APPLICATION OF GEOMETRIC ALGEBRA TO THEORETICAL MOLECULAR SPECTROSCOPY

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Master of Science Thesis

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Eskişehir Technical University

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ABSTRACT

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In this thesis, the general definition of geometric algebra (Clifford algebra) and the basic principles for studying the geometric properties of this algebra are discussed. Next, 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 operators of the kinetic energy include a metric tensor, the elements of this metric tensor was expressed as the mass-weighted sum of measuring vector inner products 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.

Keywords: Geometric algebra, Operator of the kinetic energy, Covariant metric tensor, Rotational measuring vectors, Vibrational measuring vectors.

ÖZET

GEOMETRİK CEBİRİN TEORİK MOLEKÜLER SPEKTROSKOPİYE UYGULANMASI

Baghdad Abduhameed Abdullah AL-BADANI

Fizik Anabilim Dalı

Genel fizik Bilim Dalı

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Danışman: Prof. Dr. Abidin KILIÇ

Bu tezde, geometrik cebirin (Clifford cebiri) genel tanımı ve bu cebirin geometrik özelliklerini incelemenin temel ilkeleri tartışılmaktadır. Daha sonra, çok atomlu moleküllerin moleküler titreşim-dönüşünün kinetik enerjisinin operatörlerini elde etmek için genel ve pratik bir yöntem oluşturmak için geometrik cebir kullanıldı. Öte yandan, bu çok atomlu moleküllerin kinetik enerjinin kesin içsel operatörleri bir metrik tensör içerir, bu metrik tensörün elemanları, molekülün çekirdeği ile uyumlu vektör iç çarpım vektörlerini ölçmenin kütle ağırlıklı toplamı olarak ifade edildi. Oysa cismin şekil ve çerçevelerinin geometrik olarak tanımlanmış koordinatları için metrik tensörde görünen titreşim ve dönme ölçüm vektörleri, geometrik cebir kullanılarak kolayca belirlendi. Mevcut yöntem (geometrik cebir), önceki çalışmalarla mükemmel uyum içinde olan moleküler titreşim-rotasyon kinetik enerji operatörleri üretir.

Anahtar Sözcükler: Geometrik cebir, Kinetik enerji operatörü, Kovaryant metrik tensör, Dönel ölçüm vektörleri, Titreşim ölçüm vektörleri.

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Baghdad Abduhameed Abdullah AL-BADANI

10/06/2021

STATEMENT OF COMPLIANCE WITH ETHICAL PRINCIPLES AND RULES

I hereby truthfully declare that this thesis is an original work prepared by me; that I have behaved in accordance with the scientific ethical principles and rules throughout the stages of preparation, data collection, analysis and presentation of my work; that I have cited the sources of all the data and information that could be obtained within the scope of this study, and included these sources in the references section; and that this study has been scanned for plagiarism with "scientific plagiarism detection program" used by Eskişehir Technical University, and that "it does not have any plagiarism" whatsoever. I also declare that, if a case contrary to my declaration is detected in my work at any time, I hereby express my consent to all the ethical and legal consequences that are involved.

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GLOSSARY OF SYMBOLS AND ABBREVIATIONS

CA	:	Cliffored algebra
e_{i}	:	Unit bases
$\mathbf{I}$	:	pseudovector of geometric algebra
$\boldsymbol{Cl}_n$	:	n-dimensional Clifford space
$\boldsymbol{Cl}_3$	:	three-dimensional Clifford space
$\cdot$	:	Dot product
$\times$	:	Vector multiplication
$\wedge$	:	Wedge (exterior)
$\langle \ \rangle$	:	grate operator
A	:	multivector
$\lrcorner$	:	inner product
∇_{β}	:	the vector derivative operator
$\nabla_{\beta}\mathrm{q_i}$	:	vector derivatives of the coordinate $\mathrm{q_i}$
$\hat{\mathrm{T}}$	:	the kinetic energy operator
$\hat{\mathrm{V}}$	:	the potential energy operator
ϵ_o	:	the vacuum permittivity
X_{β}	:	the position of β nuclear
M	:	the molecule's mass
$e_{\beta}^{(q_i)}$	:	the measuring vector correlating with the molecule's β
Ψ_e	:	the wave function for electronic motions
Ψ_t	:	the wave function for the translational motions of the center of mass
Ψ_r	:	the wave function for rotational motions
Ψ_v	:	the wave function for vibrational motions
$\Gamma_i^{\dagger}$	:	adjoint
$g^{(q_i q_j)}$	:	contravariant metric tensor
J	:	Jacobian

1. INTRODUCTION

1.1. Literature Review

Geometric algebra is a numerical technique that simplifies the description of geometric concepts and procedures [1]. Clifford algebra, as its name suggests, also called "geometric 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]. Clifford algebra has become amongst the most important mathematical physics theories. The so-called Clifford product, in especially, is important.

Most of the geometric algebra was based on research performed in the mid-19th century. Initially, Wessel, Argand, and Gauss noticed the usefulness of complex numbers when attempting to solve several problems in 2-dimensional, and they used imaginary number exponentials, particularly in describing the rotation operation [4]. In geometric algebra, the exponential of imaginary numbers is a highly important and basic approach, particularly in establishing the rotation operation.

The complex numbers were then extended to 3-dimensional space by Hamilton, who established his renowned quaternion algebra. Quaternion algebra is the oldest the most well noncommutative algebra, and it may be thought of as a subset of geometric algebra or Clifford algebra since its fundamental components are expressed as a linear product of geometric algebra units. He began his quaternion algebra by observing that when complex numbers are described in the plane as a vector with the x-axis containing the real part and the y-axis that included the imaginary part, multiplying the vector z by the imaginary produces a new vector (also known as a complex number) at the correct angle to z. Quaternions represent the definitions of vectors and their cross-products, although they only exist in three dimensions. [5].

Quaternion algebra is quite similar to Grassmann's algebra. Hermann Günter Grassmann, the first to describe multiplication by merely providing a set of algebraic

laws, devised the outside or exterior product, which may be constructed on any vector space. Grassmann's significant discoveries are acknowledged as the first introduction of the pure principle of vector spaces over the real number field. The hyper numbers e_i were defined by Grassmann as directed unit lines, and every vector is expressed by format. [2]

$$u_i e_i \tag{1.1}$$

In this case, u_i is a scalar number. For these hyper numbers, Grassmann identified two different multiplications. These would be the inner products

$$e_i \cdot e_j = e_j \cdot e_i = \delta_{ij} \tag{1.2}$$

and the outer product

$$e_i \wedge e_j = -e_j \wedge e_i \tag{1.3}$$

Grassmann classified the outer product outcome as a directional field and used this algebra to describe things with much more than 2 dimensions. Many math historians believe that in the latter years of Grassmann's life, he identified the point and the outer product as the center product [6].

$$\vec{u}\vec{w} = \vec{u} \cdot \vec{w} + \vec{u} \wedge \vec{w} \tag{1.4}$$

Clifford's vector product will have the same formulation as the center product. Grassmann made these comments fully independently of Clifford [2]. Clifford, on the other hand, was informed with Grassmann and represented this function as well as presented the central product. Hamilton's algebra of quaternions also can be defined in this algebra. Clifford reported this finding in his 1878 publication and dubbed it geometric algebra.

Physicists had already adapted to the hybrid technique before Gibbs, despite mathematicians' efforts to create a simple unified geometric algebra. Gibbs recognized two vector products. Inner Grassmann product and Quaternion-inspired cross product The cross product of two vectors yields a third vector.

Gibbs algebra was ideally suited to handling electromagnetic issues and hence quickly gained popularity. However, because the vector product is not changeable and

cannot be applied to multi-dimensional structures, some issues have not been properly handled.

As a result, in the end of the nineteenth century, Clifford algebra created, encircled by these feeble algebras [7]. Geometric algebra unites all of these algebraic structures into coherent programming equations that retain the benefits of each of these subalgebras while also adding strong advanced features [5].

After some deployments, it provided academics optimism for the future solution of numerous problems using quaternion algebra. Unlike the other algebraic structures, it fully embraces projective geometry. As a result, Clifford algebra is the obvious algebraic tool for controlling subspaces and rotates.

David Hestenes used a completely different method to comprehending Clifford algebra. Like many scientists in the 1960s, he concentrated on field theories and particles. With this interpretation, he discovered that Dirac matrices can be viewed as vectors, opening up new insights on quantum theory and the Dirac equation.

The success of this notion prompted Hestenes to reassess what Clifford algebra might do. Hestenes contended that Clifford algebra is a native language, not merely a system of direction numbers and that conclusions should be articulated in terms of algebra and geometry outcomes rather than numbers. Hestenes spend many years trying to make Clifford algebra an acceptable language for physics while remaining true to the original, and he dubbed it geometric algebra [2].

Clifford algebra is now widely employed in numerous domains, including molecular chemistry and electromagnetic, and also engineering fields such as robots and computer vision.

Clifford's geometric algebra is an excellent language for physics since it improves the use of geometric characteristics and symmetric. Clifford algebra, in instance, provides cross products with basic mathematical formulations, notably in relativistic spacetime, and reduces the possibility of conflating pseudovectors with pseudoscalars. Reduces rotations and Lorentz changes to algebraic multiplication, increases detailed assessment to more than two dimensions, approximates cross products to $n >$ 3dimensions, and builds the unit imaginary i as a geometric object, Thus, it justifies its importance in physics by trying to extend complex analysis to ever more than two

dimensions, and more widely, it helps make computational design without matrices or tensors, merges Newtonian mechanics, relativity, quantum theory, and are more in a fixed formalism and language as easy as the algebra of the Pauli spin matrices, and therefore combines Newtonian physics, relativity, quantum theory, and more.

There are several previous experimental and analytical research studied using (GA) in physics. I can mention some of them as follows:

"Coordinates of vibration and their gradients using geometric algebra" were studied by Janne Pesonen, In this study, to form a precise vibrational kinetic energy driver of a polyatomic molecule, vibrational induction gradients are required. The traditional methods for obtaining these gradients are rather time-consuming. However, using geometric algebra, the gradients for any vibrational coordinates were easily computed as the atomic location vectors themselves were dealt with rather than their components, and thus the expressions became simple at each stage of the derivation. This is not the case when Cartesian substitution components are used to obtain the vibration energy actuator [8].

"Volume-elements of integration: A geometric algebra approach" by Janne Pesonen, In this study, geometric algebra is used to calculate the element of volume of the integral needed to determine the position, direction and shape of the molecule containing N from the atom to the center of mass of the three Cartesian coordinates, the three Euler angles, and the coordinates of the shape $(3N-6)$. As the volume element is formed by combining the resulting volume elements for each atom separately, and each of them has three coordinates. Each measurement is taken in three dimensions of physical space. [9].

1.2. Objective of Thesis

Clifford Algebra is a mathematical approach found in physics, robotics, computer-aided design (CAD), computer-aided manufacturing (CAM), and computer graphics. Clifford algebra simplifies geometric objects and specifies some essential characteristics that apply to all sorts of engineering parts. As a result, the goal of this research is to focus attention on engineering algebra and its numerous methods in 2D and 3D, as well as their use in theoretical molecular spectroscopy to more readily extract molecular vibration-rotation kinetic energy operators.

1.3. Thesis Organization

The first chapter provides a brief overview of the history of geometric algebra and its stages of development and discusses some studies that have used geometric algebra as an applied topic of research, in addition to the aims and objectives of the thesis. The basic principles of geometric algebra, as well as the geometric transformations and relations used in this algebra, are discussed in Chapter 2. The Schrödinger equation and the wave equation for polyatomic particles are discussed briefly in Chapter 3, as well as the kinetic energy operator of polyatomic particles in terms of geometric algebra. Regarding geometric algebra, Chapter 4 discusses the Lagrangian formula and variable vectors of measure. In the chapter 5 results and conclusıons.

2. GEOMETRIC ALGEBRA

2.1. Introduction

To represent geometric relations, many different algebra systems have been devised. Among these are mostly well branches of analysis' complex algebras, such as vectors, matrices, and tensor, quaternion, and algebras of spinner. Each has a particular benefit in some uses while also having significant overlap, i.e., they have several mathematical models with the same geometrical concepts [2]. To build fundamental definitions, geometric algebra uses a number of specific rules for multiplication vector. We'll go through these concepts in this section.

2.2. Fundamental Concepts

A vector is a geometric entity with direction and magnitude; it may be thought of as a space arrow [1]. A portion of the directional axis is used to geometrically define a vector. The vector's direction is shown by the line holding the vector, and the vector's magnitude is shown by the length [5].

