Article

Not peer-reviewed version

Particle Swarms in N-Dimensional Simplex Conformations Quantum Mechanical and Topological Problems

Ramon Carbó-Dorca *

Posted Date: 29 January 2026

doi: 10.20944/preprints202601.2273.v1

Keywords: simplices; hypercubes; canonical and reciprocal basis sets; simplex particle swarms; simplex topological matrices; quantum mechanical simplices; time-dependent simplices

Article

Particle Swarms in N-Dimensional Simplex Conformations Quantum Mechanical and Topological Problems

Ramon Carbó-Dorca

[1] Institut de Química Computacional i Catalisi Universitat de Girona (Catalonia) Spain

[2] Ronin Institute for Independent Research 2.0 (RIIS 2.0)

* Correspondence: ramoncarbodorca@gmail.com

Abstract

$N-$ dimensional simplices, apart of their highly symmetric properties, exhibit interesting properties, both in the structure of the coordinates of their $P=N+1$ vertices and in the uniform distances between pairs of them. Relationships of simplices with the vertices of $N-$dimensional hypercubes are also of interest. Discussing these facts in depth as an introduction, the present study examines the implications of the coordinate structure of simplices for the Theoretical and Quantum Mechanical formalism, applied to swarms of P particles located at the vertices of a simplex. Also, the properties of the topological matrices that represent such a distance-conformation will be studied. Some interesting results arise from this analysis. Among others, a paradox about the existence of swarms of P particles with $N-$dimensional simplex-vertex distance structure and the possibility of overcoming it, allowing the description of an $N-$dimensional description of the particles' location. A brief discussion on the time-dependence of simplex coordinates is also provided.

Keywords: simplices; hypercubes; canonical and reciprocal basis sets; simplex particle swarms; simplex topological matrices; quantum mechanical simplices; time-dependent simplices

---

1. Introduction

Interest in hypercubes has been a common research topic in this laboratory since the dawn of the century; see, for example, references [1–10].

Such scientific exploration history has promoted a varied number of applications, including the earlier redefinition of fuzzy sets and the induction of new general and solid algorithms to distinguish elements of a set, which in turn induced the concept of tagged sets [11–13], used in molecular structure-properties relations [8,9,12], and quantum similarity problems [9,12,13].

From the mathematical point of view, hypercubes, among other things, allowed us to generalize the concept of sign to vectors and matrices [14] and formalize the structure of vector spaces [8,13]. The role of simplices within hypercubes was also studied [15].

Therefore, the present article must be considered a continuation of such previous work, begun 25 years ago. Being the simplices an infinite set of highly symmetric structures in any dimension and homothetic size, perhaps such a simplex, excuse the redundancy, simple constructs might be suitable for this journal.

The paper will be organized as follows. *First*, the construction of simplices will be presented with as much originality as possible. *Next*, the representation of particle swarms using a simplex structure will be discussed, with emphasis on its topological nature. The role and algebraic properties of matrices bearing the simplex structure will also be studied within this part. *After this*, the role of the unity matrix in this study of particle simplices will be presented. The paper will *continue* by discussing the nature of the overlap and Gaussian functions centered at simplex vertices. To be *followed* by a schematic description of how to build the usual quantum-mechanical integrals entering particle interactions. *And then*, the structure of the quantum-mechanical particle swarm energy and Hückel-like matrices within a simplex framework will be discussed. *Before* the discussion and conclusions that close this study, some considerations for constructing a possible time-dependent simplices forms will be presented.

2. Construction of N-Dimensional Simplices and Their Relations with Hypercubes

An N-dimensional tetrahedron or simplex can be easily constructed using first the equidistant set of vectors of the canonical basis set as vertices:

$$\mathbf{C}_N = \left\{ |\mathbf{v}_I\rangle = |\mathbf{e}_I\rangle \,\middle|\, I = 1, N \right\} \quad (1)$$

corresponding to the columns of the $(N \times N)$ unit matrix:

$$\mathbf{I}_N = \left\{ I_{IJ} = \delta_{IJ} \,\middle|\, I, J = 1, N \right\} \quad (2)$$

And in a second step, a simplex of such a dimension has an extra vertex $|\mathbf{v}_{N+1}\rangle = |\mathbf{v}_P\rangle$, a new vector equidistant from all the canonical basis set elements.

To obtain the extra vertex which really defines the simplex, one must be aware that the squared Euclidean distance between two elements of the set $\mathbf{C}_N$, can be easily calculated using the set of equalities:

$$\begin{gathered} \forall I, J = 1, N \wedge I \neq J : D^2 = D_{IJ}^2 = \left\| |\mathbf{e}_I\rangle - |\mathbf{e}_J\rangle \right\|^2 = \\ \langle \mathbf{e}_I | \mathbf{e}_I \rangle + \langle \mathbf{e}_J | \mathbf{e}_J \rangle - 2 \langle \mathbf{e}_I | \mathbf{e}_J \rangle = 1 + 1 - 2 \cdot 0 = 2 \end{gathered} \quad (3)$$

therefore, the squared distance matrix between the set $\mathbf{C}_N$ corresponds to a $(N \times N)$ structure, which can be written as:

$$\mathbf{D}^{[2]} = \left\{ D_{IJ}^2 = 2\delta(I \neq J) \,\middle|\, I, J = 1, N \right\} \quad (4)$$

where the expression $\delta(I \neq J)$ is a logical Kronecker delta, here equivalent to:

$$\delta(I \neq J) = 1 - \delta(I = J) \equiv 1 - \delta_{IJ} \quad (5)$$

In general, being L any logical expression, a logical Kronecker delta might be defined in such a way that:

$$\delta[L = .true.] = 1 \wedge \delta[L = .false.] = 0 \quad (6)$$

Now, the extra vertex of the simplex can be calculated as a homothecy of the N-dimensional unity vector $|\mathbf{1}\rangle$, that is:

$$|\mathbf{v}_P\rangle = \lambda |\mathbf{1}\rangle = \lambda (1,1,1,\ldots,1)^T \quad (7)$$

 doi:10.20944/preprints202601.2273.v1

In such a way that the squared Euclidean distance from the vector $|\mathbf{v}_P\rangle$ to any element of the set $\mathbf{C}_N$, will be equal to 2. Therefore, one can set the N equivalent equations:

$$\forall I=1,N: \left\| |\mathbf{e}_I\rangle - |\mathbf{v}_P\rangle \right\|^2 = \left\| |\mathbf{e}_I\rangle - \lambda|\mathbf{1}\rangle \right\|^2 = \\ \langle \mathbf{e}_I|\mathbf{e}_I\rangle + \lambda^2\langle \mathbf{1}|\mathbf{1}\rangle - 2\lambda\langle \mathbf{e}_I|\mathbf{1}\rangle = 1+\lambda^2 N - 2\lambda = 2, \quad (8)$$

that results in the definition of the homothecy of the unity vector as the higher root of the polynomial:

$$N\lambda^2 - 2\lambda - 1 = 0 \Rightarrow \lambda = N^{-1}\left(1 \pm \sqrt{N+1}\right) \quad (9)$$

considering that the negative sign will provide negative homotheties of the unity vector, so the most immediate action consists of only using the positive sign of the square root.

2.1. Comparison with Hypercubes

Now one can compare this simplex result with the structure of the N-dimensional hypercubes. Binary hypercubic structures can be defined as 2^N sequences of N bits as vertices, but, for computational purposes, the set of $\{0,1\}$ binary elements can also be taken as being natural numbers, transforming a binary or Boolean hypercube into, say: a unit natural one.

The canonical basis set is common to both simplex and hypercubic structures; however, the vertex $|\mathbf{v}_P\rangle$, except in the case $N=3$, when $\lambda=1$ and the result $|\mathbf{v}_P\rangle = |\mathbf{1}\rangle$, matches a canonical hypercube vertex, the one which, in binary form, can be called after Mersenne. In any other dimension $N \neq 3$, a canonical simplex cannot match its hypercubic counterpart. That is, the vertex $|\mathbf{v}_P\rangle$ cannot be equal to a hypercube one.

It is worth noting that the complete match between the simplex and the hypercube occurs only in the three-dimensional case.

2.2. Simplex Homotheties

However, simplices and hypercubes can be constructed with distances different from the canonical ones by multiplying each vertex by the same scalar, obtaining a homothetic structure with the same form but different vertex distances.

Of course, one can construct simplices with smaller or greater inter-vertex distances than the canonical structure as defined here. This will be possible by performing the same homothecy to every vertex, with a homothetic factor h greater than 1 or less than 1 to enlarge or reduce the structure of the vertices and thus the distances between them.

2.3. Centroid of any Simplex

Therefore, the set of N-dimensional simplex vertices can be written, using $P=N+1$, as: $\mathbf{V}_N = \{\mathbf{C}_N; |\mathbf{v}_P\rangle\}$, the set of the canonical basis $\mathbf{C}_N$ already defined in the equation **Error! Reference source not found.**, where is arbitrarily taken to be the first N vertices of the simplex.

Another interesting feature of simplices is the simple structure of the *centroid* of an N-dimensional simplex.

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 29 January 2026 doi:10.20944/preprints202601.2273.v1

A vector that is equidistant from all the simplex vertices can be described as the mean of the sum of all the simplex vertices vectors in the set $\mathbf{V}_N$, that is:

$$\begin{aligned} |\mathbf{c}_N\rangle &= (N+1)^{-1}\left(\sum_{I=1}^{N}|\mathbf{e}_I\rangle + |\mathbf{v}_P\rangle\right) \\ &= (N+1)^{-1}\left[1+N^{-1}\left(1+\sqrt{N+1}\right)\right]|\mathbf{1}\rangle \\ &= (N+1)^{-1}[1+\lambda]|\mathbf{1}\rangle = \theta|\mathbf{1}\rangle \Leftarrow \theta = (N+1)^{-1}[1+\lambda]. \end{aligned} \tag{10}$$

This expression becomes quite simple when: $N=3$. As one obtains $\theta = \frac{1}{2}$, in this case, a coincident result with the centroid of the 3-dimensional unit cube.

2.4. Characterization of Simplices

Being the N-dimensional simplex nature described by the set of vertices $\mathbf{V}_N = \{\mathbf{C}_N; |\mathbf{v}_P\rangle\}$, one might add some precise definitions to the two parts of any simplex. The set $\mathbf{C}_N$ can be referred to as the *canonical* simplex *vertices*, and the vector $|\mathbf{v}_P\rangle$ can be named as the *rotor vertex*.

It has been chosen this way, as one can consider such a vector $|\mathbf{v}_P\rangle$ as some well-defined axis in the direction of the Mersenne vertex $|\mathbf{1}\rangle$, around which one can rotate the canonical vertices without destroying their structure or the fixed Euclidean distances between them and the rotor vertex. Any simplex is invariant under an arbitrary rotation performed by the rotor vertex as the rotation axis.

The cardinality of the canonical set of vertices is augmented or diminished by one element as the dimension of the simplex structure does the same.

In fact, what characterizes a simplex as such is precisely the set of $\mathbf{C}_N$, while the extra rotor vertex can be observed as a consequence of the dimension choice, which selects the canonical simplex vertices and thus formalizes the rotor vertex as such.

