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AN INVESTIGATION OF MOLECULAR SPECTROSCOPY WITH GEOMETRIC ALGEBRA

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ABSTRACT

In this study Geometric Algebra was used to create a general and practical method for obtaining the operators of the kinetic energy of the molecular vibration-rotation of polyatomic molecules. On the other hand, these polyatomic molecules' precise intrinsic kinetic energy operators include a metric tensor. The elements of this metric tensor were expressed as the mass-weighted sum of measuring vector inner product vectors compatible with the molecule's nucleus. Whereas, the vibrational and rotational measuring vectors that appear in the metric tensor for any geometrically defined coordinates of the shape and frames of the body were easily determined using geometric algebra. The current method (geometric algebra) generates molecular vibration-rotation kinetic energy operators that are in perfect agreement with earlier studies.
Finally, we have used the Lagrangian Formulation where the component of kinetic energy was expressed in the form of generalized velocities.Using geometric products, we discovered the relation between the covariant metric tensor and the contravariant metric tensor.

Keywords: Geometric Algebra, Operator of the kinetic energy, covariant metric tensor, Rotational measuring vectors, Vibrational measuring vectors

1. INTRODUCTION

Algebra is the branch of mathematics that deals with general statements of relations, utilizing letters and other symbols to represent specific sets of numbers, values, vectors, etc., in the description of such relations. There are basic rules by which an expression can be algebraic. These basic rules are

$a(b+c) = ab + ac$	Distributive property
$a(b+c) = (b+c)$	Commutative property
$a(bc) = b(ac) = c(ab)$	Combination property
$a + 0 = a, \quad a \cdot 1 = a$	Identity property
$a + (-a) = 0, \quad a \cdot 1a = 1$	Inverse property

Where a, b and c are arbitrary numbers.
Geometric algebra is a numerical technique that simplifies the description of geometric concepts and procedures [1]. Geometric algebra also called "Clifford algebra" and sometimes called "hyper complex numbers" to describe a generalization of the complex number and the quaternions, was first introduced by William Kingdon Clifford in 1878, in his article "Grasman's Application of Extended Algebra" in the American Journal of Pure and Applied Mathematics [2].

Clifford was much more affected by Grassmann's research and utilized it as a starting point for establishing geometric algebra and combining external and internal products into a distinct engineering product, a new product form [3].

Geometric algebra is also an algebra because it provides the basic rules for algebra. Geometric algebra makes simple definitions with some special rules used for the product of vectors. It is an algebra that extends real number systems and is an ideal language for physics, often used in mathematical physics. Clifford Algebra contains the elements of area and volume, thanks to the basic elements it contains.

The expression of geometric algebra,

$$\vec{a}\,\vec{b} = \vec{a}\cdot\vec{b} + \vec{a}\wedge\vec{b} \tag{1}$$

Here $\vec{a}\cdot\vec{b}$ is the dot product and is a scalar expression. The expression $\vec{a}\wedge\vec{b}$ is the outer product. The outer product expression is denoted by the wedge sign " ∧ ". The outer product is neither a scalar nor a vector. It is a new element called the bivectors.

Clifford Algebra has three orthogonal unit base vectors $\hat{e}_1, \hat{e}_2, \hat{e}_3$. Since these unit basis vectors are perpendicular to each other, ${\hat{e}_1}^2 = {\hat{e}_2}^2 = {\hat{e}_3}^2 = 1$.

The oriented plane area of the square with sides e_1 and e_2 is expressed by the product e_1e_2, that is a new type of quantity known as a bivector. As shown in figure 1. Write for short $e_{12} = e_1e_2$.

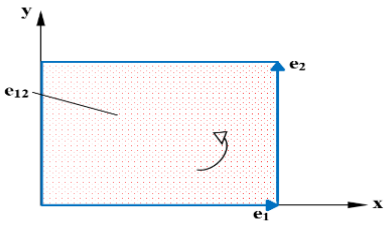


Figure 1. Express the Bivectors

1.1. Relations and Geometric Transformations

In geometrical algebra, every geometric point being expressed as a vector, and each geometric parameter may be explained in terms of its exceptional qualities without the need of any external coordinate frames. Any vector $\vec{s}$, for instance, may be divided into parallel and orthogonal components. Figure 2. Depicts the computation of the component of $\vec{s}$ in the direction of $\vec{r}$ when the two vectors form an angle of $0 < \theta < 180$ degrees.

