NaSTech JOURNAL OF NATURAL SCIENCES AND TECHNOLOGIES
2024, 3(2), pp. 327-336, DOI: 10.5281/zenodo.14543012

AN INVESTIGATION OF THE KINETIC ENERGY OPERATOR OF A POLYATOMIC MOLECULE WITH GEOMETRIC ALGEBRA

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ABSTRACT

Physics concepts require mathematical frameworks to be understood and supported as an algebraic expression. Mathematicians and physicists have introduced and explored a variety of algebras throughout history. One of these is Clifford Algebra, often known as geometric algebra.

This work developed a general and useful method for deriving the operators of the kinetic energy of polyatomic molecules using Geometric Algebra. The kinetic energy operator of a polyatomic molecule contains the vibrational and rotational kinetic energy operators.

The gradients of vibrational coordinates form the exact vibrational kinetic energy operator of a polyatomic molecule. The conventional methods utilized for obtaining these gradients can often be extremely laborious. However, the gradients for any vibrational coordinate can be readily computed using geometric algebraic techniques. These gradients are the measuring vectors. so, the components of the reciprocal metric tensor g_{ij} readily form that emerges in the exact internal kinetic energy operators of polyatomic molecules. On the other hand, Finding the measuring vectors for the rotational degrees of freedom is more difficult because the components of the total angular momentum operator are not conjugated to any rotational coordinates. Nonetheless, using geometric algebraic methods without any restrictions on the number of particles in the system, rotational measuring vectors for any geometrically defined body frame may be easily computed and this is what we show in this paper.

Keywords: Geometric Algebra, kinetic energy of polyatomic molecules, measuring vectors, vibrational kinetic energy operator, rotational kinetic energy operators.

1. INTRODUCTION

The purpose of the molecule's Hamiltonian operator must be to explore the molecular system's internal dynamics in some way. In practical application, the kinetic and potential energy operators can be expressed in certain coordinates [1]. If the Born-Oppenheimer approximation is valid, the potential energy operator can be easily generated. However, in addition to vibration, the internal motion of the molecule also includes rotation. This complicates theoretical explanations of the internal motion of the molecular system, even when employing rectilinear coordinates [2].

This work aims to investigate a simple algebraic way to obtain the operators of the kinetic energy of polyatomic molecules. These polyatomic molecules' precise intrinsic kinetic energy operators include a metric tensor. The measuring vector expresses the elements of this metric tensor. 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 will be determined using geometric algebra [3].

2. FUNDAMENTALS OF GEOMETRIC ALGEBRA

Today Physics is blended with different mathematical formalisms, each introduced to handle some specific problems. For example, the vector algebra developed by Gibbs, matrix algebra, and complex algebra [4].

These algebraic systems are combined into geometric algebra, which creates a cohesive mathematical language with the strengths of each subalgebra while also introducing potent new features [5].

In the Clifford Algebra, another product is beneficial in addition to an exterior product. This multiplication operator is denoted by a wedge (∧).

For that reason, vectors can be divided and multiplied by other vectors and by any element by any other element. such that, instead of influencing their components, they can be directly manipulated.

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The geometric product for arbitrary vectors $\vec{a}$ and $\vec{b}$ are defined as

$$ab = a \bullet b + a \wedge b \tag{1}$$

Here $a \bullet b$ is the dot product and is a scalar expression. The expression $a \wedge b$ is the outer product. The wedge sign " $\wedge$ " denotes the outer product expression. The outer product is neither a scalar nor a vector. It is a new element called the bivectors [6].

And from vectors $\vec{a}$ and $\vec{b}$ we can define ba product as

$$ba = a \bullet b - b \wedge a \tag{2}$$

from Eq.1 and Eq.2 we can see the commutative rule $a \bullet b = b \bullet a$, in conjunction with the anticommutative rule $a \wedge b = - b \wedge a$.