The alignment of the standard lines and areas to the surfaces is indicated by vectors. Only the directions matter; dimensions are unimportant. These vectors are referred as direction vectors. They are normally multiplied by an appropriate number by unit vectors of unit magnitude since their dimensions are immaterial [1].

Vectors are investigated for 1-D subspaces in spaces of 2 and greater sizes, but they are ignored in spaces of 2 and bigger sizes. Because 1-D subspaces are still considered an idea, they serve as a basis for the subspace idea. With the help of these perspectives, multidimensional subspace forms are constructed using vectors [5].

Subspaces are defined and expressed as mathematics using operators in geometric algebra. Geometric algebra is an algebra that allows planes to be described and orientation fields to be defined in two-dimensional subspaces. In this algebra, subspaces of various dimensions can be combined, subtracted, multiplied, and divided, resulting in particular geometric connections [10].

We take the plane $\mathbb{R} \times \mathbb{R} = \{(\alpha, \beta) \mid \alpha, \beta \in \mathbb{R}\}$. A linear pattern is created by addition.

$$(\alpha_1 , \beta_1) + (\alpha_2 , \beta_2) = (\alpha_1 + \alpha_2 , \beta_1 + \beta_2) \quad (2.1)$$

as well as scaling

$$\gamma(\alpha, \beta) = (\gamma\alpha , \gamma\beta) \quad (2.2)$$

where $\gamma \in \mathbb{R}$. The plane $\mathbb{R} \times \mathbb{R}$ is turned into a straight line $\mathbb{R}^2$ by the linear structure.

When we take a basis (e_1 , e_2) of $\mathbb{R}^2$ that is

$$e_1 = (1,0) \quad \text{and} \quad e_2 = (0,1) \quad (2.3)$$

The length of r is Introduced by $r = \alpha e_1 + \beta e_2$ as

$$|r| = \sqrt{\alpha^2 + \beta^2} \quad (2.4)$$

$\mathbb{R}^2$becomes a Euclidean plane, often known as $\mathbb{R}^2$, The unit vectors e_1 , and e_2 are the basic vectors.

$$|e_1| = 1, |e_2| = 1 \quad (2.5)$$

The unit vectors e_1 , e_2 are orthogonal $e_1 \perp e_2$ [3].

Let $\vec{A} , \vec{B}$ be arbitrary vectors such that $\vec{A} = a_1 e_1 + a_2 e_2$, $\vec{B} = b_1 e_1 + b_2 e_2 \in \mathbb{R}^2$.

$$\vec{A} \cdot \vec{B} = a_1 b_1 + a_2 b_2 \quad (2.6)$$

The symmetric scalar product

$$\vec{A} \cdot \vec{B} = \vec{B} \cdot \vec{A} \quad (2.7)$$

If the two vectors $\vec{A} , \vec{B}$ are orthogonal $\vec{A} \perp \vec{B}$, their scalar product $\vec{A} \cdot \vec{B} = 0$ (vanishes).

The non-commutative (nonsymmetric) associative product for $\mathbb{R}^2$vectors is then introduced. If the vector Z is multiplied by itself or squared, $ZZ = Z^2$, the vector's square must match the vector's length, $Z^2 = |Z|^2$.We create a product for vectors in coordinate form that does the following

$$(\alpha e_1 + \beta e_2)^2 = \alpha^2 + \beta^2 \quad (2.8)$$

We can apply the distributive rule without assuming commutativity [10], which gives

$$\alpha^2 e_1^2 + \beta^2 e_1^2 + \alpha\beta (e_1 e_2 + e_2 e_1) = \alpha^2 + \beta^2 \quad (2.9)$$

This is achievable if the orthogonal unit vectors e_1 , e_2 obey the multiplication laws [1]

$$e_1^2 = e_2^2 = 1 \quad \& \quad e_1 e_2 = -e_2 e_1 \tag{2.10}$$

which is equivalent to

$$| e_1 | = | e_2 | = 1 \quad \& \quad e_1 \perp e_2 \tag{2.11}$$

As illustrated in figure 2.1, the oriented plane area of the square with sides e_1 and e_2 is expressed by the product $e_1 e_2$, that is a new type of quantity known as a bivector., As shown in figure 2.1. Write for short $e_{1\,2} = e_1 e_2$

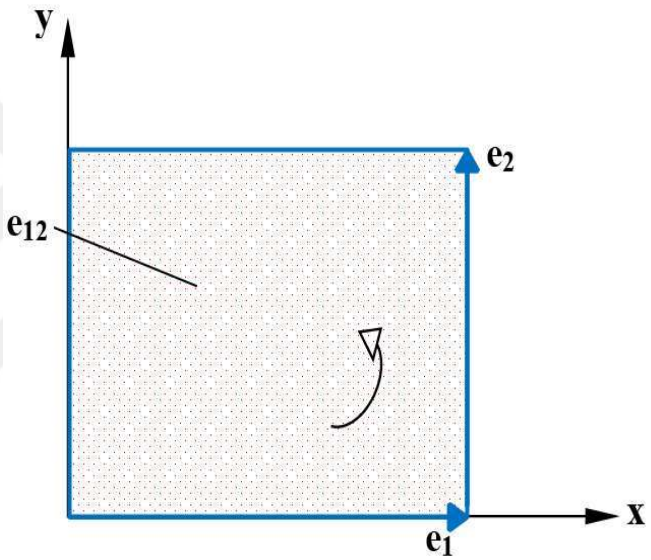

Figure 2.1. *Express the Bivectors*

In Using Clifford algebra, another product that is particularly helpful in addition to the point product may be generated with the assistance of the operator. This is known as an exterior product. This multiplication operator is denoted by a wedge (∧). If $\vec{a}$ and $\vec{b}$ are two vectors, whose outer product (wedge product) is given in the form $\vec{a} \wedge \vec{b}$ [11].

We construct two vectors $\vec{a} = a_1 \ e_1 + a_2 \ e_2$, $\vec{b} = b_1 e_1 + b_2 e_2$ Clifford product was its product of a scalar and a bivector.

$$ab = a_1 b_1 + a_2 b_2 + (a_1 b_2 - a_2 b_1) e_{12} \tag{2.12}$$

The scalar product "$\vec{a}$ dot $\vec{b}$",

$$\vec{a} \cdot \vec{b} = a_1 b_1 + a_2 b_2 \tag{2.13}$$

The exterior product "$\vec{a}$ wedge $\vec{b}$".

$$\vec{a} \wedge \vec{b} = (a_1 b_2 - a_2 b_1) e_{12} \tag{2.14}$$

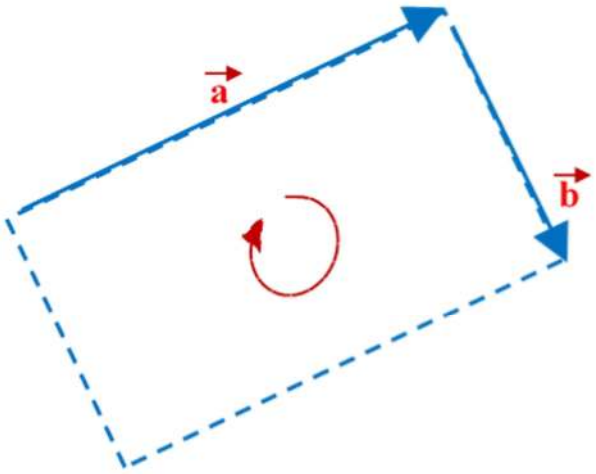

Figure 2.2. *Express the extend of vector* $\overrightarrow{(a)}$ *to vector* $\overrightarrow{(b)}$

The plane shown in figure 2.2 is a 2D subspace known as a bivector. The matching geometric shape is a parallelogram with a directed magnitude. $\vec{a}$ and $\vec{b}$ The rotation of the vector is in the clockwise direction. This parallelogram's area is $|a_1 b_2 - a_2 b_1|$.

The inverse extension of the vector $\vec{b}$ over the vector $\vec{a}$ leads to the same region as in figure 2.3.The outer product in the mathematical equation is not interchangeable, has the same magnitude but rotate in different directions. This is easily communicated by writing [11]

$$\vec{a} \wedge \vec{b} = -\vec{b} \wedge \vec{a} \tag{2.15}$$

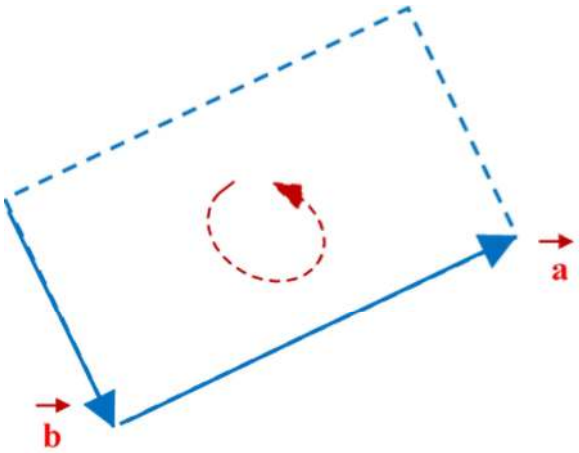

Figure 2.3. *Express the extend of vector* $\overrightarrow{(b)}$ *to vector* $\overrightarrow{(a)}$

When we take $\vec{a},\vec{b},\vec{c}$ are vectors an γ is scalar, we find

$$(\gamma\vec{a}) \wedge \vec{b} = \gamma(\vec{a} \wedge \vec{b}) \tag{2.16}$$

$$\lambda(\vec{a} \wedge \vec{b}) = (\vec{a} \wedge \vec{b})\,\gamma \tag{2.17}$$

$$\vec{a} \wedge (\vec{b} + \vec{c}) = (\vec{a} \wedge \vec{b}) + (\vec{a} \wedge \vec{c}) \tag{2.18}$$

Note: The bivector valued exterior product $\vec{a} \wedge \vec{b} = (a_1 b_2 - a_2 b_1)e_{12}$, which represents a plane area, should not be confused with the vector-valued cross product $\vec{a} \times \vec{b} = (a_1 b_2 - a_2 b_1)e_3$.

From Eq.s (2.12), (2.13) and (1.14) the Clifford product (geometric product) provide in the form

$$\vec{a}\vec{b} = \vec{a} \cdot \vec{b} + \vec{a} \wedge \vec{b} \tag{2.19}$$

The commutative rule $\vec{a} \cdot \vec{b} = \vec{b} \cdot \vec{a}$, in conjunction with the anticommutative rule in Eq (2.14), This implies the $\vec{a}\vec{b}$ to $\vec{b}\vec{a}$ relationship. Consequently

$$\vec{b}\vec{a} = \vec{a} \cdot \vec{b} - \vec{b} \wedge \vec{a} \tag{2.20}$$

By summing and subtracting Eqs. (2.19) and (2.20), we obtain

$$\vec{a} \cdot \vec{b} = \frac{1}{2}(\vec{a}\vec{b} + \vec{b}\vec{a}) \tag{2.21a}$$

and

$$\vec{a} \wedge \vec{b} = \frac{1}{2}(\vec{a}\vec{b} - \vec{b}\vec{a}) \tag{2.21b}$$

From Eqs.(2.21a) and (2.21b)

$$\vec{a}\vec{b} = \vec{b}\vec{a} \quad \Leftrightarrow \quad \vec{a} \wedge \vec{b} = 0 \quad \Leftrightarrow \quad \vec{a}\vec{b} = \vec{a} \cdot \vec{b} \quad \Leftrightarrow \quad \vec{a} \parallel \vec{b}$$

$$\vec{a}\vec{b} = -\vec{b}\vec{a} \quad \Leftrightarrow \quad \vec{a} \cdot \vec{b} = 0 \quad \Leftrightarrow \quad \vec{a}\vec{b} = \vec{a} \wedge \vec{b} \quad \Leftrightarrow \quad \vec{a} \perp \vec{b}$$

The inner product $\vec{a} \cdot \vec{b}$ 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 $\vec{a}\vec{b} = \vec{b}\vec{a}$.

As a result, the product $\vec{a}\vec{b}$ contains knowledge about the vectors' relative directions. Orthogonality is denoted by anticommutativity, while collinearity is denoted by commutativity [12].

A given vector in n-dimensional space can be represented by unit base vectors $(e_1, e_2, e_3, \ldots, e_n)$. In these 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.