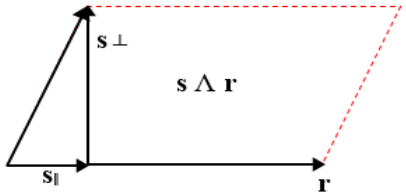


Figure 2. Decomposition of $\vec{s}$ vector to components along and perpendicular to a vector $\vec{r}$

The parallel variable is the scalar multiple of the unit vector $\frac{r}{|r|}$.

$$s_{\parallel} = |s|\cos\theta\frac{r}{|r|} = |s||r|\cos\theta\frac{r}{|r|^2} \tag{2}$$

In other words, the parallel component $s_{\parallel}$ is the scalar product $s\cdot r = |s||r|\cos\theta$ multiplied by the vector $r^{-1} = \frac{r}{|r|^2}$, also known as the vector $\vec{r}$ inverse. As a result

$$s_{\parallel} = (s\cdot r)\frac{r}{|r|^2} = (s\cdot r)\,r^{-1} \tag{3}$$

The perpendicular component $s_{\perp}$ is defined as the difference

$$s_{\perp} = s - s_{\parallel} = s - (s\cdot r)\,r^{-1} = (sr - s\cdot r)\,r^{-1} = (s\wedge r)\,r^{-1} \tag{4}$$

The reflection of s across the line u as shown in figure 3(a). Is acquired by sending $s = s_{\parallel} + s_{\perp}$ to $s' = s_{\parallel} - s_{\perp}$ where $s_{\parallel} = (s\cdot u)u^{-1}$. The mirror image u′of u for s is then

$$s' = usu^{-1} \tag{5}$$

We may represent the dot and outer products in Eq (2) in regards of the angle between both the vectors θ.

$$\vec{s}\cdot\vec{r} = \frac{1}{2}(\vec{s}\,\vec{r} + \vec{r}\,\vec{s}) = |\vec{s}|\,|\vec{r}\,|\cos\theta \tag{6}$$

$$\vec{s} \wedge \vec{r} = \frac{1}{2}(\vec{s}\vec{r} - \vec{r}\vec{s}) = i|\vec{s}|\,|\vec{r}|\sin\theta \tag{7}$$

Eqs. (6) and (7) how to construct the geometric product of unit vectors, which results in a useful formula for rotating a vector in a plane. If the unit bivector for the longitudinal plane the unit vectors $\vec{s}$ and $\vec{r}$ is i then the geometric product is represented as [4]

$$\vec{s}\vec{r} = \cos\theta + i\sin\theta = e^{i\theta} \tag{8}$$

The $e^{i\theta}$ exponential, commonly known as a two-dimensional rotor.
As seen in figure 3(b), multiplying a vector s by the rotor produces a new vector s', which is the old vector rotated in the i plane by the angle θ.

$$s' = s\,e^{i\theta} = s\cos\theta + si\sin\theta \tag{9}$$

Since the unit bivector i ant commutes with every vector s in the e_1e_2 plane, the rotated vector can also be expressed as:

$$s\cos\theta + si\sin\theta = s\cos\theta - is\sin\theta = e^{-i\theta}s \tag{10}$$

Furthermore, we have

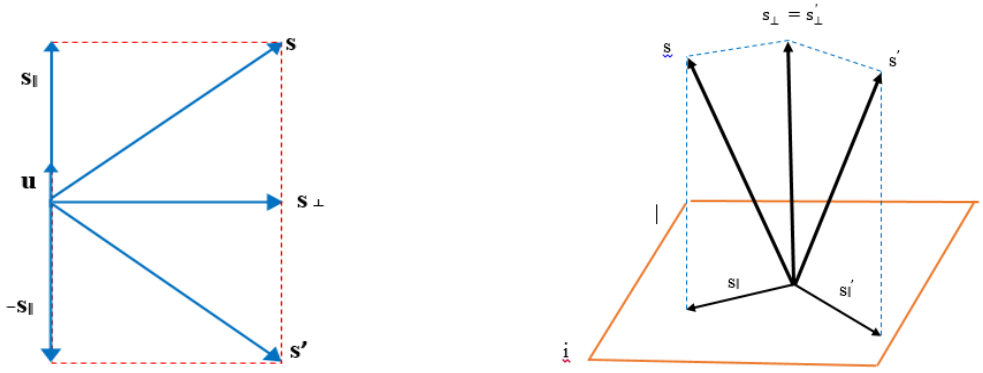
$$\cos\theta + i\sin\theta = (\cos\frac{\theta}{2} + i\sin\frac{\theta}{2})^2 \tag{11}$$

And the rotated vector also has the form y^{-1} as where

$$y = e^{i\theta/2} \quad \text{And} \quad y^{-1} = e^{-i\theta/2} \tag{12}$$

The same Eq (8) applies to the rotation of any Multivector B (a vector, a bivector, etc., or any combination thereof).
If Multivector B rotates across a bivector angle φ , then B' is obtained by sandwiching the multivector B between rotation plane exponentials.

$$B' = e^{-i\varphi/2}\,B\;e^{i\varphi/2} \tag{13}$$



(**a**) (**b**)