The canonical set of vertices primarily validates the basic structure of a simplex in any dimension, as it does in a hypercube, too.

In this manner, the canonical simplex set of vertices, when considered as the canonical basis vectors, is also present as the vertex elements of the hypercubic structure in the same dimension.

The difference lies in the connection that the simplices bear between the canonical vertices with their squared distance, which is the same for all of them.

However, this homogeneous distance among simplex vertices is not a choice that the canonical basis set permits to be implemented in any hypercube, as the distances between vertices are not homogeneous in this construction.

2.5. The Simplex Particle Swarm Paradox

After the presentation of the structure of simplices, one can ask for the possibility that a set of P particles (or objects) can be displayed in such a manner that the distances between them are all equal. The results, however, show that in three-dimensional space, only four particles or objects can fit such a distance structure.

It has been shown that simplices in N-dimensional spaces can hold P particles only at homogeneous distances. Thus, to describe a particle swarm without restrictions, spaces with more

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 29 January 2026 doi:10.20944/preprints202601.2273.v1

than three dimensions are to be used. Note, though, that the usual classical or quantum mechanical picture involves particle swarms in three-dimensional space.

Therefore, it seems that within the usual particle-space descriptions, there cannot be any number greater than four particles at the same distance from the rest. That is, the topology of a swarm cannot be a simplex when the number of particles of the swarm becomes greater than four. Yet one can ask why, in four or larger dimensional spaces, geometry opposes the possibility that all the swarm components are at a unique distance from each other?

Such a situation can be translated into a macroscopic three-dimensional reality, in which only four objects can be arranged in a configuration with equal distances between them.

A paradox seems to develop here. One can consider arbitrary swarms of P three-dimensional particles subjected to mechanical scrutiny, but if $P>4$, they cannot be located in a simplex-vertex structure, which allows the location of infinite structures of this sort.

For example, given the number of particles P, the dimension of the simplex will be $N=P-1$. Still, an infinite number of homothetic versions of the original simplex might be available via the homothecy parameter h, as every homothetic simplex can also hold P particles.

This situation must be treated as a mechanical impossibility for three-dimensional particles, or, to overcome it, one must agree that a simplex particle swarm must be described in *N*-dimensional spaces.

That is, to overcome this paradox, P particles at homogeneous distances must be described in spaces with $N=P-1$ dimensions.

The problem of *experimental* observation of a system in a framework of more than 3 dimensions seems to have been recently solved, as a study published a year ago reports observations in 37 dimensions [24] of a photonic system as a landscape of non-classical context.

This situation and the possibility of studying simplex-structured particles in N-dimensional spaces will be discussed in the forthcoming sections.

2.6. Alternative Simplices Based on the Reciprocal Basis Set

Besides the structure of the simplices previously defined, $\mathbf{V}_N=\{\mathbf{C}_N;|\mathbf{v}_P\rangle\}$, essentially based on the canonical basis set and the corresponding rotor vertex, one might consider picking up an alternative to the canonical basis set: the *reciprocal* canonical basis set $\mathbf{R}_N$, which corresponds to the set of column vectors issuing from the subtraction of the unit matrix from the unity matrix:

$$\begin{aligned}\mathbf{C}_N\equiv\mathbf{I}_N\Leftrightarrow\mathbf{R}_N\equiv\mathbf{1}_N-\mathbf{I}_N\Leftarrow\mathbf{1}_N=\{1_{IJ}=1|\forall I,J=1,N\}\\ \Rightarrow\mathbf{R}_N=\{\forall I,J=1,N:R_{IJ}=\delta[I\neq J]\}\\ \Rightarrow\forall I=1,N:|\mathbf{r}_I\rangle=\{\forall J=1,N:r_{JI}=R_{JI}\}\end{aligned} \quad (11)$$

The squared distance between two reciprocal basis set vectors is also 2, with the elements of $\mathbf{R}_N$, and one needs to obtain the *reciprocal rotor vector* $|\mathbf{u}_P\rangle$, using a similar technique to that used before with the canonical basis set, also choosing a homothecy of the unity vector:

$$\begin{aligned}|\mathbf{u}_P\rangle=\upsilon|\mathbf{1}\rangle\rightarrow\forall I:\langle\mathbf{u}_P|\mathbf{u}_P\rangle-2\langle\mathbf{u}_P|\mathbf{r}_I\rangle+\langle\mathbf{r}_I|\mathbf{r}_I\rangle=2\\ \rightarrow\forall I:N\upsilon^2-2(N-1)\upsilon+(N-3)=0\end{aligned} \quad (12)$$

which leads to the result:

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 29 January 2026 doi:10.20944/preprints202601.2273.v1

$$\forall I: \upsilon = \frac{1}{N}\left((N-1) \pm \sqrt{(N-1)^2 - N(N-3)}\right) = \frac{1}{N}\left((N-1) \pm \sqrt{N+1}\right) \quad (13)$$

Now, in this homothetic structure, the dimension $N = 3$ allows obtaining two natural square roots, namely: $\upsilon = \frac{4}{3}$ and $\upsilon = 0$; this is a different situation from the previously obtained one within the canonical basis set vertices framework. Then, taking the zero-root value, one can see that $|\mathbf{u}_P\rangle = |\mathbf{0}\rangle$. Therefore, the reciprocal simplex in this case might be symbolized by $\mathbf{U}_3 = \{\mathbf{R}_3; |\mathbf{0}\rangle\}$. This three-dimensional reciprocal simplex contains a set of $P = N+1 = 4$ vertices of a three-dimensional cube.

