_2 \pm \frac{1}{2}, m_2}(\theta_2, \phi_2). \end{aligned} \tag{6}$$

2.1. Ground state of water molecule

The water molecule model used is a fermion system, due to the two protons. Then, the protons follow the Pauli exclusion principle. For the ground state, $l_1 = l_2 = 0$ and $m_1 = m_2 = 0$, therefore, one of the spin protons must have $+1/2$ value and the other the $-1/2$ value. The total angular momentum takes the value $j = 0, 1$ and the only two states allowed are

$$\begin{aligned} |0; 0 >^{(0,0)}_{(\frac{1}{2}, \frac{1}{2})} &= \left|\frac{1}{2}, \frac{1}{2}; -\frac{1}{2}, \frac{1}{2}\right\rangle_{00}, \\ |1; 0 >^{(0,0)}_{(\frac{1}{2}, \frac{1}{2})} &= \left|\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\right\rangle_{00}. \end{aligned} \tag{7}$$

2.2. First excited state of water molecule

The first excited state must occur with $l_i = 1$ and the other remains in $l_i = 0$. For this case, all combinations of the quantum numbers are allowed. To exemplify, it is taken $l_1 = 1$, then, $j_1 = 1/2, 3/2$; then, the six states can be obtained by

Eq. (2). The quantum numbers for the second proton are $l_2 = 0$ and $s_2 = 1/2$, then $j_2 = 1/2$. The calculations are simplified by considering the angular momentum rise and fall operators, instead of the Clebsh-Gordan coefficients. The two spaces are described below.

2.2.1. Space generated by $j_1 = 1/2$ and $j_2 = 1/2$

The total angular momentum j has two possible values: 1 and 0.

1. Case $j = 1$: The three states are.

$$\begin{aligned}
|1,1\rangle^{(1,0)}_{(\frac{1}{2},\frac{1}{2})} &= \left|\frac{1}{2},\frac{1}{2};\frac{1}{2},\frac{1}{2}\right\rangle_{10}\\
|1,0\rangle^{(1,0)}_{(\frac{1}{2},\frac{1}{2})} &= \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2},\frac{1}{2};-\frac{1}{2},\frac{1}{2}\right\rangle_{10}\right.\\
&\quad\left.+\left|\frac{1}{2},\frac{1}{2};\frac{1}{2},-\frac{1}{2}\right\rangle_{10}\right)\\
|1,-1\rangle^{(1,0)}_{(\frac{1}{2},\frac{1}{2})} &= \left|\frac{1}{2},\frac{1}{2};-\frac{1}{2},-\frac{1}{2}\right\rangle_{10}.
\end{aligned}\tag{8}$$

The first state could be obtained immediately due to the known conditions of sum of angular momentum. The other two were obtained from applying the descent operator to the first state. The same procedure was used for the other states, as shown below.

2. Case $j = 0$: There is only one state giving by

$$\begin{aligned}
|0,0\rangle^{(1,0)}_{(\frac{1}{2},\frac{1}{2})} &= \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2},\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right\rangle_{10}\right.\\
&\quad\left.-\left|\frac{1}{2},\frac{1}{2};-\frac{1}{2},\frac{1}{2}\right\rangle_{10}\right).
\end{aligned}\tag{9}$$

2.2.2. Space generated by $j_1 = 3/2$ and $j_2 = 1/2$

The total angular momentum j has two possible values: 2 and 1.

1. Case j=2: The five states are

$$\begin{aligned}
|2,2\rangle^{(1,0)}_{(\frac{3}{2},\frac{1}{2})} &= \left|\frac{3}{2},\frac{1}{2};\frac{3}{2},\frac{1}{2}\right\rangle_{10}\\
|2,1\rangle^{(1,0)}_{(\frac{3}{2},\frac{1}{2})} &= \sqrt{\frac{3}{4}}\left|\frac{3}{2},\frac{1}{2};\frac{1}{2},\frac{1}{2}\right\rangle_{10}\\
&\quad+\frac{1}{2}\left|\frac{3}{2},\frac{1}{2};\frac{3}{2},-\frac{1}{2}\right\rangle_{10}\\
|2,0\rangle^{(1,0)}_{(\frac{3}{2},\frac{1}{2})} &= \frac{1}{\sqrt{2}}\left(\left|\frac{3}{2},\frac{1}{2};-\frac{1}{2},\frac{1}{2}\right\rangle_{10}\right.\\
&\quad\left.+\left|\frac{3}{2},\frac{1}{2};\frac{1}{2},-\frac{1}{2}\right\rangle_{10}\right)\\
|2,-1\rangle^{(1,0)}_{(\frac{3}{2},\frac{1}{2})} &= \frac{1}{2}\left|\frac{3}{2},\frac{1}{2};-\frac{3}{2},\frac{1}{2}\right\rangle_{10}\\
&\quad+\sqrt{\frac{3}{4}}\left|\frac{3}{2},\frac{1}{2};-\frac{1}{2},-\frac{1}{2}\right\rangle_{10}\\
|2,-2\rangle^{(1,0)}_{(\frac{3}{2},\frac{1}{2})} &= \left|\frac{3}{2},\frac{1}{2};-\frac{3}{2},-\frac{1}{2}\right\rangle_{10}.
\end{aligned}\tag{10}$$