Figure 3. (a) Reflection of s along u ;(b) Rotation of vector s in the plane i

1.2. Internal Coordinate Gradients

In geometric algebra, the gradients $\nabla_\beta q_i$ are the vector derivatives of the coordinate q_i with respect to the spatial position vector x_β , that is

$$\nabla_\beta q_i = \partial_{x_\beta} q_i \tag{14}$$

The vector derivative operator ∇_β is expressed in some coordinates using the chain rule as

$$\nabla_\beta = \sum_i (\nabla_\beta q_i)\frac{\partial}{\partial q_i} \tag{15}$$

Where we utilize the subscript β in the vector round as to underline that these conclusions apply to several vector elements $x_1, x_2, \dots$.
Much of the calculations for gradients resemble those of the usual scalar calculus. For example, If F and G are vectors, the vector differentiation is distributive

$$\nabla_\beta(F + G) = \nabla_\beta F + \nabla_\beta G \tag{16}$$

Furthermore, if $\gamma = \gamma(x_\beta)$ seems to be a scalar-valued function, therefore

$$\nabla_\beta(\gamma G) = (\nabla_\beta \gamma)G + \gamma \nabla_\beta G \tag{17}$$

If $F = f(x_\beta)$, the definitions of its divergence and curl are as follows

$$div_\beta f = \nabla_\beta \cdot f \tag{18}$$

By using geometric product definition we can write

$$\nabla_\beta f = \nabla_\beta \cdot f + \nabla_\beta \wedge f = \nabla_\beta \cdot f + i\nabla_\beta \times f \tag{19}$$

As a result, the scalar component of the Eq (19) is the divergence, and the other component is the curl. Because the last form is restricted to three dimensions, it is better to conceive of the curl as the bivectors element of the vector derivative. [5].
In general, the vector derivative $\nabla_\beta F$, F is constructed for all elements F, not only vectors and scalars

$$\nabla_\beta F = \nabla_\beta \cdot F + \nabla_\beta \wedge F \tag{20}$$

Eqs (16) and (17) provide distributive vector differentiation but, in practice, the operator of the vector derivative doesn't quite actually commute with Multivector, so the product rule should be phrased as

$$\nabla_\beta(FG) = \dot{\nabla_\beta}\dot{F}\, G + \dot{\nabla_\beta} F\, \dot{G} \tag{21}$$

2. THE SCHRODINGER EQUATION FOR MOLECULES

Materials are composed of atoms, which also are composed of electrons and nuclei. To the highest extent imaginable, the wave function which represents molecule with N nuclei and P electrons characterizes the molecule's status. When studying the interior motions of molecules, we must consider the movements of a substantial amount of charged particles related to each other. All molecular characteristics, such as energy state and molecular geometry, may potentially be determined using the wave function that exists in the Schrodinger equation.

$$(\hat{\mathrm{T}} + \hat{\mathrm{V}})\Psi = \mathrm{E}\Psi \tag{22}$$

Where $\hat{\mathrm{T}}$ is the operator of the kinetic energy, $\hat{\mathrm{V}}$ is the operator of the potential energy, Ψ is the wave function and E is the energy.

When the Schrodinger equation is solved, many wavefunctions Ψn and their related energies E_n are obtained, which adequately characterize the movements of the constituent particles of the molecule. Every E_n is an energy amount which the molecule can still have, also known as a level of energy that the molecule may hold [1].
If the required boundary conditions are considered. The operator of the kinetic energy $\hat{\mathrm{T}}$ and the operator of the potential energy $\hat{\mathrm{V}}$ both are affected by the locations of electron$\mathrm{X}_{\mathrm{N}+1}, \mathrm{X}_{\mathrm{N}+2}, \dots, \mathrm{X}_{\mathrm{N}+\mathrm{P}}$ s as well as the locations of nuclei $\mathrm{X}_1, \mathrm{X}_2, \dots, \mathrm{X}_\mathrm{N}$.
If electrons and nuclei are represented as points charges and relativity influences and spin are ignored, the operator of the potential energy and the operator of the kinetic energy can be represented as

$$\hat{\mathrm{T}} = -\frac{h^2}{8\pi^2}\sum_{\beta=1}^{\mathrm{N}+\mathrm{P}}\frac{\nabla_\beta^2}{m_\beta} \tag{23}$$

$$\hat{\mathrm{V}} = \frac{e^2}{8\pi\epsilon_o}\sum_{\beta}^{\mathrm{N}+\mathrm{P}}\sum_{\beta\neq\alpha}^{\mathrm{N}+\mathrm{P}}\frac{\mathrm{Z}_\beta\,\mathrm{Z}_\alpha}{|\mathrm{X}_\beta - \mathrm{X}_\alpha|} \tag{24}$$

Where ∇_β denotes to the vector derivative operator with respect to the position X_β, h represents Planck constant, m_β is the mass of the particle β, e is the unit charge $(e = 1.6019 \times 10^{-19}\mathrm{C})$, Z_β is the charge number of the particle β(it is -1 for an electron) and $(\epsilon_o = 8.854 \times 10^{-12}\mathcal{T}^{-1}C^2m^{-1})$ is the vacuum permittivity.