We begin with the vectors $\vec{a}$ and $\vec{b}$, which are determined by the two-dimensional Euclidean planes unit base vectors e_1 and e_2 . a_1, a_2, b_1, b_2 scalars .We may express the vectors a and b in the following ways

$$\vec{a} = (a_1, a_2) \quad \text{or} \quad \vec{a} = a_1\ e_1 + a_2\ e_2$$

$$\vec{b} = (b_1, b_2) \quad \text{or} \quad \vec{b} = b_1\, e_1 + b_2\, e_2$$

and the outer product (wedge product),

$$\vec{a} \wedge \vec{b} = (a_1\, e_1 + a_2\, e_2) \wedge (b_1 e_1 + b_2 e_2)$$

$$= (a_1 e_1 \wedge b_1 e_1) + (a_1\, e_1 \wedge b_2\, e_2) + (a_2\, e_2 \wedge b_1 e_1) + a_2\ e_2 \wedge b_2\, e_2$$

$$= (a_1\ b_1 e_1 \wedge e_1) + (a_1\ b_2\, e_1 \wedge e_2) + (a_2\ b_1\, e_2 \wedge e_1) + (a_2\, b_2\, e_2 \wedge e_2) \tag{2.22}$$

In the outer product (wedge product),

$$(e_1 \wedge e_2) = e_{12} = \mathbf{I} \tag{2.23}$$

$$(e_2 \wedge e_1) = e_{21} = -e_{12} = -\mathbf{I} \tag{2.24}$$

Also because the vector cannot extend itself to form an area

$$(e_1 \wedge e_1) = 0 \quad \text{and} \quad (e_2 \wedge e_2) = 0 \tag{2.25}$$

We may create a table including all geometric product combinations with unit bases. for the two-dimensional Clifford space, The geometric product variants are shown in Table 2.1.

Table 2.1. *Possible unit basis combinations for the outer product in* Cl_2

$\wedge$	1	e_1	e_2	**I**
1	1	e_1	e_2	**I**
e_1	e_1	1	**I**	e_2
e_2	e_2	$-$**I**	1	$-e_1$
I	**I**	$-e_2$	e_1	-1

Where $\mathbf{I} = e_{12}$ and **I** is named as pseudovector of geometric algebra two-dimensional.

The wedge product over two dimensions is obtained by adding Eqs (2.23), (2.24), and (2.25) to Eq (2.22)

$$\vec{a} \wedge \vec{b} = (a_1\ b_2 - a_2\ b_1)\, e_{12} = (a_1\ b_2 - a_2\ b_1)\ \mathbf{I} \tag{2.26}$$

If we select the vectors $\vec{a}$ and $\vec{b}$ in three-dimensional euclidean space, we have the unit base vectors e_1 , e_2 and e_3 .

$$\vec{a} = a_1\ e_1 + a_2\ e_2 + a_3\ e_3 \quad \& \quad \vec{b} = b_1\, e_1 + b_2\, e_2 + b_3\, e_3$$

and the outer product (wedge product),

$$\begin{aligned} \vec{a} \wedge \vec{b} &= (a_1\ e_1 + a_2\ e_2 + a_3\ e_3) \wedge (b_1\, e_1 + b_2\, e_2 + b_3\, e_3) \\ &= (a_1\ e_1 \wedge b_1\, e_1) + (a_1\ e_1 \wedge b_2\, e_2) + (a_1\ e_1 \wedge b_3\, e_3) \\ &+ (a_2\ e_2 \wedge b_1\, e_1) + (a_2\ e_2 \wedge b_2\, e_2) + (a_2\ e_2 \wedge b_3\, e_3) \\ &+ (a_3\ e_3 \wedge b_1\, e_1) + (a_3\ e_3 \wedge b_2\, e_2) + (a_3\ e_3 \wedge b_3\, e_3). \end{aligned} \tag{2.27}$$

From Eqs (2.23) and (2.25) for $i \neq j$

$$e_i \wedge e_i = 0 \tag{2.28}$$

$$e_i \wedge e_j = e_{ij} \tag{2.29}$$

$$e_j \wedge e_i = -e_{ij} \tag{2.30}$$

Table 2.2 shows the geometric product possibilities of a three-dimensional Clifford space $\boldsymbol{Cl_3}$.

Table 2.2. *Possible unit base combinations for the outer product throughout* Cl_3

$\wedge$	$\mathbf{1}$	$\mathbf{e_1}$	$\mathbf{e_2}$	$\mathbf{e_3}$	$\mathbf{e_{12}}$	$\mathbf{e_{13}}$	$\mathbf{e_{23}}$	$\mathbf{I}$
$\mathbf{1}$	1	e_1	e_2	e_3	e_{12}	e_{13}	e_{23}	I
$\mathbf{e_1}$	e_1	1	e_{12}	e_{13}	e_2	e_3	I	e_{23}
$\mathbf{e_2}$	e_2	$-e_{12}$	1	e_{23}	$-e_1$	$-I$	e_3	$-e_{13}$
$\mathbf{e_3}$	e_3	$-e_{13}$	$-e_{123}$	1	I	$-e_1$	$-e_2$	e_{12}
$\mathbf{e_{12}}$	e_{12}	$-e_2$	e_1	I	-1	$-e_{23}$	e_{13}	$-e_3$
$\mathbf{e_{13}}$	e_{13}	$-e_3$	$-I$	e_1	e_{23}	-1	$-e_{12}$	e_2
$\mathbf{e_{23}}$	e_{23}	I	$-e_3$	e_2	$-e_{13}$	e_{12}	-1	$-e_1$
$\mathbf{I}$	I	e_{23}	$-e_{13}$	e_{12}	$-e_3$	e_2	$-e_1$	-1

Where $\mathbf{I} = e_{123}$. So that the Eq (2.27) will equal to

$$\vec{a} \wedge \vec{b} = (a_1\ b_2 - a_2\ b_1)e_{12} + (a_1\ b_3 - a_3\ b_1)e_{13} + (a_2\ b_3 - a_3\ b_2)\, e_{23} \tag{2.31}$$

The outer product of two vectors in three-dimensional Euclidean space was represented by the equation that is in the above.

Suppose we choose three vectors, $\vec{a}$, $\vec{b}$, and $\vec{c}$, the outer product of a vector $\vec{a}$ with such a bivector is expressed as $\vec{b} \wedge \vec{c}$ These are referred as a trivector, and a trivector $\vec{a} \wedge (\vec{b} \wedge \vec{c})$ may be defined as

$$\vec{a} \wedge (\vec{b} \wedge \vec{c}) = \frac{\overrightarrow{a\,b} \wedge \vec{c} + \vec{b} \wedge \overrightarrow{ca}}{2} = (\vec{a} \wedge \vec{b}) \wedge \vec{c} \tag{2.32}$$

This means that now the outer product of a bivector as well as a vector is symmetric.

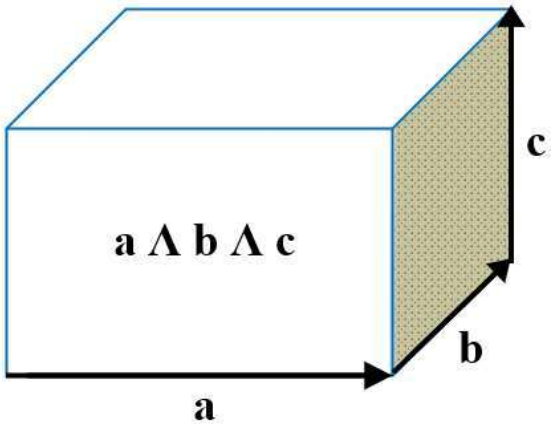

Figure 2.4. *Express the trivector*

As Extending a bivector to a third vector, as shown in figure 2.4, results in a directional volume element. This is known as a trivector. A 3-dimensional subspace is generated by the outer product of trivectors such as with a, b, and c. Unit base vectors in three-dimensional Euclidean space have been defined as

$$\mathrm{e}_1 \wedge \mathrm{e}_2 \wedge \mathrm{e}_1 = \mathrm{e}_{123} = \mathbf{I} \tag{2.33}$$

The concepts of scalar, vector, bivectors, and trivector were previously examined in 0-dimensional, 1-dimensional, 2-dimensional, 3-dimensional space. Now, the concept of k-degree will be expressed, showing the size of the subspace. 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 two and three dimensions in Tables 2.3 and 2.4, respectively.

Table 2.3. *Two-dimensional space degrees*

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

Table 2.4. *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
trivector	$\{e_{123}\}$	1

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

$$\binom{n}{k} = \frac{n!}{(n-k)!\,k!} \tag{2.34}$$

Here n is the dimension and k seems to be the base degree. For instance, in 3-dimensional space, when $n = 3, k = 1$, the number of bivector bases was

$$\binom{3}{1} = \frac{3!}{(3-1)!\,1!} = 3$$

This same geometric algebra of subspaces has been created by the unit bases that make up n spaces. It is termed the n-grade Clifford space and is shown as $\mathrm{cl_n}$. For instance, the unit bases for such two-dimensional Clifford space $\mathrm{cl_n}$ could be $\{1, \mathrm{e}_1, \mathrm{e}_2, \mathrm{e}_{12}\} = \{1, \mathrm{e}_1, \mathrm{e}_2, \mathbf{I}\}$.

Every portion of the two-dimensional Clifford space geometrical algebra was explained using linear combinations of unit base degrees. For instance, unit bases in three-dimensional Clifford space, cl_3 are $\{1, \mathrm{e}_1, \mathrm{e}_2, \mathrm{e}_3, \mathrm{e}_{12}, \mathrm{e}_{13}, \mathrm{e}_{23}, \mathrm{e}_{123}\}$.

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

$$\sum_{k=0}^{n}\binom{n}{k} = 2^{\mathrm{n}} \tag{2.35}$$

This Eq. (2.35) generates a large number of planes based on the mentioned algebraic combinations. Table 2.5 displays how to find the equation for a large number of geometric algebra.

Table 2.5. *cl_n unit's bases*

$\mathbf{cl_n}$	**Base Element**	**Total**
cl_0	$\{1\}$	2^0=1
cl_1	$\{1; e_1\}$	2^1=2
cl_2	$\{1; e_1, e_2; e_{12}\}$	2^2=4
cl_3	$\{1; e_1, e_2, e_3; e_{12}, e_{13}, e_{23}; e_{123}\}$	2^3=8
cl_4	$\{1; e_1, e_2, e_3, e_4; e_{12}, e_{13}, e_{14}, e_{23}, e_{24}, e_{34}; e_{123}, e_{124}, e_{134}, e_{234}; e_{1234}\}$	2^4=16

The element A in cl_n is represented with

$$A = a_0 + a_{11}e_1 + \cdots + a_{1i}e_n + a_{21}e_1e_2 + \cdots + a_{2i}e_1e_n + \cdots + a_{di}e_1e_2 \ldots\ldots e_n \quad (2.36)$$

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 in $(n + 1)$ as well as subspaces

$$cl_n = \Lambda^0\mathbb{R}^n + \Lambda^1\mathbb{R}^n + \ldots + \Lambda^n\mathbb{R}^n \quad (2.37)$$

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

The elements *A* of the Clifford algebra cl_n in Eq (2-36) 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 has 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 [13].

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.

$$A = \langle A\rangle_0 + \langle A\rangle_1 + \cdots + \langle A\rangle_n \quad (2.38)$$

Where $\langle A \rangle_p$ the p -vector portion of A, is the project of $A \in cl_n$ into $\Lambda^p \mathbb{R}^n$. $\langle \quad \rangle$ Is called the operator of the grade [12]. 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 $\vec{a} \rfloor \vec{b}$ produces a scalar 0

$$\langle \vec{a} \rangle_1 \rfloor \langle \vec{b} \rangle_1 = \langle \overrightarrow{ab} \rangle_0 \tag{2.39}$$

The vector is obtained by projecting the vector onto the bivector **B**

$$\langle \vec{a} \rangle_1 \rfloor \langle \mathbf{B} \rangle_2 = \langle \vec{a}\, \mathbf{B} \rangle_{2-1} \tag{2.40}$$

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

$$\langle \vec{a} \rangle_1 \wedge \langle \vec{b} \rangle_1 = \langle \overrightarrow{ab} \rangle_2 \tag{2.41}$$

This rule is applicable in general

$$\langle \mathbf{A} \rangle_s \rfloor \langle \mathbf{B} \rangle_t = \langle \mathbf{AB} \rangle_{s-t} \qquad \text{If} \quad s \leq t \tag{2.42}$$

$$\langle \mathbf{A} \rangle_s \rfloor \langle \mathbf{B} \rangle_t = 0 \qquad \text{If} \quad s > t \tag{2.43}$$

$$\langle \mathbf{A} \rangle_s \wedge \langle \mathbf{B} \rangle_t = \langle \mathbf{AB} \rangle_{s+t} \tag{2.44}$$

2.3. 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. The above principles may be easily algebraically manipulated to produce an endless number of geometrical equations. Any vector $\vec{s}$, for instance, may be divided into parallel and orthogonal components. Figure 2.5 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.