Similarly to the canonical vertex case in three dimensions, instead of the Mersenne vertex, the reciprocal zero vertex is involved. As a result, the three-dimensional cube holds two sets of different vertices describing a tetrahedron.

The reciprocal simplex structure, which can be symbolized in general by: $\mathbf{U}_N = \{\mathbf{R}_N; |\mathbf{u}_P\rangle\}$ has been commented on so far, for completeness's sake. Still, given the simplicity of the canonical simplex $\mathbf{V}_N = \{\mathbf{C}_N; |\mathbf{v}_P\rangle\}$ construction, this framework will remain the usual one from now on.

The reciprocal canonical vertex form remains a possibility, which will not be used thereafter.

2.7. Matrix Representation of Canonical and Reciprocal Basis Sets and the Topological Structure of the Simplices

According to the equation **Error! Reference source not found.**, the canonical and reciprocal basis sets are related to the matrices $\mathbf{C}_N = \mathbf{I}_N$ and $\mathbf{R}_N = \mathbf{1}_N - \mathbf{I}_N$, respectively. Thus, they are complementary in the sense that:

$$\mathbf{C}_N + \mathbf{R}_N = \mathbf{1}_N \quad (14)$$

hence the adjective form *reciprocal*, given to the basis set contained in the columns or rows of $\mathbf{R}_N$.

In the following sections, the matrix $\mathbf{R}_N$ will also be symbolized by $\mathbf{T}_N$ to highlight its role in the *topological* description of graphs in general and simplices in the present discussion.

In the next parts of the present discussion, the roles of both basis sets matricial representations will be shown in many instances.

3. Topological Representation of Particle Simplices

First, to have a look at the simplex particle swarms, one can describe and study their Hückel-like topological structure.

Particularly, considering $P = N+1$ equivalent particles, and assuming that they are at the same distance D from one another, can be supposed standing in a global position made of *N*-dimensional tetrahedral or simplex structures.

Thus, the whole particle swarm might be associated with an operator $(P \times P)$ and a matrix representation, irrespective of the dimension chosen, that can be constructed in the form:

$$\mathbf{\Omega} = \alpha\mathbf{I} + \beta\mathbf{T} \quad (15)$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 29 January 2026 doi:10.20944/preprints202601.2273.v1

where $\{\alpha,\beta\}$ are two parameters associated with one particle and two particles situated at a distance D, respectively; $\mathbf{I}=\left(I_{IJ}=\delta_{IJ}\middle|I,J=1,P\right)$ is the diagonal unity matrix as defined in the equation **Error! Reference source not found.**, and the off-diagonal matrix $\mathbf{T}$ corresponds to a matrix employed earlier in the equation **Error! Reference source not found.**, but named $\mathbf{R}$ for linear algebra purposes, that can be expressed by means of the matrix $\mathbf{1}$, the unity matrix also which is a $(P\times P)$ square matrix with all its elements equal to the natural unit:

$$\mathbf{1}=\left\{1_{IJ}=1\middle|I,J=1,P\right\} \tag{16}$$

In turn, defining a unity vector in the same manner:

$$\langle\mathbf{1}|=(1,1,1,\ldots,1,\ldots,1)\Leftrightarrow|\mathbf{1}\rangle=\langle\mathbf{1}|^{T} \tag{17}$$

also, the unity matrix can be computed as a tensor product of such a vector:

$$\mathbf{1}=|\mathbf{1}\rangle\langle\mathbf{1}|=|\mathbf{1}\rangle\otimes|\mathbf{1}\rangle=\langle\mathbf{1}|\otimes\langle\mathbf{1}| \tag{18}$$

Finally, one can write: $\mathbf{T}=\mathbf{1}-\mathbf{I}$, in the same manner as the squared distance matrix in the equation **Error! Reference source not found.**, and therefore, the elements of the matrix $\mathbf{T}$ can also be defined using a logical Kronecker delta as:

$$\mathbf{T}=\left\{T_{IJ}=\delta\left[I\neq J\right]\right\} \tag{19}$$

Note again that this matrix was already also defined when it is described in the equation **Error! Reference source not found.**, and named $\mathbf{R}$, within the section dealing with the reciprocal basis set definition.

Eigensystem of the Topological Matrices

The matrices $\mathbf{\Omega}$ in the equation **Error! Reference source not found.** possess a particular eigensystem, as indeed one can write the eigenvalue equation:

$$\mathbf{\Omega}|\mathbf{x}\rangle=\omega|\mathbf{x}\rangle, \tag{20}$$

that is equivalent to writing the sequence:

$$\begin{gathered}(\alpha\mathbf{I}+\beta\mathbf{T})|\mathbf{x}\rangle=\omega|\mathbf{x}\rangle\Rightarrow\alpha|\mathbf{x}\rangle+\beta\mathbf{T}|\mathbf{x}\rangle=\omega|\mathbf{x}\rangle\Rightarrow\\ \mathbf{T}|\mathbf{x}\rangle=\left(\frac{\omega-\alpha}{\beta}\right)|\mathbf{x}\rangle=\tau|\mathbf{x}\rangle\Rightarrow\tau=\left(\frac{\omega-\alpha}{\beta}\right)\Leftrightarrow\omega=\alpha+\beta\tau\end{gathered} \tag{21}$$

Thus, the eigenvalue equation to be solved is:

$$\mathbf{T}|\mathbf{x}\rangle=\tau|\mathbf{x}\rangle \tag{22}$$

in order to obtain the eigenvalues of $\mathbf{\Omega}$.