Two vectors' outer and inner products can be represented in terms of the geometric product, and vice versa

$$a \bullet b = \frac{1}{2}(ab + ba) \tag{3}$$

and

$$a \wedge b = \frac{1}{2}(ab - ba) \tag{4}$$

From Eqs. (3) and (4)

$$\vec{a}\vec{b} = \vec{b}\vec{a} \quad \Leftrightarrow \quad \vec{a} \wedge \vec{b} = 0 \quad \Leftrightarrow \quad \vec{a}\vec{b} = \vec{a} \bullet \vec{b} \quad \Leftrightarrow \quad \vec{a} \parallel \vec{b}$$
$$\vec{a}\vec{b} = -\vec{b}\vec{a} \quad \Leftrightarrow \quad \vec{a} \bullet \vec{b} = 0 \quad \Leftrightarrow \quad \vec{a}\vec{b} = \vec{a} \wedge \vec{b} \quad \Leftrightarrow \quad \vec{a} \perp \vec{b} \tag{5}$$

The inner product $\vec{a} \bullet \vec{b}$ is symmetric and notices that vectors $\vec{a}$ and $\vec{b}$ are orthogonal if and only if $\vec{a}\vec{b} = -\vec{b}\vec{a}$.

The outer product $\vec{a} \wedge \vec{b}$ is antisymmetric (and associative) and vanishes whenever the two vectors are collinear, that is $\vec{a}$ and $\vec{b}$ are collinear (or linearly dependent) if and only if $\vec{a}\vec{b} = \vec{b}\vec{a}$.

A given vector in n-dimensional space can be represented by unit base vectors $(e_1, e_2, e_3, \ldots, e_n)$. In other words, any vector may be written as a linear combination of base vectors. A linear combination can also be used to describe the bivector.

The concepts of scalar, vector, bivectors, and tri vector are $0-$dimensional, $1-$dimensional, 2-dimensional, and $3-$dimensional space respectively. Now, the idea of $k-$degree will be expressed, showing the subspace size where k refers to the degree order.

Scalars receive a grade of 0, vectors receive a grade of 1, bivectors receive a rating of 2, and trivectors receive a grade of 3. It continues as 4^{th} degree, 5^{th} degree, and so on in high-dimensional space. This notation is n-degree for n-dimensional space. Degrees are shown in three dimensions in Table 1.

Table 1. Three-dimensional space degrees

k	Base element	Total
scalar	$\{1\}$	1
vector	$\{e_1, e_2, e_3\}$	3
bivectors	$\{e_{12}, e_{23}, e_{23}\}$	3

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tri vector	$\{e_{123}\}$	1

It's also critical to understand how many k-degrees exist in n-dimensional space. The binomial multiplier does this

$$\binom{n}{k} = \frac{n!}{(n-k)!k!} \tag{6}$$

Here n is the dimension and k seems to be the base degree.

The overall number of algebra unit bases may well be calculated by adding the unit bases of all grade levels.

$$\sum_{k=0}^{n} \binom{n}{k} = 2^n \tag{7}$$

The element A in Cl_n is represented with.

$$A = a_0 + a_{11}e_1 + \ldots + a_{1i}e_n + a_{21}e_1e_2 + \ldots + a_{2i}e_1e_n + \ldots + a_{di}e_1e_2 \ldots\ldots e_n \tag{8}$$

Here $d = 2^n - 1$ and $i = \binom{n}{k}$ for the real numbers a_{ki}. Consequently, the vector space cl_n can also be subdivided into $(n + 1)$ as well as subspaces.

$$Cl_n = \Lambda^0\mathbb{R}^n + \Lambda^1\mathbb{R}^n + \ldots + \Lambda^n\mathbb{R}^n \tag{9}$$

Every subspace seems to have a dimension $\binom{n}{k}$.

The elements A of the Clifford algebra Cl_n in Eq (8) are called Multivector, and those of $\Lambda^p\mathbb{R}^n$, p -vectors.