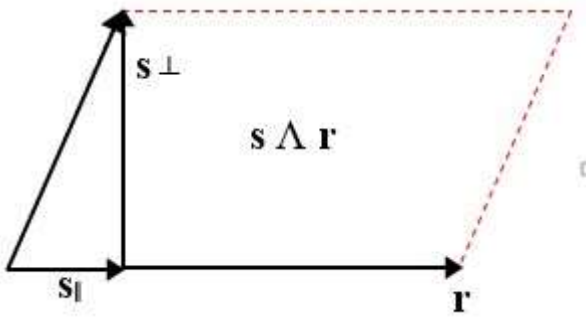

Figure 2.5. *Decomposition of s ⃗vector to components along and perpendicular to a vector r ⃗*

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

$$\mathrm{s}_{\parallel} = |\mathrm{s}| \cos\theta \frac{\mathrm{r}}{|r|} = |\mathrm{s}||\mathrm{r}| \cos\theta \frac{\mathrm{r}}{|r|^2} \tag{2.45}$$

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

$$\mathrm{s}_{\parallel} = (\mathrm{s} \cdot \mathrm{r}) \frac{\mathrm{r}}{|r|^2} = (\mathrm{s} \cdot \mathrm{r})\, r^{-1} \tag{2.46}$$

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

$$\mathrm{s}_{\perp} = \mathrm{s} - \mathrm{s}_{\parallel} = \mathrm{s} - (\mathrm{s} \cdot \mathrm{r})\, r^{-1} = (\mathrm{sr} - \mathrm{s} \cdot \mathrm{r})\, \mathrm{r}^{-1} = (\mathrm{s} \wedge \mathrm{r})\, \mathrm{r}^{-1} \tag{2.47}$$

The reflection of s across the line u as shown in figure 2.6 is acquired by sending $s = s_{\parallel} + s_{\perp}$ to $s' = s_{\parallel} - s_{\perp}$ where $\mathrm{s}_{\parallel} = (\mathrm{s} \cdot \mathrm{u})\mathrm{u}^{-1}$. The mirror image u′of u for s is then

$$\mathrm{s}' = \mathrm{usu}^{-1} \tag{2.48}$$

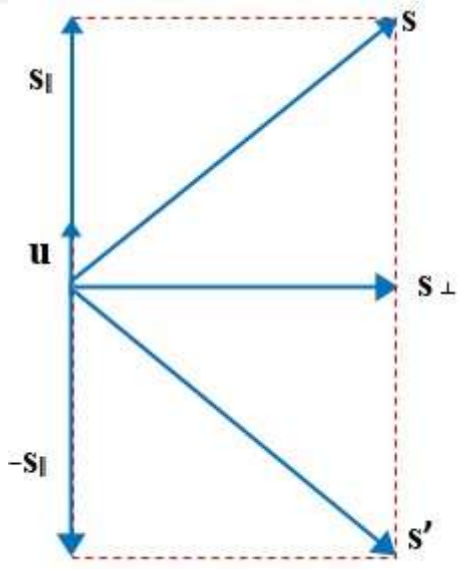

Figure 2.6. *Reflection of s along u*

We may represent the dot and outer products in Eq (2.14) in regards of the angle between both the vectors θ.

$$\vec{\mathrm{s}} \cdot \vec{\mathrm{r}} = \frac{1}{2}(\vec{\mathrm{s}}\vec{\mathrm{r}} + \vec{\mathrm{r}}\vec{\mathrm{s}}) = |\vec{\mathrm{s}}|\,|\vec{\mathrm{r}}|\, \cos\theta \tag{2.49}$$

$$\vec{s} \wedge \vec{r} = \frac{1}{2}\left(\vec{s}\vec{r} - \vec{r}\vec{s}\right) = i|\vec{s}|\,|\vec{r}|\sin\theta \tag{2.50}$$

Eqs. (2.49) and (2.50) 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 [9]

$$\vec{s}\vec{r} = \cos\theta + i\sin\theta = e^{i\theta} \tag{2.51}$$

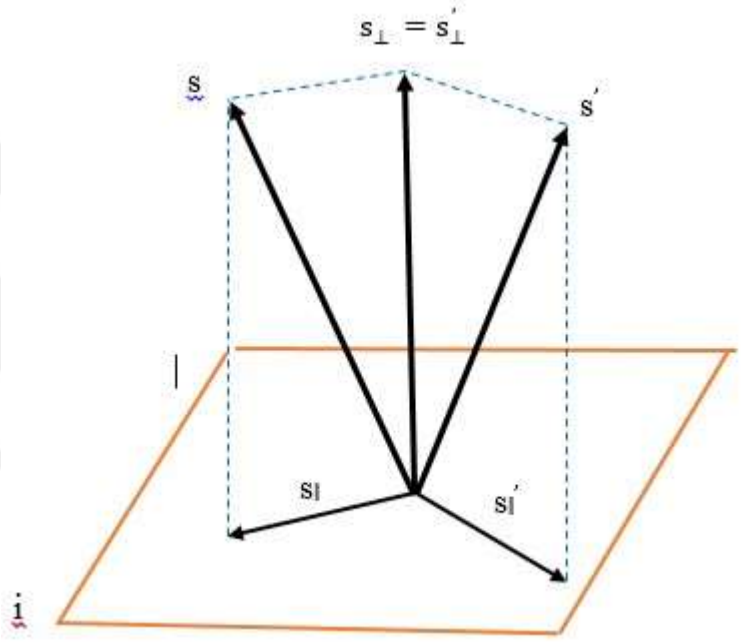

Figure 2.7. *Rotation of s vector s in the plane i*

The $e^{i\theta}$ exponential, commonly known as a two-dimensional rotor, is defined in Eq (2.51). As seen in figure 2.7, 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.

$$s' = s\,e^{i\theta} = s\cos\theta + si\sin\theta \tag{2.52}$$

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:

$$s\cos\theta + si\sin\theta = s\cos\theta - is\sin\theta = e^{-i\theta}s \tag{2.53}$$

Furthermore, we have

$$\cos\theta + i\sin\theta = \left(\cos\frac{\theta}{2} + i\sin\frac{\theta}{2}\right)^2 \tag{2.54}$$

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

$$y = e^{i\theta/2} \text{ and } y^{-1} = e^{-i\theta/2} \tag{2.55}$$

The same Eq (2.51) 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.

$$B' = e^{-i\varphi/2} B \; e^{i\varphi/2} \tag{2-56}$$

In ordinary vector algebra, such a simple equation does not exist. Geometric algebra is claimed to be the most successful means of representing rotations.

The spinor $e^{D/2}$, which specifies the total rotation of two sequential rotations, the first $e^{A/2}$, then the second $e^{B/2}$, is calculated by multiplying

$$e^{D/2} = e^{A/2}\, e^{B/2} \tag{2.57}$$

2.4. 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

$$\nabla_\beta q_i = \partial_{x_\beta} q_i \tag{2.58}$$

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

$$\nabla_\beta = \sum_i (\nabla_\beta q_i) \frac{\partial}{\partial q_i} \tag{2.59}$$

Where we utilize the subscript β in the vector round as to underline that these conclusions apply to several vector elements $x_1, x_2, \ldots$.

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

$$\nabla_\beta (F + G) = \nabla_\beta F + \nabla_\beta G \tag{2.60}$$

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

$$\nabla_\beta(\gamma G) = (\nabla_\beta \gamma)G + \gamma \nabla_\beta G \tag{2.61}$$

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

$$div_\beta f = \nabla_\beta \cdot f \tag{2.62}$$

$$curl_\beta f = \nabla_\beta \times f \tag{2.63}$$

By using geometric product definition we can write

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

$$= \nabla_\beta \cdot f + i\nabla_\beta \times f \tag{2.64}$$

As a result, the scalar component of the vector derivative of f is the divergence, and the dual 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

$$\nabla_\beta F = \nabla_\beta \cdot F + \nabla_\beta \wedge F \tag{2.65}$$

Eqs (2.60) and (2.61) 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

$$\nabla_\beta(FG) = \dot{\nabla}_\beta \dot{F}\, G + \dot{\nabla}_\beta F\, \dot{G} \tag{2.66}$$

Any internal coordinate's gradient may be evaluated using simple function derivatives in combination with the product and chain principles. Some of these essential identities may be easily measured by stating as in Eq (2-59) and applying

$$u_k u_j = -u_j u_k \qquad \text{For} \quad k \neq j \quad \text{and} \quad u_k^2 = 1 \tag{2.67}$$

As an instance,

$$\nabla_\beta X_\beta = \sum_{k,j}^{3} u_k u_j \frac{\partial x_{\beta_j}}{\partial x_{\beta_k}} = \sum_{k}^{3} u_k u_k \frac{\partial x_{\beta_k}}{\partial x_{\beta_k}} = 3 \tag{2.68}$$

$$\nabla_\beta\, a \cdot X_\beta = \sum_k^3 u_k \left(a \cdot \frac{\partial X_\beta}{\partial x_{\beta_k}} \right) = \sum_k^3 u_k\, a \cdot u_k = a = \nabla_\beta\, X_\beta \cdot a \tag{2.69}$$

For any regardless of X_β, by employing the product rule

$$\nabla_\beta x_\beta^2 = \nabla_\beta\, X_\beta \cdot X_\beta = \hat{\nabla_\beta} \hat{X_\beta} \cdot X_\beta + \hat{\nabla_\beta} X_\beta \cdot \hat{X_\beta} = 2X_\beta \tag{2.70}$$

Wher $x_\beta = |X_\beta|$

For instance, if $F\ (\lambda\ (x_\beta)$ has become a multivector function of the scalar parameter λ(x),

$$\nabla_\beta\, F\ \left(\lambda\left(x_\beta\right)\right) = \nabla_\beta\, \lambda\left(x_\beta\right) \frac{\partial F}{\partial \lambda} \tag{2.71}$$

Using the above-mentioned criteria, the following results may be proved:

$$\nabla_\beta\, X_\beta = 3 \tag{2.72}$$

$$\nabla_\beta\, X_\beta a = 3a \tag{2.73}$$

$$\nabla_\beta\, a\, X_\beta = -a \tag{2.74}$$

$$\nabla_\beta\, X_\beta \cdot B_p = pB_p \tag{2.75}$$

$$\nabla_\beta\, X_\beta \wedge B_p = (3-p)B_p \tag{2.76}$$

$$\nabla_\beta\, (X_\beta \times a) \cdot b = a \times b \tag{2.77}$$

$$\nabla_\beta\, (X_\beta \times a) \cdot (b \times c) = ba \cdot c - ca \cdot b \tag{2.78}$$

$$\nabla_\beta\, |X_\beta - a|^k = k|X_\beta - a|^{k-2}(X_\beta - a) \tag{2.79}$$

$$\nabla_\beta\, |X_\beta - a|^k (X_\beta - a) = (k+3)\, |X_\beta - a|^k \tag{2.80}$$

Where a, b, and c are vectors, $B_p = b_1 \wedge \ldots \wedge b_p$ is a p-blade independent of a vector x_β $(p = 1, 2, and\ 3)$, and $k = 0, \pm 1, \pm 2, \pm 3, ..$

3. OPERATORS FOR KINETIC ENERGY IN POLYATOMIC MOLECULES

3.1. 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. When the Schrodinger Eq(3.1) is solved, many wavefunctions Ψ_n 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].

$$\left(\hat{\mathrm{T}} + \hat{\mathrm{V}}\right)\Psi = \mathrm{E}\Psi \tag{3.1}$$

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.

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 electrons $\mathrm{X}_{\mathrm{N}+1}, \mathrm{X}_{\mathrm{N}+2}, \ldots, \mathrm{X}_{\mathrm{N}+\mathrm{P}}$ as well as the locations of nuclei $\mathrm{X}_1, \mathrm{X}_2, \ldots, \mathrm{X}_{\mathrm{N}}$.

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

$$\hat{\mathrm{T}} = -\frac{h^2}{8\pi^2}\sum_{\beta=1}^{\mathrm{N}+\mathrm{P}}\frac{\nabla_\beta^2}{m_\beta} \tag{3.2}$$

$$\hat{\mathrm{V}} = \frac{e^2}{8\pi\epsilon_o}\sum_{\beta}^{\mathrm{N}+\mathrm{P}}\sum_{\beta\neq\alpha}^{\mathrm{N}+\mathrm{P}}\frac{\mathrm{Z}_\beta\,\mathrm{Z}_\alpha}{|\mathrm{X}_\beta - \mathrm{X}_\alpha|} \tag{3.3}$$

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.