2.1. Approximation of Born-Oppenheimer

Analytical solutions to the Schrodinger equation exist just for two-body systems such as that of the hydrogen atom, and it is complicated to solve it analytically for molecules containing more than two particles; nevertheless, some assumptions must have been made in order to identify approximate solutions.The Born-Oppenheimer approximation is one of these simplifications.

The effect, the electrons' motion can be interpreted as if the nuclei were stationary in space, and the electronic Schrodinger equation can be solved separately for each value of the nuclear coordinates. That is, there is an approximate wavefunction that describes electron motions independently of a second wavefunction that describes nuclei motions.

The Schrodinger equation, which is dependent on both nuclei and electron coordinates, is written as

$$\left(\widehat{\mathrm{T}}_e + \widehat{\mathrm{V}}_e\right)\Psi_e + \left(\widehat{\mathrm{T}}_{nucl} + \widehat{\mathrm{V}}_{nucl}\right)\Psi_{nucl} = \mathrm{E}_e\Psi_e + \mathrm{E}_{nucl}\Psi_{nucl} \tag{25}$$

The mathematical analysis of nuclear movements is simplified through separating nuclear movements into vibrational, rotational, and translational modes.We may get the translational, vibrational, and rotational modes and energies of the molecule under inquiry by resolving the Schrodinger [1].

$$\left(\widehat{\mathrm{T}}_{nucl} + \widehat{\mathrm{V}}_{nucl}\right)\Psi_{nucl} = \mathrm{E}_{nucl}\Psi_{nucl} \tag{26}$$

2.2. The Representation of Coordinates

Each atom in a group of N atoms that are just not related to each other can move around freely in three dimensions. To characterize their movement, $3N$ coordinates are essential .To describe the molecule's shape, a system of $3N - 6$ translationally and rotationally invariant internal coordinates q_i is utilized. Three translationally invariant angles of Euler χ, θ, ϕ, may be utilized to determine the rotation of the entire molecule.The angles of the Euler have been used to connect the orientations of many an orthonormal fixed axis system of molecule $\{\upsilon_1', \upsilon_2', \upsilon_3'\}$ to a normal orthonormal space-fixed frame $\{\upsilon_1, \upsilon_2, \upsilon_3\}$.

$$\upsilon_i' = R^\dagger \upsilon_i R \tag{27}$$

Where R is the rotor that was described by

$$R = e^{i\chi\upsilon_3/2}e^{i\theta\upsilon_1/2}e^{i\phi\upsilon_3/2} = e^{i\chi\upsilon_3'/2}e^{i\theta\upsilon_1'/2}e^{i\phi\upsilon_3'/2} = e^{i\phi\upsilon_3/2}e^{i\theta n_2/2}e^{i\chi\upsilon_3'/2} \tag{28}$$

When n_2 is determined by the formula

$$n_2 = \frac{\upsilon_3 \times \upsilon_3'}{|\upsilon_3 \times \upsilon_3'|} \tag{29}$$

The position of the molecule may be parametrized using three Cartesian coordinates. The location of the molecule can be parametrized by three Cartesian coordinates

$$\boldsymbol{X} = \sum_{\beta=1}^{N} \frac{m_\beta X_\beta}{M} \tag{30}$$

From Eq (30), M is the molecule's mass, and it's written as

$$\mathrm{M} = \sum_{\beta}^{\mathrm{N}} m_\beta \tag{31}$$

The chain rule describes the vector derivative operator ∇_β as

$$\nabla_\beta = \sum_{i}^{3\mathrm{N}} e_\beta^{(q_i)} \frac{\partial}{\partial q_i} \tag{32}$$

From Eq (32), q_i denotes the internal coordinates, which are understood that

$$q_{3N-5} = \phi, \qquad q_{3N-4} = \theta, \qquad q_{3N-3} = \chi$$

$$q_{3N-2} = X_1, \quad q_{3N-1} = X_2\,, \quad q_{3N} = X_3 \tag{33}$$

$e_\beta^{(q_i)}$ is the measurement vector that corresponds to the nucleus β and coordinates $q_i$of the molecule.

$$e_\beta^{(q_i)} = \nabla_\beta q_i \tag{34}$$

The term "measuring vector" $e_\beta^{(q_i)}$comes from the fact that the vector takes the measure of the rate of change in the coordinate $q_i(\mathrm{X}_\beta)$ for any given rate of change $\frac{d\mathrm{X}_\beta}{dt}$ of the nuclear position X_β as [6]

$$\frac{dq_i}{dt} = \sum_\beta^N e_\beta^{(q_i)} \cdot \frac{dX_\beta}{dt} \tag{35}$$

By geometric algebra, internal coordinates may be discussed in terms of nucleus position vectors. Their gradients can then be obtained with algebraic expressions by modifying the atomic position vectors. After that, we'll utilize this knowledge to characterize the operator of the kinetic energy of a polyatomic molecule.