In special, (0-vectors) are real numbers with dim $(\Lambda^0\mathbb{R}^n) = 1$. (1-vectors) are vectors with dim $(\Lambda^1\mathbb{R}^n) = n$ and $\Lambda^1\mathbb{R}^n$ has the basis $\{e_1, e_2, \ldots., e_n\}$. (2-vectors) are bivectors and have the basis $\{e_1e_2, e_1e_3, \ldots, e_1e_n\}$. Finally, ($n$-vectors) with $\dim(\Lambda^n\mathbb{R}^n) = 1$, and has as basis $\{e_1e_2\ldots\ldots e_n\}$, the (n-vectors) are called the pseudo scalars of Cl_n .

Essentially arbitrary multi-vectors will just be denoted by non-bold upper case like A. A_P Would be used to describe p-vectors. A could be defined as any multi-vector A[7].

$$A = \langle A\rangle_0 + \langle A\rangle_1 + \ldots + \langle A\rangle_n \tag{10}$$

Where $\langle A\rangle p$ the p-vector portion of A, is the project of A $\in Cl_n$ into $\Lambda^p\mathbb{R}^n$. $\langle\ \rangle$ Is called the operator of the grade. Using this notation, it is possible to reframe the description of the inner and outer product or service in terms of its degree. If $\vec{a}$ and $\vec{b}$ vectors, the inner product of $\vec{a} \lrcorner \vec{b}$ produces a scalar 0

$$\langle\vec{a}\rangle_1 \lrcorner \langle\vec{b}\rangle_1 = \langle\vec{a}b\rangle_0 \tag{11}$$

The vector is obtained by projecting the vector onto the bivector $\mathbf{B}$

$$\langle\vec{a}\rangle_1 \lrcorner \langle\mathbf{B}\rangle_2 = \langle\vec{a}\,\mathbf{B}\rangle_{2-1} \tag{12}$$

The external product of vectors $\vec{a}$ and $\vec{b}$ can be expressed as

$$\langle\vec{a}\rangle_1 \wedge \langle\vec{b}\rangle_1 = \langle\vec{ab}\rangle_2 \tag{13}$$

This rule is applicable in general.

$$\langle\mathbf{A}\rangle_s \lrcorner \langle\mathbf{B}\rangle_t = \langle\mathbf{AB}\rangle_{s-t} \qquad \text{If} \quad s \leq t \tag{14}$$

$$\langle \mathbf{A} \rangle_s \lrcorner \langle \mathbf{B} \rangle_t = 0 \qquad \text{If} \quad s > t \tag{15}$$

$$\langle A \rangle_s \wedge \langle B \rangle_t = \langle AB \rangle_{s+t} \tag{16}$$

The inverse of the vector **b** is given by.

$$\boldsymbol{b}^{-1} = \frac{\boldsymbol{b}}{b^2} \tag{17}$$

and it fulfills.

$$bb^{-1} = b^{-1}b = 1 \tag{18}$$

It has been quite formal to introduce geometric algebra in such a basic way. However, an infinite number of geometrical relations can be extracted by performing a straightforward algebraic operation on the laws. For instance, multiplying any vector $\boldsymbol{b}$ by $\boldsymbol{nn^{-1}}$ can be broken down into the components parallel ($\boldsymbol{b}_{\parallel}$) and orthogonal ($\boldsymbol{b}_{\perp}$) to a given vector $\boldsymbol{n}$. This leads to

$$bnn^{-1} = \frac{bnn}{n^2} = \frac{(bn)n}{n^2} = \frac{1}{n^2}(b \bullet n + b \wedge n)n = b_{\parallel} + b_{\perp} \tag{19}$$

Similarly, any vector $\boldsymbol{b}$ can be decomposed to the parallel ($\boldsymbol{b}_{\parallel}$) and orthogonal ($\boldsymbol{b}_{\perp}$) to some given plane