As every distance between the two charged particles is a variable, in the Schrodinger equation, the number of variables normally increase as the molecule's size increaseses. As a consequence, the two-particle hydrogen atom's Schrodinger equation has been obtained numerically. But for any atom containing particles bigger than the hydrogen atom, just approximate solutions can be determined. However, because more specificity comes at the expense of more accurate measurements, estimated results with extremely high precision can be achieved.

3.2. Approximation of Born-Oppenheimer

Analytical solutions to Eq (3.1) exists 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 Born-Oppenheimer approach takes into consideration the significant variation in nuclei and electron masses. The Born-Oppenheimer approach is based on the assumption that the mass of a molecule's atomic nucleus is substantially higher than that of an electron by more than 1000 times. Due to this difference, nuclei move significantly slower than electrons, which may respond practically instantly to nuclear displacements. Furthermore, the mutual force of attraction of $\frac{\mathrm{Z}e^2}{r^2}$ operates on an atomic nucleus and an electron related to having opposing charges, and as a response of this force, all particles accelerate, with the difference between atomic nuclei acceleration and electron acceleration exceeding 2000. Since this quantity of acceleration is negatively proportional to mass, That's the difference between the acceleration of electron and the acceleration of atomic nuclei [14].

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 electronic energy E_e obtained by solving the electronic Schrodinger equation at the nuclear configuration $\{\mathrm{X}_1, \mathrm{X}_2, \dots, \mathrm{X}_\mathrm{N}\}$is equivalent to the price of the potential

$V_{nucl}(\mathrm{X}_1, \mathrm{X}_2, \ldots, \mathrm{X}_\mathrm{N})$ that the nuclei get owing to mutual repulsion and electron fast mobility [16].

The mathematical analysis of nuclear movements is simplified through separating nuclear movements into vibrational, rotational, and translational modes. Vibrational motions allow the distances between both the component nuclei to shift. The rotating movements change the location of the whole molecule in space.The translational motion is the 3D movement of a whole molecule. Determining the velocity of a molecule's center of mass can also be used to identify it.

Because the wave function of the molecule can be modeled as the wave function for electronic movements Ψ_e, the wave function for translational motions of the mass center Ψ_t, the wave function for rotational motions Ψ_r, and the wave function for vibrational motions Ψ_v as a result of dividing the nuclear motions, the wave equation of the molecule can be written as

$$\Psi_{molecule} = \Psi_e \Psi_t \Psi_r \Psi_v \tag{3.4}$$

The nuclei's wave function, on the other hand, $\Psi_{nucl} = \Psi_t \Psi_r \Psi_v$ so that the Eq (3.4) can write as

$$\Psi_{molecule} = \Psi_e \Psi_{nucl} \tag{3.5}$$

We describe the Hamiltonian for a molecule using the approximation

$$\mathrm{H}_{molecule} = \mathrm{H_e} + \mathrm{H}_t + \mathrm{H}_r + \mathrm{H}_v = \mathrm{H_e} + \mathrm{H_{nucl}} \tag{3.6}$$

The multiple electronic, vibrational, and rotational movements, on the other hand, are distinct of one another. The Schrödinger wave equation may be written using Eqs (3.4) and (3.6)

$$\mathrm{H}_{molecule}\Psi_{molecule} = (\mathrm{H_e} + \mathrm{H}_t + \mathrm{H}_r + \mathrm{H}_v)\Psi_e \Psi_t \Psi_r \Psi_v$$

$$\mathrm{H}_{molecule}\Psi_{molecule} = \Psi_\mathrm{t}\Psi_\mathrm{r}\Psi_\mathrm{v}(\mathrm{H_e}\Psi_\mathrm{e}) + \Psi_r \Psi_v \Psi_e(\mathrm{H}_t\Psi_t)$$

$$+\Psi_e \Psi_t \Psi_v(\mathrm{H}_r\Psi_r) + \Psi_e \Psi_t \Psi_r(\mathrm{H}_v\Psi_v)$$

$$\mathrm{H}_{molecule}\Psi_{molecule} = \Psi_\mathrm{t}\Psi_\mathrm{r}\Psi_\mathrm{v}(\mathrm{E}_e\Psi_e) + \Psi_r \Psi_v \Psi_e(\mathrm{E}_t\Psi_t)$$

$$+\Psi_e \Psi_t \Psi_v(\mathrm{E}_r\Psi_r) + \Psi_e \Psi_t \Psi_r(\mathrm{E}_v\Psi_v)$$

$$H_{molecule}\Psi_{molecule} = (E_e + E_t + E_r + E_v)\,\Psi_e\Psi_t\Psi_r\Psi_v \tag{3.7}$$

$$H_{molecule}\Psi_{molecule} = E_{molecule}\Psi_{molecule} \tag{3.8}$$

From Eqs (3.7) and (3.8), the energy of the molecule is

$$E_{molecule} = E_e + E_t + E_r + E_v \tag{3.9}$$

A molecule's energy is the total of the energies produced by various forms of motion. We may express Schrodinger's equation as follows by using aforementioned formulae

$$H_{molecule}\Psi_{molecule} = E_e\Psi_e + E_{nucl}\Psi_{nucl} \tag{3.9}$$

Using the Eq (3.1) operator of The kinetic energy and the operator of potential energy are combined to form the Hamiltonian operator

$$H_{molecule}\Psi_{molecule} = \left(\hat{T}_{molecule} + \hat{V}_{molecule}\right)\Psi_{molecule}$$

$$\left(\hat{T}_e + \hat{V}_e\right)\Psi_e + \left(\hat{T}_{nucl} + \hat{V}_{nucl}\right)\Psi_{nucl} = E_e\Psi_e + E_{nucl}\Psi_{nucl} \tag{3.10}$$

The Schrodinger equation, which is dependent on both nuclei and electron coordinates, is written as Eq (3.10), and we can obtain the Schrodinger equation that is solely reliant on nuclei coordinates from Eq (3.10)

$$\left(\hat{T}_{nucl} + \hat{V}_{nucl}\right)\Psi_{nucl} = E_{nucl}\Psi_{nucl} \tag{3.11}$$

We may get the translational, vibrational, and rotational modes and energies of the molecule under inquiry by resolving the Schrodinger Eq (3.11) [1].

3.3. 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. The overall number of movements in a molecule remains unchanged when the same atoms are joined together, but it is more convenient to restructure how we define them.

In a Atomic nuclei hold virtually constant locations in respect to one another in a molecule created of many atoms. The motion of the molecule's center of mass is distinct, and thus needs three coordinates to characterize. To create a better approximation, the

motion of the center of mass is regardless of how the atoms move in regard to the center of mass or each other. As a result, the coordinates remain $3N-3$ after doing this.

The amount of accessible rotational movements is determined by the number of different axes that the molecule may rotate around. We can use any combination of three or more non-parallel axes in 3D space, and the molecule may be thought to rotate around each one independently of its motion over to the other axes, resulting in an axis being represented as a group of any three other axes. This means that the molecule can have a maximum of three unique rotating movements [16].

If the molecule seems to be linear, that is, its atoms have been arranged in a single direction, we can also use the axis of the molecular as being one of the rotation axes, with another two axes selected to be perpendicular to each other and to the axis of the molecular , so we can see how the rotation in around molecular axis is not a rotation at all and has no impact on the direction of the molecular . As a consequence, if the molecule is linear, we still need two coordinates to characterize all rotational movements. The residual coordinates are $3N-5$ after the necessary coordinates for representing the movements of the transitional and rotational have been applied.

Vibrations are the movements that are utilized to characterize how atoms move in respect to one another. Fundamental vibrations must have been explained using the coordinates left over after the movements of the translational and rotational have been defined. A non-linear molecule takes $3N-6$ coordinates to identify its vibrations, whereas a linear molecule takes $3N-5$ coordinates.

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 $\chi,\theta,\phi,$ 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 $\{\upsilon_1,\upsilon_2,\upsilon_3\}$.

$$\upsilon_i' = R^{\dagger}\upsilon_i R \tag{3.12}$$

Where R is the rotor that was described by

$$R = e^{i\chi\upsilon_3/2}e^{i\theta\ \ _1/2}e^{i\phi\upsilon_3/2} = e^{i\chi\ \ '_3/2}e^{i\theta\upsilon_1'/2}e^{i\phi\ \ '_3/2} = e^{i\phi\upsilon_3/2}e^{i\theta n_2/2}e^{i\chi\upsilon_3'/2} \tag{3.13}$$

When n_2 is determined by the formulae

$$n_2 = \frac{v_3 \times v_3'}{|v_3 \times v_3'|} \tag{3.14}$$

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

$$\boldsymbol{X} = \sum_{\beta=1}^{N} \frac{m_\beta X_\beta}{M} \tag{3.15}$$

From Eq (3-15), M is the molecule's mass, and it's written as

$$\mathrm{M} = \sum_{\beta}^{\mathrm{N}} m_\beta \tag{3.16}$$

The chain rule describes the vector derivative operator ∇_β as

$$\nabla_\beta = \sum_{i}^{3\mathrm{N}} e_\beta^{(q_i)} \frac{\partial}{\partial q_i} \tag{3.17}$$

From Eq (3.17), q_i denotes the internal coordinates, which are understood that

$$q_{3N-5} = \phi, \qquad q_{3N-4} = \theta, \qquad q_{3N-3} = \chi$$
$$q_{3N-2} = X_1, \quad q_{3N-1} = X_2\,, \quad q_{3N} = X_3 \tag{3.18}$$

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

$$e_\beta^{(q_i)} = \nabla_\beta q_i \tag{3.19}$$

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 [16]

$$\frac{dq_i}{dt} = \sum_{\beta}^{N} e_\beta^{(q_i)} \cdot \frac{dX_\beta}{dt} \tag{3.20}$$

By geometric algebra, internal coordinates may be discussed in terms of nucleus position vectors. Their gradients can then be obtained algebraic expressions by modifying the atomic position vectors, as discussed in Section 2.4 of Chapter 1. After

that, we'll utilize this knowledge to characterize the operator of the kinetic energy of a polyatomic molecule .

3.4. Frames for Body

Each fixed location vector for body can be rotated to the fixed location vector for space as seen from Eq(3.13) ,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

$$s_\beta = R^\dagger s'_\beta R \tag{3.21}$$

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 [17].

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

$$a = \sum_\beta c_\beta X_\beta \tag{3.22}$$

$$b = \sum_\beta d_\beta X_\beta \tag{3.23}$$

The internal coordinates can affect the coefficients c_β and d_β, where

$$a \times b \neq 0 \tag{3.24}$$

where these vectors are not collinear

$$\sum_\beta c_\beta = 0 \tag{3.25}$$

$$\sum_\beta d_\beta = 0 \tag{3.26}$$

The axes of the body are represented as

$$v'_3 = \frac{a}{|a|} \tag{3.27}$$

$$v'_2 = \frac{a \times b}{|a \times b|} \tag{3.28}$$

$$v_1' = v_2' \times v_3' \tag{3.29}$$

Since any value for a and b can be chosen, the measurement vectors for the rotational part can be easily obtained using the present system (geometric algebra) by defining the body axes (or directions a and b) as will be discussed later [16,18].

3.5. Operators for Kinetic Energy in Polyatomic Molecules in Terms of Geometric Algebra

Since the beginning of modern quantum theory, the subject of Hamiltonian quantification of multi-particle systems such as polyatomic particles has piqued researchers' interest. While the operator for potential energy is the same as in the classical situation, quantization the operator for kinetic energy is more difficult, particularly in confined systems.

The majority of the issues are caused by operator ordering and establishing the quantum mechanical counterparts of classical values. several prescriptions were used to obtain a correct expression for the operator of the kinetic energy in classical mechanics, with the equivalent in quantum mechanics. In general, most prescriptions do not provide a correct expression for the quantum mechanical operator of kinetic energy [18]. This is true if the representation is sought by replacing the momentum of generalized p_i in the classical Hamiltonian with the operator of the partial derivative $-i\hbar\frac{\partial}{\partial q_i}$, or by using correspondence concepts like rule of Weyl or ordering of Born-Jordan [20].

Regardless of the ordering of the generalized velocities and components of the covariant metric tensor. By substituting the generalized velocity $\dot{q}_i$, the classical Lagrangian cannot be converted into a valid quantum mechanical operator of the kinetic energy [21].

We will use 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 the operator of the angular mome .

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

$$\hat{\mathrm{T}}^{(nucl)} = -\frac{h^2}{8\pi^2}\sum_{\beta}^{\mathrm{N}}\frac{1}{m_\beta}\nabla_\beta^2 \tag{3.30}$$

Where m_β is the mass of the atom β and ∇_β is the vector derivative (gradient) operator with respect to the spatial position X_β of the nucleus β.