Each fixed location vector for body can be rotated to the fixed location vector for space as seen from Eq (28) ,if we have a fixed location vector for body s'_β is rotated to the fixed location vector for space $s_\beta = \mathrm{X}_\beta - \mathbf{X}$ by

$$s_\beta = R^\dagger s'_\beta R \tag{36}$$

Where R is the rotor that is influenced by the axes of body.
Each option of the body's axes provides a reference orientation in which the body's axes coincide with the fixed frame of space. The change of the molecule orientation for a given shape is equivalent to the change in the orientation of the body's axis, but it is independent of any specific option of body frame. But, if the molecule is deformed (that is if the shape in the initial and final is changed), the rotation of the molecule would be determined by the choice of the body's axis [7].

3. OPERATORS FOR KINETIC ENERGY IN POLYATOMIC MOLECULES IN TERMS OF GEOMETRIC ALGEBRA

We used geometric algebra to obtain a representation of the operator of the kinetic energy for an atomic molecule N, at least in principle, by directly expressing the operator of a gradient in terms of generalized coordinates or by components of operators of the quasi momentum such as the operator of the angular moment .

For an atomic molecule N the expression of the operator of the kinetic energy

$$\hat{\mathrm{T}}^{(nucl)} = -\frac{h^2}{8\pi^2}\sum_\beta^{\mathrm{N}} \frac{1}{m_\beta}\nabla_\beta^2 \tag{37}$$

Where m_β is the mass of the atom β. the operator of kinetic energy reads as

$$\hat{\mathrm{T}} = -\frac{h^2}{8\pi^2}\sum_\beta^{\mathrm{N}}\sum_j^{3\mathrm{N}} \frac{1}{m_\beta}\nabla_\beta \cdot e_\beta^{(q_j)}\frac{\partial}{\partial q_j} \tag{38}$$

The Eq (38) may be written in a number of different ways, one of which is a ” contravariant metric tensor $g^{(q_iq_j)}$” such that the $g^{(q_iq_j)}$ is giving in the form

$$g^{(q_iq_j)} = \sum_\beta^{\mathrm{N}} \frac{1}{m_\beta} e_\beta^{q_j} \cdot e_\beta^{q_i} \tag{39}$$

The official results of the classical tensor analysis show that [22]

$$\sum_{\beta}^{\mathrm{N}} \frac{1}{m_\beta} \nabla_\beta \cdot e_\beta^{(q_j)} \frac{\partial}{\partial q_j} = \frac{1}{z^{-1/2}} \sum_i \frac{\partial}{\partial q_i} z^{-1/2} g^{(q_i q_j)} \frac{\partial}{\partial q_j} \tag{40}$$

Where $z = det\ g^{(q_i q_j)}$ is the contravariant metric tensor determinant.The operator of the kinetic energy is as follows

$$\hat{\mathrm{T}}^{(nucl)} = -\frac{h^2}{8\pi^2} \sum_{ij}^{3\mathrm{N}} \left(\frac{\partial}{\partial q_i} + \frac{1}{z^{-1/2}} \frac{\partial z^{-1/2}}{\partial q_i} \right) g^{(q_i q_j)} \frac{\partial}{\partial q_j} \tag{41}$$

To be more specific, it is assumed that all integrations are done over the volume-element $d\tau = Jdq_1 dq_2$ ..., where $J = \left| det\ g^{(q_i q_j)} \right|^{-1/2} = z^{-1/2}$, where J is called Jacobian.
If the volume element $d\tau_k = kdq_1 dq_2$ ..., is used instead of the volume element $d\tau = Jdq_1 dq_2$ ..., the corresponding operator of kinetic energy $\hat{T}_k$ is provided as [8].

$$\hat{T}_k^{(nucl)} = J^{1/2} k^{-1/2} \hat{T}^{(nucl)} k^{1/2} J^{-1/2} \tag{42}$$

The vibrational and rotational degrees of freedom are completely isolated from translation.
If we have the matrix $[\omega]$ with elements $[\omega]_{ij} = g^{(q_i q_j)}$as follows:

$$\begin{bmatrix} \omega^{(int)} & 0 \\ 0^T & \omega^{(tranl)} \end{bmatrix} \tag{43}$$

This Martic is split into a translational and internal block .
The measurement vectors for the coordinates of cartesian of the center of mass can be written as

$$e_\beta^{(\mathrm{X}_i)} = \nabla_\beta \mathrm{X}_i = \sum_{\alpha}^{\mathrm{N}} \nabla_\beta \frac{m_\alpha \upsilon_i \cdot \mathrm{X}_\alpha}{M} = \frac{m_\alpha}{M} \upsilon_i \tag{44}$$