$\boldsymbol{U = r \wedge s}$ as [6]

$$b_{\parallel} = (b \bullet U)U^{-1} \tag{20}$$

$$b_{\perp} = (b \wedge U)U^{-1} \tag{21}$$

The reflection of $\boldsymbol{b}$ across the line $\boldsymbol{u}$ is acquired by sending $\boldsymbol{b = b_{\parallel} + b_{\perp}}$ to $\boldsymbol{b^{-1} = b_{\parallel} - b_{\perp}}$where $\boldsymbol{b_{\parallel} = (b \bullet u)u^{-1}}$. The mirror image $\boldsymbol{u'}$of $\boldsymbol{u}$ for $\boldsymbol{b}$ is then.

$$b' = ubu^{-1} \tag{22}$$

We may represent the dot and outer products for the two vectors $\boldsymbol{b}$ and $\boldsymbol{n}$ regarding the angle between these vectors $\boldsymbol{\theta}$.

$$\vec{b} \bullet \vec{n} = \frac{1}{2}(\vec{b}\vec{n} + \vec{n}\vec{b}) = |\vec{b}||\vec{n}| \cos\theta \tag{23}$$

$$\vec{b} \wedge \vec{n} = \frac{1}{2}(\vec{b}\vec{n} - \vec{n}\vec{b}) = i|\vec{b}||\vec{n}| \sin\theta \tag{24}$$

The geometric product of unit vectors can be constructed using equations (23) and (24), yielding a useful method for rotating a vector in a plane. The geometric product is expressed as follows if the unit bivector for the longitudinal plane is $\boldsymbol{i}$ equal to the unit vectors ($\vec{\boldsymbol{b}}$) and ($\vec{\boldsymbol{n}}$).

$$\vec{b}\vec{n} = \cos\theta + i \sin\theta = e^{i\theta} \tag{25}$$

When a vector s is multiplied by the $\boldsymbol{e^{i\theta}}$ exponential, also referred to as a two-dimensional rotor, a new vector $\mathbf{b}'$ is created. This new vector is the previous vector rotated by an angle θ in the $\boldsymbol{i}$ plane.

$$b' = b\, e^{i\theta} = b\cos\theta + bi \sin\theta \tag{26}$$

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

$$b\cos\theta + bi \sin\theta = b\cos\theta - ib \sin\theta = e^{-i\theta} b \tag{27}$$

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The vector derivatives of the coordinate q_i for the spatial position vector x_β are known as the gradients $\nabla_\beta q_i$ in geometric algebra.

$$\nabla_\beta q_i = \partial_{x_\beta} q_i \tag{28}$$

The chain rule can be used to express the vector derivative operator ∇_β in certain coordinates as

$$\nabla_\beta = \sum_i (\nabla_\beta q_i)\frac{\partial}{\partial q_i} \tag{29}$$

In the vector round, we use the subscript β to emphasize that these findings apply to several vector elements, $x_1, x_2, \ldots$

The computations for gradients are largely like those in standard scalar calculus. For instance, distributive vector differentiation exists if X and Y are vectors.

$$\nabla_\beta (X + Y) = \nabla_\beta X + \nabla_\beta Y \tag{30}$$

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

$$\nabla_\beta (\gamma X) = (\nabla_\beta \gamma) X + \gamma \nabla_\beta X \tag{31}$$

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

$$div_\beta y = \nabla_\beta \cdot y \tag{32}$$

$$curl_\beta y = \nabla_\beta \times y \tag{33}$$

By using geometric product definition, we can write

$$\nabla_\beta y = \nabla_\beta \cdot y + \nabla_\beta \wedge y$$

$$= \nabla_\beta \cdot y + i\nabla_\beta \times y \tag{34}$$

Consequently, the curl is the dual component, and the divergence is the scalar component of the vector derivative of y.

Not just vectors and scalars but all elements Y are produced for the vector derivative $\nabla_\beta Y$

$$\nabla_\beta Y = \nabla_\beta \cdot Y + \nabla_\beta \wedge Y \tag{35}$$

Eqs provide distributive vector differentiation. (30) and (31); however, as the operator of the vector derivative doesn't genuinely commute with Multivector in practice, the product rule should be expressed as [5]

$$\nabla_\beta (XY) = \grave{\nabla}_\beta \grave{X} Y + \grave{\nabla}_\beta X \grave{Y} \tag{36}$$

3. KINETIC ENERGY OPERATOR FOR POLYATOMIC MOLECULAR.

A molecule is a group of two or more atoms that form the smallest identifiable unit into which a pure substance can be divided and still retain the composition and chemical properties of that substance.