When the representation of coordinate of Eq (3.17) is replaced into Eq (3.30), the operator of kinetic energy reads as

$$\hat{\mathrm{T}} = -\frac{h^2}{8\pi^2}\sum_\beta^{\mathrm{N}}\sum_j^{3\mathrm{N}}\frac{1}{m_\beta}\nabla_\beta \cdot e_\beta^{(q_j)}\frac{\partial}{\partial q_j} \tag{3.32}$$

The Eq (3.32) may be written in a number of different ways, one of which is a " covariant metric tensor $g^{(q_iq_j)}$" such that the $g^{(q_iq_j)}$ is giving in the form

$$g^{(q_iq_j)} = \sum_\beta^{\mathrm{N}}\frac{1}{m_\beta}e_\beta^{q_j}\cdot e_\beta^{q_i} \tag{3.33}$$

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

$$\sum_\beta^{\mathrm{N}}\frac{1}{m_\beta}\nabla_\beta \cdot e_\beta^{(q_j)}\frac{\partial}{\partial q_j} = \frac{1}{z^{-1/2}}\sum_i\frac{\partial}{\partial q_i}z^{-1/2}g^{(q_iq_j)}\frac{\partial}{\partial q_j} \tag{3.34}$$

Where $z = det\ g^{(q_iq_j)}$ is the covariant metric tensor determinant.

The operator of the kinetic energy is as follows

$$\hat{\mathrm{T}}^{(nucl)} = -\frac{h^2}{8\pi^2}\sum_{ij}^{3\mathrm{N}}\left(\frac{\partial}{\partial q_i}+\frac{1}{z^{-1/2}}\frac{\partial z^{-1/2}}{\partial q_i}\right)g^{(q_iq_j)}\frac{\partial}{\partial q_j} \tag{3.35}$$

To be more specific, it is assumed that all integrations are done over the volume-element $d\tau = Jd\ _1dq_2$ ..., where $J = \left|det\ g^{(q_iq_j)}\right|^{-1/2} = z^{-1/2}$, where J is called Jacobian.

If the volume element $d\tau_k = kdq_1dq_2$ ..., is used instead of the volume element $d\tau = Jd\ _1dq_2$ ..., the corresponding operator of kinetic energy $\hat{T}_k$ is provided as [22].

$$\hat{T}_k^{(nucl)} = J^{1/2}k^{-1/2}\hat{T}^{(nucl)}k^{1/2}J^{-1/2} \tag{3.36}$$

The vibrational and rotational degrees of freedom are completely isolated from translation.

If we have the matrix $[\omega]$ with elements $[\omega]_{ij} = g^{(q_iq_j)}$as follows:

$$\begin{bmatrix}\omega^{(int)} & 0\\ 0^T & \omega^{(tranl)}\end{bmatrix} \tag{3.37}$$

This Martic is split into a translational and internal block .where $\omega^{(tranl)}$ denotes a translational block of size 3×3, $\omega^{(int)}$ an internal block of size $(3N-3) \times (3N-3)$, 0 denotes a $(3N-3) \times 3$ block of zeros, and 0^T denotes a $3 \times (3N-3)$ block of zeros.

The measurement vectors for the coordinates of Cartesian of the center of mass can be written as

$$e_{\beta}^{(\mathrm{X}_i)} = \nabla_{\beta} \mathrm{X}_i = \sum_{\alpha}^{\mathrm{N}} \nabla_{\beta} \frac{m_{\alpha} v_i \cdot \mathrm{X}_{\alpha}}{M} = \frac{m_{\alpha}}{M} v_i \tag{3.38}$$

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

$$\sum_{\beta} \nabla_{\beta} q_i = 0 \tag{3.39}$$

$$\sum_{\beta} \nabla_{\beta} B_i = 0 \tag{3.40}$$

When Eqs (3.37), (3.38), (3.39) and (3-40) are taken into account, The internal and translational parts can be combined to form the operator of the kinetic energy.

$$\widehat{\mathrm{T}}^{(nucl)} = \widehat{\mathrm{T}}^{(int)} + \widehat{\mathrm{T}}^{(transl)} \tag{3.41}$$

The internal part

$$\widehat{\mathrm{T}}^{(int)} = -\frac{h^2}{8\pi^2} \sum_{ij}^{3\mathrm{N}-3} \left(\frac{\partial}{\partial q_i} + \frac{1}{z^{-1/2}} \frac{\partial z^{-1/2}}{\partial q_i} \right) g^{(q_i q_j)} \frac{\partial}{\partial q_j} \tag{3.42}$$

The translational part

$$\widehat{\mathrm{T}}^{(transl)} = -\frac{h^2}{8\pi^2} \sum_{i=1}^{3} \frac{\partial^2}{\partial \mathrm{X}_i^2} \tag{3.43}$$

It is common to represent the rotational portion of each gradient operator in the forms of the components of the fixed body $\hat{\imath}_i = v_i' \cdot \hat{\mathrm{I}}$ of the angular momentum operator $\hat{\mathrm{I}}$, rather than the partial derivative operators $\frac{\partial}{\partial B_i}$,from the [4] we can see the relation

$$\left(\nabla_{\beta} \phi\right) \frac{\partial}{\partial \phi} + \left(\nabla_{\beta} \theta\right) \frac{\partial}{\partial \theta} + \left(\nabla_{\beta} \chi\right) \frac{\partial}{\partial \chi} = \sum_{i}^{3} e_{\beta}^{(L_i)} \hat{\imath}_i \tag{3.44}$$

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

$$e_{\beta}^{(L_k)} = \nabla_a \left[(a \cdot \nabla_{\beta} v_i') \cdot v_j' \right] \tag{3.45}$$

Where $e_{\beta}^{(L_k)}$related to the nucleus β and the kth part of the angular momentum operator L.

The kinetic energy operator's internal component in Eq (3.41) can be written succinctly as

$$\hat{\mathrm{T}}^{(int)} = -\frac{h^2}{8\pi^2}\sum_{ij}^{3N-3}\hat{\Gamma}_i^{\dagger}\, g^{(q_i q_j)}\hat{\Gamma}_j \tag{3.46}$$

The $\hat{\Gamma}_j$ in equation (3.46) 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 covariant metric tensor [23].

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

$$g^{(ij)} = \sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(q_i-3)}\cdot e_{\beta}^{(q_j-3)} \qquad \text{for } (i,j = 4,5,\ldots,3N-3) \tag{3.7a}$$

$$g^{(q_i q_j)} = \sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(q_i)}\cdot e_{\beta}^{(q_j)} = \sum_{\beta}^{N}\frac{1}{m_\beta}(\nabla_\beta q_i)\cdot(\nabla_\beta q_j) \quad \text{for } (i,j = 1,2,\ldots,3N-6) \tag{3.7b}$$

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

$$\mathrm{g^{(ij)}} = \sum_{\beta}^{\mathrm{N}}\frac{1}{\mathrm{m_\beta}}\mathrm{e}_{\beta}^{(\mathrm{q_i}-3)}\cdot\mathrm{e}_{\beta}^{(\mathrm{L_j})} \quad \text{for } (i = 4,5,\ldots,3N-3) \quad \text{and } j = (1,2,3) \tag{3.48a}$$

$$g^{(L_j q_i)} = \sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(L_j)}\cdot\nabla_\beta q_i \quad \text{for } (\mathrm{i} = 1,2,\ldots,3\mathrm{N}-6) \quad \text{and } j = (1,2,3) \tag{3.48b}$$

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

$$g^{(ij)} = g^{(L_i L_j)} = \sum_{\beta}^{N}\frac{1}{m_\beta}e_{\beta}^{(L_i)}\cdot e_{\beta}^{(L_j)} \qquad \text{for } i,j = (1,2,3) \tag{3.49}$$

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

$$\nabla_{\beta} B_j = e_{\beta}^{(B_j)} = \sum_{i=1}^{3} e_{\beta}^{(L_i)} A_{ij}^{-1} \tag{3.50}$$

Where ($B_1 = \phi$, $B_1 = \theta$, *and* $B_1 = \chi$ are the same as before), A_{ij}^{-1} is the element of the matrix's inverse as $A_{ij}^{-1} = [A]_{ij}^{-1}$, that's the matrix is $[A]_{ij} = n_i \cdot \upsilon_j'$, n_i is the vectors of nodal lines ($n_1 = \upsilon_3, n_2 = \frac{\upsilon_3 \times \upsilon_3'}{|\upsilon_3 \times \upsilon_3'|} = \frac{\upsilon_3 \times \upsilon_3'}{\sin\theta}$ and $n_3 = \upsilon_3'$).

The matrix [A] is

$$[A] = \begin{bmatrix} \sin\theta \sin\chi & \sin\theta\, c & \\ \cos\chi & -\sin\chi & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{3.51a}$$

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

$$[A]^{-1} = \begin{bmatrix} \frac{\sin\chi}{\sin\theta} & \cos\chi & -\frac{\cos\theta \sin\chi}{\sin\theta} \\ \frac{\cos\chi}{\sin\theta} & -\sin\chi & -\frac{\cos\theta \cos\chi}{\sin\theta} \\ 0 & 0 & 1 \end{bmatrix} \tag{3.51b}$$

As a result, It is possible to write

$$g^{(B_j B_l)} = \sum_{\beta}^{N} \frac{1}{m_\beta} e_{\beta}^{(B_j)} \cdot e_{\beta}^{(B_l)} = \sum_{ik}^{3} \sum_{\beta}^{N} \frac{1}{m_\beta} e_{\beta}^{(L_i)} \cdot e_{\beta}^{(L_k)} A_{ij}^{-1} A_{kl}^{-1} = \sum_{ik}^{3} g^{(L_i L_k)} A_{ij}^{-1} A_{kl}^{-1} \tag{3.52}$$

$$g^{(B_j q_l)} = \sum_{\beta}^{N} \frac{1}{m_\beta} e_{\beta}^{(B_j)} \cdot e_{\beta}^{(q_l)} = \sum_{ik}^{3} \sum_{\beta}^{N} \frac{1}{m_\beta} e_{\beta}^{(L_i)} \cdot e_{\beta}^{(q_l)} A_{ij}^{-1} = \sum_{i}^{3} g^{(L_i q_l)} A_{ij}^{-1} \tag{3.53}$$

Where q_l is a coordinate for a shape.

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

$$z' = (\sin\theta)^2 z \tag{3.54}$$

(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 (X_1, X_2, X_3) respectively).

The determinant z' is strictly determined by the shape coordinates. Since the components of the metric tensor can be complex functions of the coordinates of shape, evaluating z' using traditional methods can be boring. The volume-element of integration $d\tau$ can be described using geometric algebra as a product of N volume-elements, each with a set of three coordinates [24].

$$d\tau = |d^3X_1||d^3X_2| \dots |d^3X_N| = Jd\ {}_1dq_2 \dots dq_{3N-6}d\phi d\theta d\chi dX_1 dX_2 dX_3$$

as a product, the volume element is produced

$$d\tau = \frac{|d^3r_1||d^3r_2|\dots|d^3r_N|}{|det[c]|^3} \tag{3.55}$$

Where $r_\beta = \sum_\alpha^N c_\beta^\alpha \mathrm{X}_\alpha \ \ (\beta = 1,2, \dots N-1)$ are certain linear combinations of the position vectors of nuclear, where r_N is the center-of-mass position vector.The $N \times N$ matrix $[c]$ contains elements $[c]_{ij} = c_i^{(j)}$ It is not impacted by the positions of the nuclear [25].

The bond vectors $s_{\alpha\beta} = \mathrm{X}_\beta - \mathrm{X}_\alpha$ are ideal choices for transcriptionally invariant $r_N$vectors, such as lengths of bonds and angles for the valences. The volume-elements $\left|d^3r_\beta\right|$ are given specifically in terms of angles of Euler, coordinates of shape, and Cartesian coordinates for the center-of-mass as follwing [25]

$$|d^3r_1| = \frac{d\phi d\theta dq_1}{|(\nabla_{r_1}\phi)\wedge(\nabla_{r_1}\theta)\wedge(\nabla_{r_1}q_1)|} = \frac{r_1^3 \sin\theta\ d\phi d\theta dq_1}{|r_1\cdot(\nabla_{r_1}q_1)|} \tag{3.56}$$

$$|d^3r_2| = \frac{d\chi\ \ {}_2dq_3}{\left|\left(\nabla_{r_2}\chi\right)\wedge\left(\nabla_{r_2}q_2\right)\wedge\left(\nabla_{r_2}q_3\right)\right|}$$

$$= \frac{r_2\ \sin^2\theta_{12} d\chi dq_2 dq_3}{|(v_{r_1}\times v_{r_2})\wedge(\nabla_{r_2}q_2)\wedge(\nabla_{r_2}q_3)|} \tag{3.57}$$

$$\left|d^3r_\beta\right| = \frac{dq_i dq_j dq_k}{\left|\left(\nabla_{r_\beta}q_i\right)\wedge\left(\nabla_{r_\beta}q_j\right)\wedge\left(\nabla_{r_\beta}q_k\right)\right|} \ \text{for}\ \beta = 2,3,\dots,N-1 \tag{3.58}$$

$$|d^3r_N| = dX_1 dX_2 dX_3 \tag{3.59}$$

This form, unlike all others, works for any arbitrary coordinates of the shape q_i.