2. Case j=1: There are three states giving by

$$\begin{aligned}
|1,1\rangle^{(1,0)}_{(\frac{3}{2},\frac{1}{2})} &= \sqrt{\frac{3}{4}}\left|\frac{3}{2},\frac{1}{2},\frac{3}{2},-\frac{1}{2}\right\rangle_{10}\\
&\quad-\frac{1}{2}\left|\frac{3}{2},\frac{1}{2};\frac{1}{2},\frac{1}{2}\right\rangle_{10}\\
|1,0\rangle^{(1,0)}_{(\frac{3}{2},\frac{1}{2})} &= \frac{1}{\sqrt{2}}\left(\left|\frac{3}{2},\frac{1}{2};\frac{1}{2},-\frac{1}{2}\right\rangle_{10}\right.\\
&\quad\left.-\left|\frac{3}{2},\frac{1}{2};-\frac{1}{2},\frac{1}{2}\right\rangle_{10}\right)\\
|1,-1\rangle^{(1,0)}_{(\frac{3}{2},\frac{1}{2})} &= \frac{1}{2}\left|\frac{3}{2},\frac{1}{2};-\frac{1}{2},-\frac{1}{2}\right\rangle_{10}\\
&\quad-\sqrt{\frac{3}{4}}\left|\frac{3}{2},\frac{1}{2};-\frac{3}{2},\frac{1}{2}\right\rangle_{10}.
\end{aligned}\tag{11}$$

Acording to [19], the energy of this water molecule model is $E_{l_1,l_2} = [\hbar^2/2md_o^2]l_1(l_1+1) + [\hbar^2/2md_o^2]l_2(l_2+1) + V$, which is degenerated. Clearly, this degeneracy persists even when the total angular momentum is considered, since it only depends on l_i. It was found that this degeneration is shifted when a constant magnetic field is considered (see Sec. 4 of [19]). In Sec. 3.4, it is found the shifted energy by the interaction of the total angular momentum with a constant magnetic field.

2.3. State function for identical protons

It was mentioned that the water molecule is a fermion system, then, to consider the protons as identical particles, the wave function must be antisymmetric. The Eq. (6) becomes

$$\Psi_{l_1,l_2;m_1,m_2;\frac{1}{2},\pm\frac{1}{2}}(\theta_1,\phi_1,\theta_2,\phi_2)=\frac{1}{\sqrt{2}} \times \begin{vmatrix} \Phi_{l_1\pm\frac{1}{2},m_1}(\theta_1,\phi_1) & \Phi_{l_2\pm\frac{1}{2},m_2}(\theta_1,\phi_1) \\ \Phi_{l_1\pm\frac{1}{2},m_1}(\theta_2,\phi_2) & \Phi_{l_2\pm\frac{1}{2},m_2}(\theta_2,\phi_2) \end{vmatrix}, \quad (12)$$

where the 2 × 2 determinant is the Slater determinant.

3. Interaction of water molecule with an external magnetic field

The water molecule model used for this analysis is like a hydrogen atom. Then, the presence of the water molecule in a constant magnetic field can be treated as the anomalous Zeeman effect, where the protons would be the analogous to the electron in the hydrogen atom. Therefore, it turns out interesting to obtain the fine structure of water molecule, through the spin-orbit interaction and the relativistic correction. These latter properties, due to the contribution of the movement of protons. This study is made with the purpose of obtaining the breaking of energy degeneration, through the total Hamiltonian of the system.