The shape and rotational coordinates' translational invariance (abbreviated as $B_1 = \phi$, $B_2 = \theta$, and $B_3 = \chi$ for short),is

$$\sum_\beta \nabla_\beta q_i = 0 \quad \text{And} \quad \sum_\beta \nabla_\beta B_i = 0 \tag{45}$$

When Eqs (43), (44) and (45) are taken into account, The internal and translational parts can be combined to form the operator of the kinetic energy.

$$\widehat{\mathrm{T}}^{(nucl)} = \hat{\mathrm{T}}^{(int)} + \hat{\mathrm{T}}^{(transl)} \tag{46}$$

The internal part

$$\hat{\mathrm{T}}^{(int)} = -\frac{h^2}{8\pi^2} \sum_{ij}^{3\mathrm{N}-3} \left(\frac{\partial}{\partial q_i} + \frac{1}{z^{-1/2}} \frac{\partial z^{-1/2}}{\partial q_i} \right) g^{(q_i q_j)} \frac{\partial}{\partial q_j} \tag{47}$$

The translational part

$$\hat{\mathrm{T}}^{(transl)} = -\frac{h^2}{8\pi^2} \sum_{i=1}^{3} \frac{\partial^2}{\partial \mathrm{X}_i^2} \tag{48}$$

It is common to represent the rotational portion of each gradient operator in the forms of the components of the fixed body $\hat{\imath}_i = \upsilon_i' \cdot \hat{\mathrm{I}}$ of the angular momentum operator $\hat{\mathrm{I}}$, rather than the partial derivative operators $\frac{\partial}{\partial B_i}$,from the [9] we can see the relation

$$\left(\nabla_\beta \phi\right) \frac{\partial}{\partial \phi} + \left(\nabla_\beta \theta\right) \frac{\partial}{\partial \theta} + \left(\nabla_\beta \chi\right) \frac{\partial}{\partial \chi} = \sum_i^3 e_\beta^{(L_i)} \hat{\imath}_i \tag{49}$$

The measuring vectors $e_\beta^{(L_k)}$ are obtained as

$$e_\beta^{(L_k)} = \nabla_a \left[(a \cdot \nabla_\beta \upsilon_i') \cdot \upsilon_j' \right] \tag{50}$$

Where $e_{\beta}^{(L_k)}$related to the nucleus β and the kth part of the angular momentum operator $\hat{\mathrm{I}}$.The kinetic energy operator's internal component in Eq (47) can be written succinctly as

$$\hat{\mathrm{T}}^{(int)} = -\frac{h^2}{8\pi^2}\sum_{ij}^{3N-3}\hat{\Gamma}_i^{\dagger}\, g^{(q_i q_j)}\hat{\Gamma}_j \tag{51}$$

The $\hat{\Gamma}_j$ refers to component of the body-frame $\frac{\hat{\imath}_i}{\hbar}$ of the overall angular momentum operator for degrees of rotational freedom $(i = 1,2,3)$ and partial derivative operator for shape coordinates $\frac{\partial}{\partial q_{i-3}}$ for degrees of vibrational freedom $i = 4,5,\ldots 3N-3$.

The $\Gamma_i^{\dagger}$ is called "adjoint" and is the same as $\hat{\Gamma}_j$ for degrees of rotational freedom and it is $\frac{\partial}{\partial q_{i-3}} + z'^{\frac{1}{2}}\frac{\partial z'^{\frac{1}{2}}}{\partial q_{i-3}}$ for the shape coordinates $(i = 4,5,\ldots 3N-3)$, where $(z' = det\; g^{(ij)})$ is the determinant of the contravariant metric tensor [10].

The contravariant metric tensor $g^{(ij)}$ or $g^{(q_i q_j)}$ with elements of vibrational is

$$g^{(ij)} = \sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(q_{i-3})}\cdot e_{\beta}^{(q_{j-3})} \qquad \text{for } (i,j = 4,5,\ldots,3N-3) \tag{52a}$$

$$g^{(q_i q_j)} = \sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(q_i)}\cdot e_{\beta}^{(q_j)} = \sum_{\beta}^{N}\frac{1}{m_\beta}(\nabla_\beta q_i)\cdot(\nabla_\beta q_j) \quad \text{for } (i,j = 1,2,\ldots,3N-6) \tag{52b}$$

The contravariant metric tensor $g^{(ij)}$ or $g^{(L_j q_i)}$ with Elements of Coriolis are

$$g^{(\mathrm{ij})} = \sum_{\beta}^{\mathrm{N}}\frac{1}{\mathrm{m}_\beta}\mathrm{e}_{\beta}^{(q_{i-3})}\cdot \mathrm{e}_{\beta}^{(\mathrm{L_j})} \quad \text{for } (i = 4,5,\ldots,3N-3) \quad \text{and } j = (1,2,3) \tag{53a}$$

$$g^{(L_j q_i)} = \sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(L_j)}\cdot\nabla_\beta q_i \quad \text{for } (\mathrm{i} = 1,2,\ldots,3\mathrm{N}-6) \quad \text{and } j = (1,2,3) \tag{53b}$$