The Jacobian J will be used to measure the inverse of the square root of the covariant metric tensor [26]

$$z'^{-1/2} = \frac{J}{si} \prod_{\beta}^{N} m_{\beta}^{3/2} \tag{3.60}$$

The measuring vectors for the rotation part for a general geometrically specified frame's of body stated formulations

$$e_{\beta}^{L_1} = -\frac{c_{\beta} v_2' + \sum_{\alpha} X_{\alpha} \cdot v_2' \nabla_{\beta} c_{\alpha}}{a} \tag{3.61}$$

$$e_{\beta}^{L_2} = \frac{c_{\beta} v_1' + \sum_{\alpha} X_{\alpha} \cdot v_1' \nabla_{\beta} c_{\alpha}}{a} \tag{3.62}$$

$$e_{\beta}^{L_3} = \frac{1}{|a \times b|} \left[b \cdot v_3' \left(c_{\beta} v_2' + \sum_{\alpha} X_{\alpha} \cdot v_2' \nabla_{\beta} c_{\alpha} \right) - a \left(d_{\beta} v_2' + \sum_{\alpha} X_{\alpha} \cdot v_2' \nabla_{\beta} d_{\alpha} \right) \right] \tag{3.63}$$

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 that 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 [16,17].

4. LAGRANGIAN FORMULATION AND COVARIANT MEASURING VECTORS

Lagrangian concepts are developed in 1788 by the Italian-French astronomer and mathematician Joseph-Louis Lagrange. They are a variant of classical physics based on the fixed action theorem. A judicious selection of variables will reduce the amount of computing required to describe and understand the motion of a N particle system. We start in this section with a summary of context information and an overview of fundamental concepts.

4.1. Kinematics

Kinematics is a branch of physics developed from classical mechanics that deals of bodies (objects), points, and body systems without considering the forces acting them to move [26].

Kinematics is a branch of analysis that is sometimes known as "geometry of motion" and is sometimes recognized as a branch of mathematics [28]. We can suppose that the coordinate kinetic system has m particles and also that the system of coordinate is Cartesian.

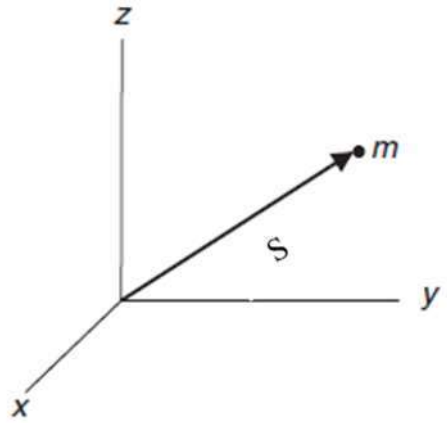

Figure 4.1. *The $\vec{s}$ vector determines a particle's position*

The time rate at which a particle's position changes is described as velocity $\mathcal{V}$, and the time rate at which its velocity changes is described as acceleration a. So, the velocity and acceleration of a particle can be represented as follows

$$\mathcal{V} = \frac{ds}{dt} = \dot{s} \tag{4.1}$$

$$a = \frac{dv}{dt} = \frac{d^2s}{dt^2} = \ddot{s} \tag{4.2}$$

The equation for acceleration a is a function of $\dot{s}, \ddot{s}$ and t. Thus Eq (4.2) is considered as the equation of motion which is a second-order differential equation in which the solution determines the position as a function of time $s = s(t)$.

The equation of motion may be theoretically and numerically solved by providing numerical solutions for every rational acceleration value and analytical solutions for particular acceleration values [9].

Object dropping, also known as projectile motion, is a common example of 2D motion that is usually applied in Cartesian coordinates (u, v) since it happens in a plane. A further instance of binary movement is an object orbiting one other object, which indicates that the particle is going to move in a circular or elliptical path, and the location of the object can be calculated by two coordinates since this motion is plane, and the coordinates have been using are the planar polar coordinates (s, θ) with the relations of transformation equations in Cartesian coordinates given below

$$x = s\cos\theta \tag{4.3}$$

$$y = s\sin\theta \tag{4.4}$$

To convert a point in the (x, y) plane into a point in the (s, θ) plane these transformations are used.

4.2. Generalized Coordinates

We shall assume that the vectors define the particle's orientation in two dimensions, the locations of a point can be defined by its rectangular coordinates (u, v) or by its polar coordinates$(s, \theta, \emptyset)$. In three dimensions, the particle's direction can be determined described using the rectangular coordinates (u, v, w), the spherical coordinates (s, θ, ϕ) or the cylindrical coordinates (ρ, ϕ, z) .

Three coordinates are needed to identify a single particle in 3 dimensions. A two-particle device requires 6 coordinates. In Cartesian coordinates, the position of two particles may be represented by a sequence of integers $(u_1, v_1, w_1, u_2, v_2, w_2)$

A system with N particles requires $3N$ coordinates and the locations of all these particles $(u_1, v_1, w_1, u_2, v_2, w_2, \dots, u_N, v_N, w_N)$ are the Cartesian coordinates.Some situations can be solved in one coordinate system, but others are easier to be solved in another. The coordinates are indicated by q_i, and the associated velocities are represented by $\dot{q}_J$. q_i Is referred to general linear coordinates [29].

The generalized coordinate's variables must properly describe every potential location of the system relative to the original location. For instance, drawing a schematic of the object in its present position ought to be achievable using only the variables of the generalized coordinates and the fixed dimensions [29]. We may select the suitable set of coordinate systems for each problem. For example, in one problem, you may use spherical coordinates, and the coordinates q_i adopt the values $(s, \theta, \emptyset)$, but in another, you may use cylindrical coordinates, and $q_i = (\rho, \phi, z)$ [3]. A system's degree of freedom is the smallest number of generalized coordinates necessary to identify its position [30].

The translation equations must be firstly understood and that is, we must know how to use the relations in order to translate from Cartesian to generalized coordinates,

$$q_1 = q_1(u_1, v_1, w_1, u_1, v_2, \dots, w_N, t)$$

$$q_2 = q_2(u_1, v_1, w_1, u_1, v_2, \dots, w_N, t)$$

.

.

.

$$q_{3N} = q_{3N}(u_1, v_1, w_1, u_1, v_2, \dots, w_N, t) \tag{4.5}$$

Inverse relations are referred by transformation formulas. Therefore, we have formula for an N-particle system,

$$u_1 = u_1(q_1, q_2, q_3, \dots, q_{3N}, t)$$

$$v_1 = v_1(q_1, q_2, q_3, \dots, q_{3N}, t)$$

.

.

$$w_1 = w_1(q_1, q_2, q_3, \dots, q_{3N}, t) \tag{4.6}$$

The letter u in this section is often used to describe all Cartesian coordinates. Thus, for a single particle (u, v, w), is written (u_1, u_2, u_3) and, for N particles $(u_1, v_1, \dots, w_N)$ is expressed as $(u_1, u_2, \dots, u_n)$.

We generally expect that if we know the transformation formulas from q_c to u_c, we could do the inverse transformation from u_c to q_c, however that's not always true. The inverse transformation is conceivable if the Jacobian determinant of Eq (4.5) isn't really zero [29]. That's means

$$\frac{\partial(q_1, q_2, \dots, q_n)}{\partial(u_1, u_2, \dots, u_n)} = \begin{vmatrix} \partial q_1/\partial u_1 & \partial q_1/\partial u_2 & \dots & \partial q_1/\partial u_n \\ \vdots & \vdots & & \vdots \\ \partial q_n/\partial u_1 & \partial q_n/\partial u_2 & \dots & \partial q_n/\partial u_n \end{vmatrix} \neq 0 \tag{4.7}$$

We'll apply Cartesian coordinates, cylindrical coordinates, or whichever coordinate system is most suitable for the case while solving problems. Mathematical analysis, on the other hand, almost usually expresses the problem with the concept of generalized coordinates$(q_1, q_2, q_3, \dots, q_n)$. As can be seen, generalized coordinates are more than just a rotating unit.

4.3. Velocity in Generalized Coordinates

As it previously stated, the position of a particle at a certain point in space can be defined using either generalized coordinates q_i or Cartesian coordinates u_i. The transformation equation connects or links these coordinate systems together (q_i) or by using Cartesian coordinates (u_i). These coordinate systems are connected or linked together by the transformation equation:

$$u_i = u_i(q_1, q_2, q_3, t) \tag{4.8}$$

It is important to note that u_i has been one of the three Cartesian coordinates of a single particle that is dependent on all of the generalized coordinates.

Because the particle's velocity in the u_i direction equals $\mathcal{V}_i$ by description, the velocity components are now specified in terms of generalized coordinates.

$$\mathcal{V}_i = \frac{du_i}{dt} \tag{4.9}$$

However, because u_i is a characteristic for q_c, we may be using the chain rule to distinguish.

$$\mathcal{V}_i = \sum_{k=1}^{3} \frac{\partial u_i}{\partial q_k} \frac{dq_k}{dt} + \frac{\partial u_i}{\partial t} = \sum_{k=1}^{3} \frac{\partial u_i}{\partial q_k} \dot{q_k} + \frac{\partial u_i}{\partial t} \tag{4.10}$$

We now have a very important relation with the partial derivative of $\mathcal{V}_i$ with regard to $\dot{q_k}$. Because the sequence of the derivatives has no effect on the combined 2nd partial derivative, we can read

$$\frac{\partial}{\partial \dot{q_j}} \frac{\partial u_i}{\partial t} = \frac{\partial}{\partial t} \frac{\partial u_i}{\partial \dot{q_j}} \tag{4.11}$$

Because the generalized velocity has no effect on u_i, u_i does not depend on $\dot{q_j}$, implying that

$$\frac{\partial u_i}{\partial \dot{q_J}} = 0 \tag{4.12}$$

We shall compute the partial derivative of velocity $\mathcal{V}_i$ with regards to $\dot{q}_J$ by Eq (4.10). This has the impact of

$$\frac{\partial \mathcal{V}_i}{\partial \dot{q}_J} = \frac{\partial}{\partial \dot{q}_J} \sum_{k=1}^{3} \frac{\partial u_i}{\partial q_k} \dot{q_k} + \frac{\partial}{\partial \dot{q}_J} \frac{\partial u_i}{\partial t}$$

And from Eq(4.12) we can write

$$\frac{\partial \mathcal{V}_i}{\partial \dot{q}_J} = \frac{\partial}{\partial \dot{q}_J} \sum_{k=1}^{3} \frac{\partial u_i}{\partial q_k} \dot{q_k} + 0$$

$$\frac{\partial \mathcal{V}_i}{\partial \dot{q}_J} = \sum_{k=1}^{3} \left(\frac{\partial}{\partial \dot{q}_J} \frac{\partial u_i}{\partial q_k} \right) \dot{q_k} + \sum_{k=1}^{3} \left(\frac{\partial u_i}{\partial q_k} \frac{\partial \dot{q_k}}{\partial \dot{q}_J} \right)$$

$$\frac{\partial \mathcal{V}_i}{\partial \dot{q}_J} = o + \sum_{k=1}^{3} \frac{\partial u_i}{\partial q_k} \delta_{ij}$$

$$\frac{\partial \mathcal{V}_i}{\partial \dot{q}_J} = \frac{\partial u_i}{\partial q_j}$$

As a result, we can conclude

$$\frac{\partial v_i}{\partial \dot{q_j}} = \frac{\partial u_i}{\partial q_j} \tag{4.13}$$

According to this connection, the Cartesian velocity v_i is connected to the generalized velocity $\dot{q_j}$ in the same manner as the Cartesian coordinate is connected to the generalized coordinate. This connection is highly useful in many extended coordinate derivations [28].

4.4. Constraints

The degrees of freedom are the separate coordinates which are used to precisely determine the position of each system component. In all physical structure, there is some degree of freedom.

To characterize the motion of a free particle in a certain system, we require three coordinates, let them be (u, v, w), which indicates that the number of degrees of freedom required to describe this system is three coordinates. In a system of two free particles, you should determine the location of all free particles. Every particle includes three degrees of freedom, for a sum of six degrees of freedom in the system. A mechanical system composed of N free particles will also have $3N$ degrees of freedom in general.