3.1. Spin-orbit coupling

As an analogy, for the hydrogen atom, the spin-oribit coupling arises from the interaction between the electron's spin magnetic moment ($\hat{\mu}_{\mathbf{s_e}}=(e/m_ec)\hat{\mathbf{S}}$, where e is the electric charge, m_e is the electron mass and c is the speed of light) and the magnetic field produced by the proton ($\mathbf{B_p}$). It is well known that the Hamiltonian is,

$$\hat{H}^e_{SO}=-\frac{1}{2m_e^2c^2}\frac{1}{r}\frac{d\hat{V}}{dr}\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}. \quad (13)$$

The magnetic moment of the protons is $\hat{\mu}_{\mathbf{s_p}}=-g(e/2m_pc)\hat{\mathbf{S}}$, where $g\sim 5.585$ [20] is the gyromangentic ratio and m_p is the proton mass. Then, the Hamiltonian associated to the proton's spin-orbit is giving by

$$\hat{H}_{SO}=-\frac{ge}{2m_p^2c}\frac{1}{r}\frac{dV}{dr}\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}. \quad (14)$$

As it is mentioned, for this water molecule model, the distance of the protons with the oxygen doubly charged negative, as well as the distance between the protons are constant, then $dV/dr=0$ and therefore $\hat{H}_{SO}=0$, *i.e.*, there is no spin-orbit coupling contribution for this water molecule model.

3.2. Relativistic correction

The kinetic energy of one proton can be approximated as:

$$\hat{T}_i=\sqrt{\hat{p}_i^2c^2+m_p^2c^4}\approx\frac{\hat{p}_i^2}{2m_p}-\frac{\hat{p}_i^4}{8m_p^3c^2}+\cdots \quad (15)$$

where $\hat{p}_i=-i\hbar\nabla_i$ is the momentum of the proton i. In spherical coordinates

$$\nabla_i^2=\frac{1}{r_i}\frac{\partial^2}{\partial r_i^2}r-\frac{1}{\hbar^2r_i^2}\hat{L}_i^2, \quad (16)$$

where,

$$\hat{L}_i^2=-\hbar^2\left[\frac{1}{\sin\theta_i}\frac{\partial}{\partial\theta_i}\left(\sin\theta_i\frac{\partial}{\partial\theta_i}\right)+\frac{1}{\sin^2\theta_i}\frac{\partial^2}{\partial\phi_i^2}\right], \quad (17)$$

is the orbital angular momentum operator of the proton i. Once again, for this model, the r_i-coordinate is constant ($r_i=d_o$), then, the momentum is purely orbital angular momentum: $\nabla^2=-(1/\hbar^2d_o^2)\hat{L}_i^2$.

The Hamiltonian is the sum of the kinetic and potential operators ($\hat{H}_i=\hat{T}_i+\hat{V}_i$), then, tacking until the second term from Eq. (15), it is obtained,

$$\hat{H}_i=\frac{\hat{p}_i^2}{2m_p}-\frac{\hat{p}_i^4}{8m_p^3c^2}+\hat{V}_i, \quad (18)$$

where, it is defined $\hat{V}_i=(e^2/2d_p)-(e^2/d_o)$. The total potential of the system is $\hat{V}=\hat{V}_1+\hat{V}_2=(e^2/d_p)-(2e^2/d_o)$, whereby Eq. (18) can be written as:

$$\hat{H}_i=\hat{H}_{0_i}-\frac{\hat{p}_i^4}{8m_p^3c^2}=\hat{H}_{0_i}+\hat{H}_{R_i}, \quad (19)$$

where,

$$\hat{H}_{0_i}=\frac{\hat{p}_i^2}{2m_p}+\hat{V}_i, \quad (20)$$

is the Hamiltonian without the magnetic field and the relativistic Hamiltonian is giving by

$$\hat{H}_{R_i}=-\frac{\hat{p}_i^4}{8m_p^3c^2}, \quad (21)$$

$\hat{p}_i^4$ can be expressed in terms of $\hat{H}_{0_i}$ and $\hat{V}_i$ using Eq. (20), obtaining

$$\hat{p}_i^4=4m_p^2[\hat{H}_{0_i}^2-2\hat{V}_i\hat{H}_{0_i}+\hat{V}_i^2]. \quad (22)$$

The energy values of $\hat{H}_{R_i}$ can be obtained to calculate the expectation value:

$$E_{R_i}=<\hat{H}_{R_i}>=-\frac{1}{8m_p^3c^2}<\hat{p}_i^4>. \quad (23)$$

The expectation value of $\hat{p}_i^4$ can be obtained using Eq. (22), then, we obtain the relativistic energy:

$$\begin{aligned} E_{R_i}&=-\frac{1}{8m_p^3c^2}<\hat{p}_i^4> \\ &=-\frac{1}{2m_pc^2}[E_{0_i}{}^2-2V_iE_{0_i}+V_i^2], \end{aligned} \quad (24)$$

where E_{0_i} is the energy without magnetic field (see Sec. 3.2 of [19]):

$$E_{0_i} = \frac{\hbar^2}{2m_p d_0^2} l_i(l_i+1) + V_i. \tag{25}$$

The energy of water molecule is $E_0 = E_{0_1} + E_{0_2}$. Finally, the total relativistic energy is

$$E_R = E_{R_1} + E_{R_2} = -\frac{1}{2m_p c^2}\Big[E_{0_1}^2 + E_{0_2}^2 - 2V_1E_{0_1} - 2V_2E_{0_2} + V_1^2 + V_2^2\Big]. \tag{26}$$

It is simple to note, that the degeneration still persists in m_1 and m_2. The contribution of the relativistic correction is considered a perturbation because it is of the order of 10^{-14} eV.