For a monatomic molecular, for example, an ideal gas (such as helium), the amount of internal total energy is the potential energy and the translational kinetic energy (vibrational kinetic energy) possessed by the atoms of an ideal gas as they bounce around randomly inside their container. Diatomic molecules (such as oxygen) and polyatomic molecules (such as water) have additional rotational motions, so they have the kinetic energy of rotation. To find the internal kinetic energy for the polyatomic molecular, we must know the vibrational and rotational degrees of freedom.

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The kinetic energy operator for a single particle in generalized coordinates q_1, q_2, and q_3 is typically obtained by replacing the kinetic energy operator with the coordinate representation of the gradient operator.

$$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2 \tag{37}$$

where $\nabla = \sum_{i=1}^{3}(\nabla q_i)\frac{\partial}{\partial q_i}$

The coordinate gradients q_i are considered the most often used coordinates, and even with traditional calculus methods, they may be determined with comparatively minimal effort.

However, finding the formulation of an N-body system's kinetic energy operator in terms of translational and shape coordinates, as well as the elements of total angular momentum, is more difficult. This work aims to investigate a simple algebraic way to obtain the operators of the kinetic energy of polyatomic molecules [8].

The components of the reciprocal metric tensor, which are present in polyatomic molecules' internal kinetic energy operators, can be expressed as the mass-weighted sum of the inner products of measurement vectors connected to the molecule's nucleus.

When it comes to vibrational degrees of freedom, the measurement vectors are just the vibrational coordinates' gradients for the nucleus's position. These can be computed via direct vectorial differentiation or by varying the relevant coordinate during the particle's path.

Finding these vectors for the rotational degrees of freedom is more challenging because there is no conjugation between the components of the total angular momentum operator and any rotational coordinates. Nonetheless, the rotational measurement vectors for any geometrically defined body frame may be easily computed using geometric algebraic methods, and there is no restriction on the number of particles in the system.

The non-relativistic kinetic energy operator $\hat{T}$ of an N-atomic molecule is given as follows if the Born-Oppenheimer approximation holds:

$$\hat{T} = -\frac{\hbar^2}{2m_\beta}\sum_{\beta}^{N}\nabla_\beta^2 \tag{39}$$

Where m_β is the mass of the atom β and ∇_β is the vector derivative (gradient) operator concerning the spatial position Y_β of the nucleus β. Specifically, it is assumed that every integration is carried out throughout the volume element $d\tau = |d^3y_1||d^3y_2|\ldots|d^3y_N|$. But for many applications, just the molecule's internal state matters. If we represent ∇_β in three Cartesian coordinates $y_i = v_i \bullet \boldsymbol{Y}$ $(i = 1,2,3)$ of the center of mass, we can easily separate the translation from the molecule's internal motions [9].

$$\boldsymbol{Y} = \sum_{\beta=1}^{N}\frac{m_\beta y_\beta}{M} \tag{40}$$

(where M is the molecule's mass, and it's written as $\mathrm{M} = \sum_{\beta}^{\mathrm{N}} m_\beta$, and $\{v_1, v_2, v_3\}$ is an orthonormal standard space-fixed frame),$3N-6$ shape coordinates q_i, and three coordinates for rotation B_i as

$$\nabla_\beta = \sum_{i=1}^{3}(\nabla_\beta\, y_i)\frac{\partial}{\partial\, y_i} + \sum_{i}^{3N-6}(\nabla_\beta\, q_i)\frac{\partial}{\partial q_i} + \sum_{I}^{3}(\nabla_\beta\, B_i)\frac{\partial}{\partial B_i}$$

$$= \sum_{i=1}^{3}\left(\frac{m_\beta}{M}\, v_i\right)\frac{\partial}{\partial\, y_i} + \sum_{i}^{3N-6}(\nabla_\beta\, q_i)\frac{\partial}{\partial q_i} + \sum_{I}^{3}(\nabla_\beta\, B_i)\frac{\partial}{\partial B_i} \tag{41}$$