The contravariant metric tensor $g^{(ij)}$ or $g^{(L_i L_j)}$ with the elements of rotational is

$$g^{(ij)} = g^{(L_i L_j)} = \sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(L_i)}\cdot e_{\beta}^{(L_j)} \qquad \text{for } i,j = (1,2,3) \tag{54}$$

The Euler angles' gradients are applied to the measurement vectors of rotational $e_{\beta}^{(L_i)}$as follows:

$$\nabla_\beta B_j = e_{\beta}^{(B_j)} = \sum_{i=1}^{3} e_{\beta}^{(L_i)}\, A_{ij}^{-1} \tag{55}$$

A_{ij}^{-1} is the element of the matrix's inverse as $\mathrm{A}_{ij}^{-1} = [\mathrm{A}]_{ij}^{-1}$, that's the matrix is $[\mathrm{A}]_{ij} = n_i\cdot\upsilon_j'$, n_i is the vectors of nodal lines ($\mathrm{n}_1 = \upsilon_3, \mathrm{n}_2 = \frac{\upsilon_3\times\upsilon_3'}{|\upsilon_3\times\upsilon_3'|} = \frac{\upsilon_3\times\upsilon_3'}{\sin\theta}$ and $\mathrm{n}_3 = \upsilon_3'$).

The matrix [A] is

$$[A] = \begin{bmatrix} sin\,\theta\, sin\,\chi & sin\,\theta\, cos\,\chi & cos\,\theta \\ cos\,\chi & -sin\,\chi & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{56a}$$

The inverse of the matrix $[\mathrm{A}]^{-1}$ is

$$[A]^{-1} = \begin{bmatrix} \frac{sin\,\chi}{sin\,\theta} & cos\,\chi & -\frac{cos\,\theta\, sin\,\chi}{sin\,\theta} \\ \frac{cos\,\chi}{sin\,\theta} & -sin\,\chi & -\frac{cos\,\theta\, cos\,\chi}{sin\,\theta} \\ 0 & 0 & 1 \end{bmatrix} \tag{56b}$$

As a result, It is possible to write

$$g^{(B_j B_l)} = \sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(B_j)}\cdot e_{\beta}^{(B_l)} = \sum_{ik}^{3}\sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(L_i)}\cdot e_{\beta}^{(L_k)}\, A_{ij}^{-1}A_{kl}^{-1} = \sum_{ik}^{3} g^{(L_i L_k)}\, A_{ij}^{-1}A_{kl}^{-1} \tag{57}$$

$$g^{(B_j q_l)} = \sum_{\beta}^{N} \frac{1}{m_\beta} e_\beta^{(B_j)} \cdot e_\beta^{(q_l)} = \sum_{ik}^{3} \sum_{\beta}^{N} \frac{1}{m_\beta} e_\beta^{(L_i)} \cdot e_\beta^{(q_l)} A_{ij}^{-1} = \sum_{i}^{3} g^{(L_i q_l)} A_{ij}^{-1} \tag{58}$$

Where q_l is a coordinate for a shape.

Since the determinant of $[\mathrm{A}]^{-1}$is $det[A]^{-1} = \frac{-1}{sin\,\theta}$, the determinants of the two contravariant metric tensor $detg^{(q_i q_j)} = z$ and $detg^{(ij)} = z'$ are related as follows

$$z' = (\sin\theta)^2 z \tag{59}$$

(where q_{3N-5}, q_{3N-4}, and q_{3N-3} indicate to the Euler angles(ϕ , θ, χ) respectively, and q_{3N-2}, q_{3N-1}, and q_{3N} indicate to the center of mass coordinates $(\mathrm{X}_1, \mathrm{X}_2, \mathrm{X}_3)$ respectively).

4. LAGRANGIAN FORMULATION AND COVARIANT MEASURING VECTORS

The component of kinetic energy for the classical Lagrangian $\mathrm{L} = \mathrm{T} - \mathrm{V}$ is expressed in the form of generalized velocities $\dot{q_i}$, as for conservative systems (given to time-independent or no limitations at all) [11].

$$T = \frac{1}{2} \sum_{ij}^{k} \dot{q_i}\, g_{q_i q_j} \dot{q_i} \tag{60}$$

Where k is the number of active coordinates and $g_{q_i q_j}$ is the covariant metric tensor can be determined by

$$g_{q_i q_j} = \sum_{\beta}^{N} m_\beta e_{q_i}^{(\beta)} \cdot e_{q_j}^{(\beta)} \tag{61}$$

Where $e_{q_i}^{(\beta)}$ The covariant measuring vectors which can be determined by the following equation

$$e_{q_i}^{(\beta)} = \frac{\partial x_\beta}{\partial q_i} \tag{62}$$

It is essential to develop the ability to relate the characteristics of covariant measurement vectors to those of contravariant measurement vectors. In the following, we will only analyze the unconstrained state wherein the number of available coordinates is $k = 3N$.