3.3. The fine structure of water molecule

The fine structure is obtained by adding the spin-orbit and the relativistic correction. As it is shown, there is no contribution of the spin-orbit correction, then, the fine structure is the relativistic correction giving by Eq. (26). It is simple to note, that the energy is degenerate.

3.4. Interaction of the proton's spin with a constant external magnetic field

The interaction of the orbital angular momentum ($\hat{\mu}_{\mathbf{L}} = -[e/2m_pc]\hat{\mathbf{L}}$) and spin angular momentum ($\hat{\mu}_{\mathbf{s_p}}$) with the magnetic field is giving by the Hamiltonian:

$$\hat{H}_{LSB} = -\frac{e}{2m_pc}[\hat{\mathbf{L}} + g\hat{\mathbf{S}}]\cdot\mathbf{B}. \tag{27}$$

For simplicity, it is considered $\mathbf{B} = B\hat{\mathbf{z}}$. Then, the hamiltonian for the water molecule placed in a constant magnetic field is:

$$\hat{H}_{LSB} = -\frac{eB}{2m_pc}[\hat{L}_{1_z} + \hat{L}_{2_z} + g(\hat{S}_{1_z} + \hat{S}_{2_z})]. \tag{28}$$

Therefore, the total Hamiltonian is giving by

$$\hat{H} = \hat{H}_0 + \hat{H}_R + \hat{H}_{LSB}. \tag{29}$$

The total energy is obtained by the expectation value of Eq. (29). E_0 and E_R are already known. Due to the lower order of magnitude of E_R, it is not considered its numerical value for Eq (29). $E_{LSB} =< \hat{H}_{LSB} >$ is obtained from Eq. (28). Then, the energy E_{LSB} is giving by,

$$E_{LSB} = -\frac{eB\hbar}{2m_pc}\Big[m_{l_1} + m_{l_2} + m_{s_1}g + m_{s_2}g\Big], \tag{30}$$

$m_{s_i} = \pm(1/2)$ and $m_{l_i} = -l_i, -l_i+1, ..., l_i-1, l_i$.

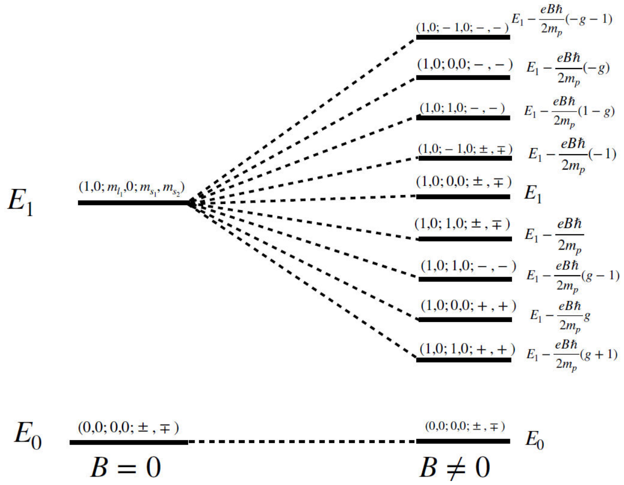

FIGURE 1. Left: Case $B = 0$. The first states are degenerated for the quantum numbers m_{l_2}, m_{s_1} and m_{s_2}. Right: Case $B \neq 0$, the degeneracy is lifted for all quantum numbers. The $\pm$ and $\mp$ indicates a spin exchange.

TABLE I. Energy levels for the ground and first excited state of the protons in the water molecule in presence of a magnetic field of $7\,T$.