However, one can also write:

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 29 January 2026 doi:10.20944/preprints202601.2273.v1

$$
\begin{aligned}
(\mathbf{1}-\mathbf{I})|\mathbf{x}\rangle = \tau|\mathbf{x}\rangle \Rightarrow \mathbf{1}|\mathbf{x}\rangle = (\tau+1)|\mathbf{x}\rangle \Rightarrow \\
\mathbf{1}|\mathbf{x}\rangle = \mu|\mathbf{x}\rangle \Rightarrow \tau = \mu - 1 \Rightarrow \omega = (\alpha-\beta)+\mu\beta
\end{aligned} \tag{23}
$$

meaning that the eigenvalues of the matrix $\mathbf{\Omega}$ are also related to the eigenvalues μ of the unity matrix $\mathbf{1}$, while the eigenvectors are the same in both matrices.

Therefore, one must examine the eigensystem of the unity matrix $\mathbf{1}$ to understand the behavior of the particle swarm in a simplex conformation.

4. Eigensystem of the Unity Matrix

The eigensystem of the unity matrix is straightforward to obtain because the secular equation to be solved is:

$$\mathbf{1}|\mathbf{x}\rangle = \mu|\mathbf{x}\rangle, \tag{24}$$

and thus it is relatively easy to study, given that the unity matrix in the equations **Error! Reference source not found.** and **Error! Reference source not found.** is the tensor product of the unity vector, as discussed in the equation **Error! Reference source not found.**.

4.1. The Principal Eigenvalue of the Unity Matrix

That is, one can rewrite the eigensystem equation **Error! Reference source not found.** as:

$$
\begin{aligned}
|\mathbf{1}\rangle\langle\mathbf{1}||\mathbf{x}\rangle = \mu|\mathbf{x}\rangle \Rightarrow |\mathbf{1}\rangle\langle\mathbf{1}|\mathbf{x}\rangle = \mu|\mathbf{x}\rangle \\
\Rightarrow \langle\mathbf{1}|\mathbf{x}\rangle|\mathbf{1}\rangle = \mu|\mathbf{x}\rangle
\end{aligned} \tag{25}
$$

but the scalar product of the unity vector $|\mathbf{1}\rangle$ by the eigenvector $|\mathbf{x}\rangle$ is easily seen to yield the complete sum $\langle|\mathbf{x}\rangle\rangle$ of the elements of the eigenvector $|\mathbf{x}\rangle$:

$$\langle\mathbf{1}|\mathbf{x}\rangle = \sum_{I=1}^{P} x_I = \langle|\mathbf{x}\rangle\rangle \tag{26}$$

Then, from the final result in the equation **Error! Reference source not found.**, it is obtained:

$$|\mathbf{x}\rangle = |\mathbf{1}\rangle \wedge \mu = \langle|\mathbf{x}\rangle\rangle = \langle|\mathbf{1}\rangle\rangle = P; \tag{27}$$

that is:

$$\mathbf{1}|\mathbf{1}\rangle = P|\mathbf{1}\rangle \tag{28}$$

that corresponds to one eigenvector and its eigenvalue for the given unity matrix.

The matching eigenvalue of the matrix of interest $\mathbf{\Omega}$, after considering the equation **Error! Reference source not found.**, can be written as:

$$\omega = (\alpha-\beta)+P\beta = \alpha + N\beta \tag{29}$$

4.2. The Degenerate Spectrum of the Unity Matrix

The remaining eigenvalues and eigenvectors of the matrix $\mathbf{1}$ can be obtained as follows.

First, one must note that the trace of the unity matrix will be the number of particles:

$$Tr|\mathbf{1}| = Tr|\mathbf{I}| = P \tag{30}$$

In any symmetric matrix, the sum of the eigenvalues corresponds to the trace of the original matrix; that is, in our case, one can write that the sum of the eigenvalues has to be P, but as one of them already has that value. Thus, the sum of the remnant eigenvalues must be zero in general. Equivalent to saying that the only way this property remains the same, whatever the dimension of the problem, is that the remnant N eigenvalues are degenerate with a value of zero. One can write thus the spectrum of $\mathbf{\Omega}$ as:

$$\mu_{N+1} = P \wedge \{\mu_I = 0 | I = 1, N\} \tag{31}$$

The attached eigenvector space for the degenerate eigenvalues must be constructed by a set of orthogonal vectors, which must also be orthogonal to the eigenvector: $|\mathbf{x}_{N+1}\rangle = |\mathbf{1}\rangle$. That is, given the set: $\{|\mathbf{x}_I\rangle | I = 1, N\}$, one will have:

$$\forall I, J = 1, N : \langle \mathbf{x}_I | \mathbf{x}_J \rangle = \delta_{IJ} \wedge \forall I = 1, N : \langle \mathbf{x}_I | \mathbf{x}_{N+1} \rangle = 0 \tag{32}$$

4.3. Eigenvector Normalization

There is a question about the normalization of the eigenvector $|\mathbf{x}_{N+1}\rangle$, which must be studied now. If this is the case, then one must be aware of the fact that the unity vector has a norm: $\langle \mathbf{1} | \mathbf{1} \rangle = P$, therefore the normalized eigenvector has to be written as:

$$\left|\mathbf{x}_{N+1}^{(\nu)}\right\rangle = \frac{1}{\sqrt{P}} |\mathbf{1}\rangle \tag{33}$$

However, if this is the choice, then the eigenvalue in the equations **Error! Reference source not found.** and **Error! Reference source not found.** transforms in:

$$\omega = \frac{1}{P} \langle \mathbf{1} | \mathbf{1} | \mathbf{1} \rangle = \frac{P}{P} \langle \mathbf{1} | \mathbf{1} \rangle = P \Leftarrow \mathbf{1} | \mathbf{1} \rangle = P | \mathbf{1} \rangle \tag{34}$$

in this way, nothing changes from the former result of the equation **Error! Reference source not found.** and the eigenvalue evaluation **Error! Reference source not found.**. A well-known property of the secular equations.