Given that the shape and rotational coordinates are translationally invariant,

$$\sum_\beta \nabla_\beta\, q_i = 0 \tag{42}$$

$$\sum_\beta \nabla_\beta\, B_i = 0 \tag{43}$$

by replacing Eq. (39) with Eq. (41), yields

$$\hat{T} = -\frac{\hbar^2}{2M}\sum_{i=1}^{3}\frac{\partial^2}{\partial y_i^2} + \hat{T}^{(int)} \tag{44}$$

where $\hat{T}^{(int)}$ denotes the kinetic energy operator portion that is only dependent on the internal coordinates. It might be stated as

$$\hat{T}^{(int)} = \sum \begin{bmatrix} -\frac{\hbar^2}{2}\left(\frac{\partial}{\partial q_i} + \frac{1}{J}\frac{\partial J}{\partial q_i}\right) g^{(q_i,q_j)}\frac{\partial}{\partial q_j} - \frac{1}{2}g^{(L_i,L_j)}\hat{l}_i\hat{l}_j \\ -\frac{\hbar}{2}g^{(L_i,q_j)}\hat{l}_i\frac{\partial}{\partial q_j} - \frac{\hbar}{2}\left(\frac{\partial}{\partial q_j} + \frac{1}{J}\frac{\partial J}{\partial q_i}\right) g^{(q_i,L_j)}\hat{l}_j \end{bmatrix} \tag{45}$$

In the orthonormal body-fixed frame $\{\acute{\upsilon}_1, \acute{\upsilon}_2, \acute{\upsilon}_3\}$, the rotation $\acute{\upsilon}_1 = \tilde{R}\upsilon_i R$ is connected to the standard laboratory-fixed frame by $\hat{l}_i = \acute{\upsilon}_i \bullet \hat{I}$, which is the ith $(i = 1,2,3)$ scalar component of the dual $\hat{I} = -i\hat{L}$ of the internal angular momentum operator[9].

$$\hat{L} = -i\hbar\sum_{\beta}^{N-1} x_\beta \times \nabla_{x_\beta} \tag{46}$$

where $x_\beta = y_\beta - \boldsymbol{Y}$ is the center of mass position of the nucleus β, and the i is the unit trivector.

The mass-weighted reciprocal metric tensor $[z]$ is composed of the vibrational, Coriolis, and rotational elements, denoted as $g^{(q_i,q_j)}$, $g^{(q_i,L_j)}$, $g^{(L_i,L_j)}$, and they are only dependent on the shape coordinates[10].

The coordinate transformation's Jacobian absolute value, denoted by J, is provided by

$$J = |det[g]^{-1/2}| \sin\theta \prod_\beta m_\beta^{-3/2} \tag{47}$$

where θ is the Euler angle between υ_3 and $\acute{\upsilon}_3$.

Instead of utilizing the volume-element $d\tau = J\, dq_1 dq_2 \ldots$, if one wants to integrate using the volume-element $d\tau_{\mathcal{K}} = \mathcal{K}\, dq_1 dq_2 \ldots$, the equivalent kinetic energy operator $\hat{T}_{\mathcal{K}}^{(int)}$ is provided as

$$\hat{T}_{\mathcal{K}}^{(int)} = J^{1/2}\mathcal{K}^{-1/2}\hat{T}^{(int)}\mathcal{K}^{1/2}J^{-1/2} \tag{48}$$