When a structure is connected to constraint forces, it is frequently required to minimize the number of coordinates utilized to define motion. Thus, the movement of a particle on a plane, for instance, may be expressed in terms of u and$v$, with the caveat that the w coordinate (specified as perpendicular to the surface) is supplied by $w = constant$.

When k requirements operate on an N -particle system, the number of generalized coordinates used to characterize the motion is $(3N - k)$. (While the number of Cartesian coordinates stays $3N$, the number of generalized (free) coordinates is$(3N - k)$.

A constraint is really a connection between coordinates if the constraint's equation (the link between coordinates) can still be written in the form

$$f(q_1, q_1, \dots, q_n, t) = 0 \tag{4.14}$$

The constraint is therefore known as holonomic.

4.5. The Equations of Lagrange for Constrained Motion

The challenge of developing a comprehensive approach for solving equations of motion under holonomic constraints stays unfinished. Lagrange devised a solution to the issue. Instead of nonparametric limitations, he employs parametric constraints.

The parametric equation for the surface is $u = u(q_1, q_2, t)$, where q_1 and q_2 are separate scalar parameters (or coordinates), and the specific t dependence provides for the possibility of the surface moving. For both fixed and variable variables, the parametric equation defines a "coordinate curve" on the area with a tangent vector at each point.

$$e_1 = \partial_{q_1} u \tag{4.15}$$

Here ∂_{q_1} denotes the derivative with regard to q_1.

As illustrated in figure 4.2, the parameter q_2 generates a tangent vector e_2 at each location on the graph.

$$e_\gamma = \partial_{q_\gamma} u \tag{4.16}$$

Here $\gamma = 1,2$.

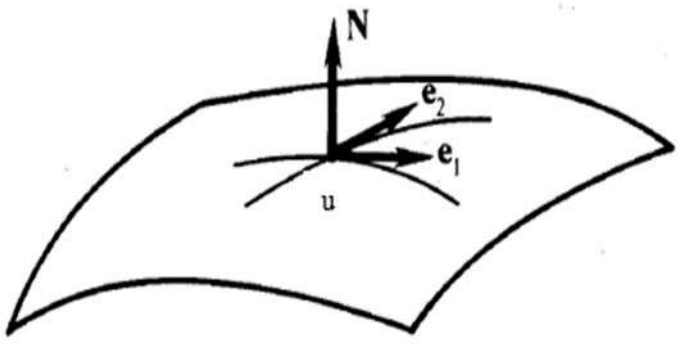

Figure 4.2. *A constraint surface's coordinate curves and tangent vectors*

The motion equation is written as follows

$$m\ddot{u} = F + N \tag{4.17}$$

Here N the constraint is force and F is an external force.

Multiplication of Eq (4.17) by e_γ , we now have

$$m\ddot{u} \cdot e_\gamma = F \cdot e_\gamma + N \cdot e_\gamma \tag{4.18}$$

Since N is perpendicular to the constraint surface, we have

$$N \cdot e_\gamma = 0 \tag{4.19}$$

So Eq (4.18) will be

$$m\ddot{u} \cdot e_\gamma = F \cdot e_\gamma \tag{4.20}$$

Here Eq (4.20) provides us the independent components of the surface equation of motion. These equations can be represented as a set of differential equations for the q_γ coordinates alone.

The parametric equation explains the trajectory of the particle on the constraint surface.

$$u = u(q_1(t), q_2(t), t) \tag{4.21}$$

As a consequence, the velocity is determined by the parametric equation.

$$\dot{u} = \sum_\gamma \dot{q_\gamma}\, \partial_{q_\gamma} u + \partial_t u \tag{4.22}$$

Whereas the total is the sum among all the values of γ Hence

$$\partial_{\dot{q_\gamma}} \dot{u} = \partial_{q_\gamma} u = e_\gamma$$

and

$$\dot{e}_\gamma = \left(\sum_\rho \dot{q}_\rho\, \partial_{q_\rho} + \partial_t\right) \partial_{q_\gamma} u = \partial_{q_\gamma} \dot{u} \tag{4.23}$$

Here $\partial_{q_\gamma} \dot{q}_\rho = 0$ for all values of γ and ρ. The left side can also be rewritten of Eq (4.19) using these facts

$$m\ddot{u} \cdot e_\gamma = m\left\{\frac{d}{dt}(\dot{u} \cdot e_\gamma) - \dot{u} \cdot \dot{e}_\gamma\right\}$$

but

$$\dot{u} \cdot e_\gamma = \dot{u} \cdot \partial_{\dot{q}_\gamma} \dot{u} = \frac{1}{2} \partial_{\dot{q}_\gamma} (\dot{u}^2)$$

and

$$\dot{u} \cdot \dot{e}_\gamma = \dot{u} \cdot \left(\partial_{q_\gamma} \dot{u}\right) = \frac{1}{2} \partial_{q_\gamma} (\dot{u}^2)$$

Hence

$$m\ddot{u} \cdot e_\gamma = \frac{d}{dt}\left(\partial_{\dot{q}_\gamma} K - \partial_{q_\gamma} K\right)$$

Here $K = \frac{1}{2} m\dot{u}^2$ represents kinetic energy of the particle

Now, new notation Q_γ is introduced as

$$Q_\gamma = F \cdot e_\gamma = F \cdot (\partial_{q_\gamma} u) \tag{4.24}$$

Eq (4.20) may be expressed as a component of force in the direction e_γ.

$$\frac{d}{dt}\left(\partial_{\dot{q}_\gamma} K\right) - \partial_{q_\gamma} K = Q_\gamma \tag{4.25}$$

This would be known as Lagrange's equation.

For apply Lagrange's equation, designate K and $Q_\gamma$as elements of q_γ and $\dot{q}_\gamma$ using the parametric formulations of constraint $u = u(q, t)$, where q alludes to the full system of coordinates q_γ . Thus, we may obtain

$$K = \frac{1}{2} m\dot{u}^2 = \frac{1}{2} \sum_\gamma \sum_\rho a_{\gamma\rho} \dot{q}_\gamma \dot{q}_\rho + \sum_\gamma b_\gamma \dot{q}_\gamma + c \tag{4.26}$$

Here the coefficients are given by

$$a_{\gamma\rho} = a_{\gamma\rho}(q, t) = m e_\gamma \cdot e_\rho$$

$$b_\gamma = b_\gamma(q, t) = m e_\gamma \cdot \partial_t u$$

$$c = c(q, t) = \frac{1}{2} m(\partial_t u)^2 \tag{4.27}$$

If the external force is conservative, $F = -\nabla V(u)$, therefore the constraint equation will be as follows

$V = V\big(u(q, t)\big) = V(q, t)$ and $Q_\gamma = -\left(\partial_{q_\gamma} u\right) \cdot \nabla V = -\partial_{q_\gamma} V$ so Lagrange's Eq(4.25) can be written as

$$\frac{d}{dt}\left(\partial_{q_\gamma} \cdot L\right) - \partial_{q_\gamma} L = 0 \tag{4.28}$$

Here $L = L(\dot{q}, q. t)$ is the previously described Lagrangian, also denoted as

$$L = K - V \tag{4.29}$$

It's critical to note that the number of coordinates in the limiting equation seems to have no bearing on how we get Lagrange's equation. All that is necessary in Eq (4.23) is to add the precise number of coordinates from Eq (4.25).

If the particle is bound to a curve rather than a surface, the parameterization equations have only one coordinate, and the motion may indeed be approximated using only one Lagrange equation. If no constraints exist, three coordinates are required, and Lagrange's technique is just a way of describing the coordinate's approximation for Newton's equation.

4.6. 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 $q_i^{\cdot}$, as for conservative systems (given to time-independent or no limitations at all) [31].

$$T = \frac{1}{2}\sum_{ij}^{k} q_i^{\cdot}\, g_{q_i q_j} q_i^{\cdot} \tag{4.30}$$

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

$$g_{q_i q_j} = \sum_{\beta}^{N} m_\beta e_{q_i}^{(\beta)} \cdot e_{q_j}^{(\beta)} \tag{4.31}$$

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

$$e_{q_i}^{(\beta)} = \frac{\partial x_\beta}{\partial q_i} \tag{4.32}$$

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 (3.20), the result is

$$\frac{\partial q_i}{\partial t} = \sum_{\beta}^{\mathrm{N}} e_{\beta}^{(q_i)} \cdot \frac{\partial \mathrm{X}_\beta}{\partial t}$$

$$\frac{\partial q_i}{\partial q_j} = \sum_{\beta}^{\mathrm{N}} e_{\beta}^{(q_i)} \cdot \frac{\partial \mathrm{X}_{\beta}}{\partial q_j} = \sum_{\beta}^{N} \frac{\partial \mathrm{X}_{\beta}}{\partial q_j} \cdot \nabla_{\beta} q_i = \delta_{ij} \tag{4.33}$$

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

$$\sum_{\beta}^{N} e_{q_i}^{(\beta)} \cdot e_{\beta}^{(q_j)} = \delta_{ij} \tag{4.34}$$

Second, by utilizing the representation of ∇_{β} in equation (3.17), it is demonstrated that

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

$$\nabla_{\beta} (A_{\bar{r}} \mathrm{X}_{\alpha}) = \delta_{\alpha\beta} \sum_{i}^{3\mathrm{N}} e_{\beta}^{(q_i)} A_{\bar{r}} \frac{\partial \mathrm{X}_{\alpha}}{\partial q_i} = \delta_{\alpha\beta} \sum_{i}^{3\mathrm{N}} e_{\beta}^{(q_i)} A_{\bar{r}} e_{q_i}^{(\alpha)} \tag{4.35}$$

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

$$(A_{\bar{r}} \mathrm{X}_{\alpha}) = A_{\bar{r}} \cdot \mathrm{X}_{\alpha} + A_{\bar{r}} \wedge \mathrm{X}_{\alpha} \tag{4.36}$$

$$(A_{\bar{r}} \mathrm{X}_{\alpha}) = (-1)^{r+1} A_{\bar{r}} \cdot \mathrm{X}_{\alpha} + (-1)^{r} A_{\bar{r}} \wedge \mathrm{X}_{\alpha} \tag{4.37}$$

and

$$\nabla_{\beta} \mathrm{X}_{\alpha} \cdot A_{\bar{r}} = \delta_{\alpha\beta} r A_{\bar{r}} \tag{4.38}$$

$$\nabla_{\beta} \mathrm{X}_{\alpha} \wedge A_{\bar{r}} = \delta_{\alpha\beta} (3 - r) A_{\bar{r}} \tag{4.39}$$

By substituting the equations (4.37), (4.38) into (4.34) , yeilds

$$\sum_{i}^{3\mathrm{N}} e_{\beta}^{(q_i)} A_{\bar{r}} e_{q_i}^{(\alpha)} = \delta_{\alpha\beta} (-1)^{r} (3 - 2r) A_{\bar{r}} \tag{4.40}$$

Where there are a number of special cases can be obtained from equation (4.39), by setting $A_{\bar{r}} = 1$ (so $r = 0$) the identity

$$\sum_{i}^{3\mathrm{N}} e_{\beta}^{(q_i)} e_{q_i}^{(\alpha)} = 3\delta_{\alpha\beta} \tag{4.41}$$

By changing the Eq (4.40) into a combination of inner and outer components

$$\sum_i^{3\mathrm{N}} e_\beta^{(q_i)} \cdot e_{q_i}^{(\alpha)} = 3\delta_{\alpha\beta} \tag{4.42}$$

$$\sum_i^{3\mathrm{N}} e_\beta^{(q_i)} \times e_{q_i}^{(\alpha)} = 0 \tag{4.43}$$

Moreover, if the inner products are explained by means of geometric products and Eq (4.39) is applied, it is easy to show that

$$\sum_k^{3N} g^{(q_i q_k)} g_{(q_k q_j)} = \delta_{ij} \tag{4.44}$$

5. RESULTS AND CONCLUSIONS

Clifford's and many others' objective, as stated in the introduction, 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 thesis 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 thesis 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.

Quantization of representations of constrained coordinate systems, on the other hand, has been a focus of significant research over the past fifty years or more. There are several methods and applications, however not all offered solutions are compatible. Geometric algebra, I think, may be applied not only to reformulate the issue but also to achieve practical advantages in determining the operators of the kinetic energy which is constrained. It should also provide an answer to the question of when and why alternative methods succeed or fail to produce a solution.

Finally, if the main goal is to comprehend nature's power, this algebra allows us to better comprehend the nature of polyatomic molecules, which are more simply stated.

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