Therefore, such an arrangement of particles in a simplex framework in any dimension corresponds to a system in which the particles' interactions apparently play no well-defined role at all, but behave homogeneously as the particle distances do.

4.4. Non-Zero Eigenvalues of the Simplex Swarms

These findings can be exemplified for the 1- and 2-dimensional cases, as one can see that:

1-D) When $N = 1$, one deals with a two-particle system, and the associated matrix is (2×2), so the eigenvalue of interest is, in the same way $\mu = 1$, thus this will give $\omega = \alpha + \beta$ using the equation **Error! Reference source not found.**.

 doi:10.20944/preprints202601.2273.v1

2-D) In the same manner with $N=2$ one has a 3-particle system and the matrix $\mathbf{\Omega}$ will be (3×3). Therefore, the equation **Error! Reference source not found.** will read in this case: $\omega=\alpha+2\beta$.

Both results are well-known from Hückel theory when a C_2 bond, or an equilateral triangular C_3 structure, are considered.

However, when higher-dimensional swarms of particles subjected to a simplex vertex framework positioning are studied, the case $N=3$, corresponding to a tetrahedral structure, can be visualized as the tetrahedron formed by equidistant C_4 bonds, yielding an eigenvalue $\omega=\alpha+3\beta$.

The cases with dimensions larger than 3 correspond to structures similar to the set of equivalent C_P simplices, which correspond to eigenvalues of the form shown in the equation **Error! Reference source not found.**: $\omega=\alpha+N\beta$.

As already commented, being structures defined in high-dimensional spaces, such swarm configurations of particles cannot exist in the usual three-dimensional reality.

Therefore, when observing these results from the point of molecular topology, one must be aware that a general framework, corresponding to a number of particles greater than 4, could never be made if the particle coordinates are such that the distance matrix can be written like: $\mathbf{D}=D\mathbf{T}$.

In other words, a swarm of $P>4$ particles cannot exist with a distance matrix of the previous form if the working space is a 3-dimensional one.

Thus, it appears that the conclusion one arrives at in this case is that a configuration of the swarm taking the form of a simplex cannot exist in N-dimensional particle swarms within $N>3$.

Then one needs to repeat that a paradox arises in the study of particle swarms. A mathematical topological Hückel-like model exists with the appropriate simplex geometry, but provides no link to three-dimensional reality.

More than this, a three-dimensional swarm of $P>4$ particles, macroscopic, microscopic, or submicroscopic, all at an arbitrary common distance D can exist only in three dimensions.

This corresponds to a puzzling situation, unless one can admit that particle swarms with such a characteristic do exist in spaces with dimensions larger than the usual three-dimensional reality.

5. Gaussian Functions Described in N-Dimensional Spaces (in a Simplex Framework): Overlap and Other Integrals

In this definition, the vectors that construct the Gaussian function can be elements of an arbitrary N-dimensional space.

Then, a simple spherical Gaussian function can be written as:

$$\gamma\left(\eta,|\mathbf{x}\rangle,|\mathbf{v}\rangle\right)=\nu\left(\eta\right)\exp\left(-\eta\left\||\mathbf{x}\rangle-|\mathbf{v}\rangle\right\|^2\right) \quad (35)$$

where η is a parameter controlling the sharpness of the Gaussian around the center, and $\nu\left(\eta\right)$ a normalization factor, such that:

$$\left\langle\gamma\left(\eta,|\mathbf{x}\rangle,|\mathbf{v}\rangle\right)\right\rangle=\int_\Delta\gamma\left(\eta,|\mathbf{x}\rangle,|\mathbf{v}\rangle\right)d|\mathbf{x}\rangle=1 \quad (36)$$

The sharpness of the Gaussian can be grasped by considering that:

 doi:10.20944/preprints202601.2273.v1

$$\lim_{\eta \to \infty} \gamma(\eta, |\mathbf{x}\rangle, |\mathbf{v}\rangle) = \delta(|\mathbf{x}\rangle - |\mathbf{v}\rangle) \tag{37}$$

where $\delta(|\mathbf{x}\rangle - |\mathbf{v}\rangle)$ is a Dirac's delta function centered at the vector $|\mathbf{v}\rangle$, and when it decreases tending to zero, the Gaussian function becomes almost coincident or parallel to the vector $|\mathbf{x}\rangle$.

The vectors $\{|\mathbf{x}\rangle, |\mathbf{v}\rangle\} \in V_N$ correspond to the variables and the location of the function's center in the chosen N-dimensional space.

This arrangement is more general than the simplex structure discussed earlier, but to center the Gaussian functions in the vertices of a simplex, one chooses the vector $\langle \mathbf{v}|$ as the vertices of the corresponding working simplex.

Under these definitions, the normalization factor is constructed as:

$$\nu(\eta) = \left(\frac{2\eta}{\pi}\right)^{\frac{N}{4}}, \tag{38}$$

as the Gaussian function **Error! Reference source not found.** can be considered as the product of one-dimensional Gaussian functions, which can be written using the expansion:

$$\exp\left(-\eta \left\| \mathbf{x}\rangle - |\mathbf{v}\rangle \right|^2\right) = \prod_{I=1}^{N} \left[\exp\left(-\eta |x_I - v_I|^2\right) \right] \tag{39}$$

5.1. Gaussian Functions Centered at a Simplex

One can suppose that at every vertex of a simplex $\mathbf{V}_N = \{\mathbf{C}_N; |\mathbf{v}_P\rangle\}$, there is situated a Gaussian function as described in the equation **Error! Reference source not found.**.