First, if $t = q_j$ is used in equation (35), the result is

$$\frac{\partial q_i}{\partial q_j} = \sum_{\beta}^{\mathrm{N}} e_\beta^{(q_i)} \cdot \frac{\partial \mathrm{X}_\beta}{\partial q_j} = \sum_{\beta}^{N} \frac{\partial \mathrm{X}_\beta}{\partial q_j} \cdot \nabla_\beta q_i = \delta_{ij} \tag{63}$$

Where $\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$

As a result, the constraint between covariant and contravariant measurements vectors is determined as follow

$$\sum_{\beta}^{N} e_{q_i}^{(\beta)} \cdot e_\beta^{(q_j)} = \delta_{ij} \tag{64}$$

Second, by utilizing the representation of ∇_βin equation (33), it is demonstrated that

$$\nabla_\beta (\, A_{\bar{r}} \mathrm{X}_\alpha) = \delta_{\alpha\beta} \sum_{i}^{3\mathrm{N}} e_\beta^{(q_i)} A_{\bar{r}} \frac{\partial \mathrm{X}_\alpha}{\partial q_i} = \delta_{\alpha\beta} \sum_{i}^{3\mathrm{N}} e_\beta^{(q_i)} A_{\bar{r}} e_{q_i}^{(\alpha)} \tag{65}$$

Where $A_{\bar{r}}$ is an r-blade that isn't affected by X_α, with $r = 0, 1, 2, 3$. From the geometric product $(\, A_{\bar{r}} \mathrm{X}_\alpha)$ is give as

$$(\, A_{\bar{r}} \mathrm{X}_\alpha) = (-1)^{r+1} A_{\bar{r}} \cdot \mathrm{X}_\alpha + (-1)^r A_{\bar{r}} \wedge \mathrm{X}_\alpha \tag{66}$$

And

$$\nabla_\beta \mathrm{X}_\alpha \cdot A_{\bar{r}} = \delta_{\alpha\beta} r A_{\bar{r}} \tag{67}$$

$$\nabla_\beta \mathrm{X}_\alpha \wedge A_{\bar{r}} = \delta_{\alpha\beta}(3-r)A_{\bar{r}} \tag{68}$$

By substituting the equations (68), (69) into (66) , yeilds

$$\sum_{i}^{3\mathrm{N}} e_\beta^{(q_i)} A_{\bar{r}} e_{q_i}^{(\alpha)} = \delta_{\alpha\beta}(-1)^r(3-2r)A_{\bar{r}} \tag{69}$$

Where there are a number of special cases can be obtained from equation (68), by setting $A_{\bar{r}} = 1$ (so $r = 0$) the identity

$$\sum_{i}^{3\mathrm{N}} e_\beta^{(q_i)} e_{q_i}^{(\alpha)} = 3\delta_{\alpha\beta} \tag{70}$$

By changing the Eq (69) into a combination of inner and outer components

$$\sum_{i}^{3\mathrm{N}} e_\beta^{(q_i)} \cdot e_{q_i}^{(\alpha)} = 3\delta_{\alpha\beta} \tag{71}$$

$$\sum_{i}^{3\mathrm{N}} e_\beta^{(q_i)} \times e_{q_i}^{(\alpha)} = 0 \tag{72}$$

Moreover, if the inner products are explained by means of geometric products and Eq (70) is applied, it is easy to show that

$$\sum_{k}^{3N} g^{(q_i q_k)} g_{(q_k q_j)} = \delta_{ij} \tag{73}$$

Eq (73) is the relation between the covariant metric tensor and contravariant metric tensor by means of geometric products.

5. RESULTS AND CONCLUSIONS

Clifford's and many others' objective was to make geometric algebra helpful in many branches of science. Because the algebra applied may provide for unexpected solutions to some problems. In this regard, David Hestenes' efforts to make geometric algebra a science language beyond algebra in Physics should be mentioned.

This study demonstrates that a general and practical method for obtaining rotational measuring vectors $\left(e_\beta^{(L_k)}\right)$ using geometrical algebra has been developed, which gives its internal products with other rotational measuring vectors and with gradients coordinates for vibration, the operator of the kinetic energy of vibration and rotational of polyatomic particles.

The conclusions of this study will allow us to write the energy expressions of polyatomic molecules much more compactly using Clifford Algebra, which will simplify our computations.

Clifford's Algebra enables us to better grasp nature and its realities. We can harness the power of mathematics for physics by employing this algebra. While Clifford Algebra is useful in robotics and dynamical systems, we now know that it also holds true in the enigmatic world of quantum physics. Everything may be understood in terms of the movements of polyatomic molecules if operators exist. We can make sense of the outcomes of applying mathematics to physics by employing operators.

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