3.1 Vibrational Degrees of Freedom

When Eq. (39) is replaced with Eq. (41) the vibrational elements of the mass-weighted reciprocal metric tensor for any vibrational coordinates q_i are obtained as follows [10]:

$$g^{(q_i,q_j)} = \sum_\beta^N \frac{1}{m_\beta} e_\beta^{(q_i)} \cdot e_\beta^{(q_j)} = \sum_\beta^N \frac{1}{m_\beta}(\nabla_\beta q_i) \bullet (\nabla_\beta q_j) \qquad \text{for } (i, j = 1,2,\ldots,3N-6) \tag{49}$$

The gradients $\nabla_\beta q_i$ are produced by calculating the vector derivative of the coordinate q_i for the position vector of the nucleus β, and the vibrational coordinates are typically expressed simply as functions of the nuclear position vectors y_β, i.e.,

$$\nabla_\beta q_i \equiv \nabla_{y_\beta} q_i = \partial_{y_\beta} q_i \tag{50}$$

or else they can be taken out of the way the coordinate q_i varies along the particle -path $y_\beta(t)$.

$$\dot{q_i} = \sum_\beta^N \dot{y_\beta}(t) \bullet \nabla_\beta q_i \tag{51}$$

($\dot{q}_i = \frac{dq}{dt}$, and t is some scalar parameter).

3.2 Rotational Degrees of Freedom

Since the elements of the angular momentum operator $\hat{L}$ are not conjugated to any rotational coordinate B_i, it is more challenging to determine the rotational and Coriolis parts of the kinetic energy operator. First, take the derivative of any arbitrary scalar function W for the Euler angles $B_1 = \phi$, $B_2 = \theta$, and $B_3 = \chi$. Now

$$\hbar \frac{\partial}{\partial B_i} W = n_i \bullet \hat{I}\, W \tag{52}$$

where $n_1 = \upsilon_3$, $n_2 = \frac{\upsilon_3 \times \upsilon_3'}{|\upsilon_3 \times \upsilon_3'|}$, and $n_3 = \upsilon_3'$ in agreement with the parametrization $R = e^{i\chi\upsilon_3/2} e^{i\theta\upsilon_1/2} e^{i\phi\upsilon_3/2} = e^{i\chi\upsilon_3'/2} e^{i\theta\upsilon_1'/2} e^{i\phi\upsilon_3'/2} = e^{i\phi\upsilon_3/2} e^{i\theta n_2/2} e^{i\chi\upsilon_3'/2}$

When body-fixed axes υ_k' are used to express n_1, n_2, and n_3 respectively, the equivalence

$$\hbar\, (\nabla_\beta B_i) \frac{\partial}{\partial B_i} = \sum_k \upsilon_k' \bullet\, n_i\, (\nabla_\beta B_i) \hat{l}_k \tag{53}$$

The rotation angle's gradient can be expressed as

$$(\nabla_\beta B_i) = \nabla_b n^{(i)} \bullet \omega^\beta(b) \tag{54}$$

where the vector $n^{(i)}$represents the reciprocal of the hybrid axis n_i, meaning that ($n^{(i)} \bullet n^{(i)} = 1$ if $i = j$ and 0 otherwise), and $\omega^\beta(b)$ is the body frame's rotational velocity due to particle β 's displacement (evaluated at point b).

$$\omega^\beta(b) = \upsilon_3 b \bullet \nabla_\beta \phi + n_2 b \bullet \nabla_\beta \theta + \upsilon_3' b \bullet \nabla_\beta \chi$$
$$= -\frac{1}{2} \sum_j^3 \upsilon_j' b \bullet \nabla_\beta \upsilon_j' = \frac{1}{2} \sum_j^3 \upsilon_j' \times (b \bullet \nabla_\beta \upsilon_j') \tag{55}$$

Following the insertion of Eq. (54) into Eq. (43) and the summation of both sides over index i,

$$\hbar\, (\nabla_\beta B_i) \frac{\partial}{\partial B_i} = \sum_k^3 \nabla_b\, [(b \bullet \nabla_\beta \upsilon_i') \bullet \upsilon_j']\, \hat{l}_k \tag{56}$$

On the right side of Eq. (56), the indices $i, j, and\ k$ are in the cyclic order. The gradient operator ∇_β, multiplied by $\hbar$, solely dependent on rotation, includes the left-hand side of Eq. (56).