Such a disposition of the functions is related to the concept of Gaussian enfolding of Euclidean spaces [16–23], by which all points of the space can be supposed to bear a Gaussian function. In this case, only the simplex vertices are enfolded with an active function and so distinguished from the rest of space, which can be supposedly enfolded with zero functions.

However, due to the simplex topological structure, one can easily define the product of two Gaussian functions located at the canonical part of the simplex.

A new Gaussian function with the following structure will appear:

$$\begin{aligned} \gamma(\eta, |\mathbf{x}\rangle, |\mathbf{p}_{IJ}\rangle) &= \gamma(\eta, |\mathbf{x}\rangle, |\mathbf{e}_I\rangle)\gamma(\eta, |\mathbf{x}\rangle, |\mathbf{e}_J\rangle) \\ &= \Gamma(2\eta, |\mathbf{x}\rangle, |\mathbf{p}_{IJ}\rangle) \Leftarrow |\mathbf{p}_{IJ}\rangle = \frac{1}{2}(|\mathbf{e}_I\rangle + |\mathbf{e}_J\rangle) \end{aligned} \tag{40}$$

where the new Gaussian function is structured like:

$$\Gamma(2\eta, |\mathbf{x}\rangle, |\mathbf{p}_{IJ}\rangle) = \left(\frac{2\eta}{\pi}\right)^{\frac{N}{2}} \exp(-\eta) \exp\left(-2\eta \left\| \mathbf{x}\rangle - |\mathbf{p}_{IJ}\rangle \right|^2\right) \tag{41}$$

In fact, this result shows that the resulting function is located between the two implied vertices.

5.2. Overlap Integrals and the Overlap of an N-Dimensional Simplex Swarm

One can try to identify the general geometric characteristics of N -dimensional swarms of particles and to define associated matrix representations with the topological signature of a simplex.

If this were successful in higher-dimensional spaces, a positive result might represent two characteristic features.

First, the obvious ability to perform quantum-mechanical calculations of simplex P particle systems in $N>3$ -dimensional spaces.

Second, the possibility that quantum-mechanical particle interactions can be studied in higher-dimensional spaces as a potential manifestation of some extended-dimensional reality.

In this section, a naïve initial attempt to implement this scheme will be sketched under the following assumptions.

(1) All particles in the swarm are equal and placed in the vertices of an N -dimensional simplex.

(2) Any particle in the chosen simplex swarm is associated with a normalized spherical Gaussian function defined in the N -dimensional space.

Also, one can take the product in the equation **Error! Reference source not found.** to rewrite the exponential of the equation **Error! Reference source not found.**:

$$\exp\left(-2\eta\left\||\mathbf{x}\rangle-|\mathbf{p}_{IJ}\rangle\right|^2\right)=\prod_{K=1}^{N}\left[\exp\left(-2\eta\left|x_K-p_{IJ;K}\right|^2\right)\right]$$
$$=\prod_{K=1}^{N}\left[\exp\left(-2\eta\left|x_K-\frac{1}{2}(\delta_{IK}+\delta_{JK})\right|^2\right)\right] \tag{42}$$

so, the overlap between two Gaussian functions representing two particles in the N -dimensional simplex could be written by means of the integral involving one of the elements of the product **Error! Reference source not found.**:

$$s=\int_{-\infty}^{+\infty}\exp\left(-2\eta\left|x-\xi\right|^2\right)dx=\left(\frac{\pi}{4\eta}\right)^{\frac{1}{2}} \tag{43}$$

then, the overlap between two Gaussian functions centered in two simplex vertices can be written:

$$S=\left(\frac{2\eta}{\pi}\right)^{\frac{N}{2}}\exp(-\eta)\left(\frac{\pi}{4\eta}\right)^{\frac{N}{2}}=\left(\frac{1}{2}\right)^{\frac{N}{2}}\exp(-\eta) \tag{44}$$

The product of every Gaussian in one canonical vertex and the one in the rotor vertex is a bit more involved, but in fact, as the rotor vertex is sought to be equidistant to the canonical vertices, this provides the same result as in the equation **Error! Reference source not found.**.

Such previous reasoning shows that one can describe particle swarms in higher-dimensional spaces without problems beyond the need to consider products of Gaussian functions with more terms than the usual 3 in the three-dimensional representation.

5.3. The Overlap Integral Matrix

Therefore, the entire overlap matrix between the Gaussian functions located at the simplex vertices is a $(P\times P)$ symmetric matrix, with the same structure as the matrices discussed after the equation **Error! Reference source not found.**.

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 29 January 2026 doi:10.20944/preprints202601.2273.v1

The differences appear because we have chosen to normalize the Gaussian functions, and also, the overlap between any pair of Gaussian functions presents the same value S. Therefore, the overlap matrix of the Gaussian simplex can be written as:

$$\mathbf{S} = \mathbf{I} + S\mathbf{T} \tag{45}$$

Such a matrix structure will remain the same when using homothetic simplices; the value of the two-vertex overlap will vary slightly, and accordingly, thereby modifying the exponent in the equation **Error! Reference source not found.** exponential function, adding the homothetic parameter h:

$$S = \left(\frac{1}{2}\right)^{\frac{N}{2}} \exp\left(-\eta h^2\right) \tag{46}$$

5.4. Eigensystem of the Overlap Matrix

The equation **Error! Reference source not found.**, has the same structure as the general simplex matrix presented in the equation **Error! Reference source not found.**. Therefore, to structure the eigensystem of the overlap matrix, one must use:

$$\mathbf{S}|\mathbf{x}\rangle = \sigma|\mathbf{x}\rangle \Rightarrow \mathbf{T}|\mathbf{x}\rangle = \left(\frac{\sigma - 1}{S}\right)|\mathbf{x}\rangle, \tag{47}$$

and one can use the previously described eigenvalues of the matrix $\mathbf{T}$, as written in the equations **Error! Reference source not found.**, resulting in the equation **Error! Reference source not found.**, finally obtaining:

$$\sigma = 1 + NS \tag{48}$$

As the overlap matrix has the same structure as the general matrix in the equation **Error! Reference source not found.**, it would be redundant to repeat the nuances discussed for the general equation and the role of the eigenvalues and eigenvectors of the unity matrix.