State	$(l_1, l_2; m_1, m_2, s_1, s_2)$	Energy (eV)
Ground	(0,0;0,0;±,∓)	-23.4
First	$(1,0;-1,0;-,-)$	-23.3977255
	$(1,0;0,0;-,-)$	-23.3977257
	$(1,0;1,0;-,-)$	-23.3977259
	$(1,0;-1,0;\pm,\mp)$	-23.3977267
	$(1,0;0,0;\pm,\mp)$	-23.3977270
	$(1,0;1,0,\pm,\mp)$	-23.3977272
	$(1,0;1,0;-,-)$	-23.3977280
	$(1,0;0,0;+,+)$	-23.3977282
	$(1,0;1,0;+,+)$	-23.3977284

It is used the notation (l_1, l_2; m_1, m_2; m_{s_1}, m_{s_2}) to represent the state of the system Eq. (6). m_{s_1} and m_{s_2} take the symbols $+$ and $-$, representing, $+1/2$ and $-1/2$, respectively. The ground state is giving by $(0,0;0,0;+,-)$, this state corresponds to E_0, as it was shown in Subsec. 2.1. In Eq. (7), the two states are orthogonal, however, they are actually representing an exchange of their spin and they are associated with the same energy. The first excited state is given by (1, 0; m_1, 0; m_{s_1}, m_{s_2}). Nine different energy values were obtained for the lifted of E_1. In Fig. 1, it is shown the lifted of E_1.

To obtain numerical values, it is used the expectation value of Eq. (29) and it is considered $B = 7$ T, to be able to compare this results with the previous in Ref. [19]. In Table I are shown the lifted values of the energy E_1. It is simple to note that the first exited state is for $(1,0;1,0;+,+)$, the second excited state occurs for $(1,0;1,0;+,+)$ and so on.

4. Discussion and conclusions

Modeling the water molecule is very important to be able to describe physical phenomena. Depending on the physical phenomenon, the model used is chosen. For the case of physics in MRI, the protons of the hydrogen atoms in the water molecules are essential. In this work, it was used a model commonly known, but never described by a wave function, which consists on three particles: the two protons from the two hydrogen atoms and the oxygen doubly charged and unstructured. Due to the electrostatic interaction, the distance between these particles is constant, the spatial wave function and the energy was obtained in a previous work [19], where the important particles in this model are the protons of the hydrogen atoms in the water molecule. For the purpose of application to MRI.

The present work is a completion of a previous work [19], where the spin of the protons is now considered. The results could be obtained analitically. Using angular momentum algebra, it was possible to obtain the total wave function, which corresponds to the total angular momentum. As an example, it was calculated the ground and first excited sate of the water molecule. The fine structure of the water molecule model, only depends on the relativistic correction and the energy is still degenerate. The degeneracy is broken when the water molecule is placed in a constant magnetic field, *i.e.*, each state corresponds to a unique energy, given by the expectation value of Eq. (29).

Two applications of this water model can be in the radiolysis of water to obtain the hydroxil molecule (OH^-) [21], which occurs when the water molecule lost a proton from the hydrogen atom. Then, this water model can be used to calculate the differential and total crossection ($d\sigma/d\Omega$ and σ, respectively) to this ionization, because it can easly remove one of the protons to consider the OH^- molecule. It can also be used to calculate $d\sigma/d\Omega$ and σ for elastic collision and some excited sate, all these functions can be obtained when calculing the scattering amplitude. For the ground state, the energy is not degenerated, as it is shown in Table I and it has a value of -23.4 eV. *i.e.* to ionize the water molecule and leave it without a proton, an energy of 23.4 eV is required. On the other hand, to know the ionization of the water molecule having lost an electron, other model is needed and in this case the energy value is around 12.6 eV [22, 23]. It is clear then that depending of the phenomenon, a different model is needed.

Another important application is the MRI, which consists in the interaction of a magnetic field with the spin of the protons of the hydrogen atoms that make up the water molecule. The spins are oriented in parallel or antiparallel to the direction of the magnetic field. Then, a RF is turned on from the RFC and the spin of the protons change the orientation: parallel becomes anti-parallel and vice versa, having an excited state of spin. When the RF turned off, the original orientation of the spins is recovered. In this transition a RF is emitted from the protons, which is detected by the RFC [17]. As a first approximation, it can be considered that the magnetic field is constant, then, each water molecule that makes up an organism, was considered placed in a constant magnetic field, therefore, the results of this work can be applied. To obtain numerical values, it was used $B = 7$ T, where clearly the energy degeneracy breaks, as it was proposed in Ref. [19], *i.e.*, for each state corresponds to a unique energy. The varition between one energy state and another is in the range of RF, as can be calculated from Table I. Thus, it is proposed the hypothesis that the RFC from the MRI device, can be programed to detect the corresponding RF from the excited states of the water molecule and therefore it will have a sharper image when carring out the MRI study, as it allows for the differentiation of the energy emission state of each water molecule within the organism. A future work is considering a variation of these results, with the obtained to consider the gradient magnetic field and consider the RF to obtain the new energy of the system.

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