The rotational g-elements can thus be expressed as follows by introducing Eq. (56) into Eqs. (39) and (41) and selecting the terms proportionate to $\hat{l}_k$

$$g^{(L_i L_k)} = \sum_\beta^N \frac{1}{m_\beta}\, e_\beta^{(L_i)} \bullet e_\beta^{(L_k)} \tag{57}$$

and the Coriolis g-elements as

$$g^{(L_k q_i)} = \sum_\beta^N \frac{1}{m_\beta}\, e_\beta^{L_k} \bullet (\nabla_\beta q_i) \quad \text{for } (i = 1,2,\ldots,3N-6) \quad \text{and } k = (1,2,3) \tag{58}$$

where

$$e_\beta^{L_k} = \nabla_b\, [(b \bullet \nabla_\beta \upsilon_i') \bullet \upsilon_j'] \tag{59}$$

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is the rotational measuring vector associated with the nucleus β: and kth component of the angular momentum operator $\hat{L}$.

If we have two directions a and b which are defined by

$$a = \sum_\beta c_\beta X_\beta \tag{60}$$

$$b = \sum_\beta d_\beta X_\beta \tag{61}$$

The internal coordinates can affect the coefficients c_β and d_β, where $a \times b \neq 0$, and these vectors are not collinear $\sum_\beta c_\beta = 0$ and $\sum_\beta d_\beta = 0$.

The axes of the body are represented as [11]

$$\upsilon_3' = \frac{a}{|a|} \tag{62}$$

$$\upsilon_2' = \frac{a \times b}{|a \times b|} \tag{63}$$

$$\upsilon_1' = \upsilon_2' \times \upsilon_3' \tag{64}$$

and the measuring vectors as

$$e_\beta^{L_1} = -\frac{c_\beta \upsilon_2' + \sum_\alpha X_\alpha \cdot \upsilon_2' \nabla_\beta c_\alpha}{a} \tag{65}$$

$$e_\beta^{L_2} = \frac{c_\beta \upsilon_1' + \sum_\alpha X_\alpha \cdot \upsilon_1' \nabla_\beta c_\alpha}{a} \tag{66}$$

$$e_\beta^{L_3} = \frac{1}{|a \times b|}\left[b \cdot \upsilon_3' \left(c_\beta \upsilon_2' + \sum_\alpha X_\alpha \cdot \upsilon_2' \nabla_\beta c_\alpha\right) - a\left(d_\beta \upsilon_2' + \sum_\alpha X_\alpha \cdot \upsilon_2' \nabla_\beta d_\alpha\right)\right] \tag{67}$$

Since the above formulas refer to any choice for a and b, the rotational measurement vectors can be easily obtained using the current system by simply defining the body's axes (or the a and b directions). As a result, the current method which is mean geometric algebra tends to be a useful technique for determining the rotational vibrational operator of the kinetic energy in situations where it is beneficial to reduce any of the Hamiltonian vibrations and rotation coupling conditions [12].

4. RESULTS AND CONCLUSIONS

The goal of Clifford and many others was to make geometric algebra useful in a wide range of scientific fields. because certain issues may have unexpected solutions when algebra is applied. In this context, it is important to highlight David Hestenes' efforts to elevate geometric algebra from algebra in physics to a science language.

This work reveals that a general and useful technique for obtaining rotational measuring vectors $e_\beta^{L_k}$ using geometric algebra has been developed. It provides its internal products with other rotational measuring vectors as well as with vibration gradient coordinates, the vibration operator of kinetic energy, and particles rotating at polyatomic speeds.

The findings of this research will enable us to use Clifford Algebra to write the energy expressions of polyatomic molecules much more compactly, which will make our computations easier.

If these operators are real, then everything can be explained in terms of the motions of polyatomic molecules. By using these operators, we can interpret the results of applying mathematics to physics.

Finally, we can see that 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 in the enigmatic world of quantum physics.

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