5.5. The Momentum and Kinetic Energy Operators in the N-Dimensional Particle Spaces

From the quantum-mechanical point of view, to continue with the N-dimensional representation of a particle swarm, one needs to define the momentum operator in the N-dimensional particle space.

In fact, it is simple to define the corresponding operator as an extended nabla over the space dimensions. For this purpose, one can outline the first-order partial derivatives operator as a vector:

$$i\left|\frac{\partial}{\partial|\mathbf{x}\rangle}\right\rangle = i\left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_I}, \ldots \frac{\partial}{\partial x_N}\right)^T \tag{49}$$

that with the appropriate atomic units will be an extension of the well-known momentum operator associated with a particle in three-dimensional space.

The kinetic energy operator is easily constructed for particle swarms of mass M:

$$K = -\frac{1}{2M}\sum_{I=1}^{N}\frac{\partial^2}{\partial x_I^2} \tag{50}$$

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 29 January 2026 doi:10.20944/preprints202601.2273.v1

thus, the kinetic energy integrals will be straightforwardly computed using the operator **Error! Reference source not found.** and the expression for the N -dimensional Gaussian functions, as in the equation **Error! Reference source not found.**.

5.6. The One- and Two-Particle Potential Integrals

The one- and two-particle potential integrals are quite similar in handling to the nuclear attraction and electronic repulsion integrals discussed by Huzinaga [25] and later on by Sanders [26].

One has only to consider the product of two Gaussian functions, as it is commented in the equations **Error! Reference source not found.** and **Error! Reference source not found.**. Such a contraction from two Gaussian functions into another one will appear once in one-particle integrals and twice in two-particle ones. Here, no further analysis of these integrals will be performed to avoid increasing the already published content in this paper.

6. Structure of the Quantum Mechanical Energy and Hückel-Like Matrices in a Simplex Framework

When considering a swarm of P particles located in a simplex set of N -dimensional coordinate sites, the tight symmetry of the swarm located in such a manner, even when considering the swarm formed by atoms in a Born-Oppenheimer approximation, one needs to see that every simplex vertex will provide and receive the same amount of combined integrals needed to build the total energy of the system.

One can write an expression schematically containing the mentioned highly symmetric situation. Therefore, a very simplified energy expression like:

$$
\begin{aligned}
\mathfrak{E}_P = H_P + R_P = \langle \mathbf{H}_P \rangle + \langle \mathbf{R}_P \rangle &= \sum_{I=1}^{P}\sum_{J=1}^{P} h_{IJ} + \sum_{I=1}^{P}\sum_{J=1}^{P}\left(\sum_{K=1}^{P}\sum_{L=1}^{P} r_{IJKL}\right) \\
&= \sum_{I=1}^{P}\sum_{J=1}^{P}\left(h_{IJ} + R_{IJ}\right) \\
&= \sum_{I=1}^{P}\left(h_{II} + R_{II}\right) + \sum_{I=1}^{P}\sum_{J=1}^{P}\delta(I \neq J)\left(h_{IJ} + R_{IJ}\right) \\
&= P\alpha_P + P(P-1)\beta_P = P\left[\alpha_P + (P-1)\beta_P\right] \\
&= P\left[\alpha_P + N\beta_P\right]
\end{aligned}
\qquad (51)
$$

with the appropriate factors and extra terms, such as exchange, if necessary, included implicitly in the integrals of the expression **Error! Reference source not found.**.

Then, the above expression describes the total energy $\mathfrak{E}_P$ of a system of particles with sufficient accuracy. Of course, considering the highly symmetric topology of the swarm.

In fact, in the final energy expression, just two parameters appear: $\{\alpha_P;\beta_P\}$, as in the old Hückel framework, but they shall be considered as dependent on P the number of particles entering the swarm, and accordingly they are sufficient to describe the whole interaction.

Also, one must be aware that, as in electronic molecular clouds, two-particle interactions can have an integral substructure associated with the exchange interaction, a consequence of the presence of electronic spins.

Finally, the final expression of the equation **Error! Reference source not found.**, indicates that one can write the total energy as an accumulation of the individual simplex energy for each particle, that is:

$$\mathfrak{E}_P = P(\alpha_P + N\beta_P) = PE_P \tag{52}$$

but the individual particle energy E_P corresponds to the eigenvalue found in the equation **Error! Reference source not found.** when discussing the eigensystem **Error! Reference source not found.**.

Thus, one retrieves, in the case of the simplex swarm of particles, the principal eigenvalue of the simplex Hückel-like eigen-equation when describing the total energy of a simplex swarm.

Then the swarm's total energy in a simplex conformation appears to be just the sum of the individual particles' energies.

7. Consideration of Time Dependence on the Simplex Structure

7.1. Time Evolution of Simplex Vertices

The set of simplex basic vertex coordinates in the chosen option of this study, being a set of the natural $\{0,1\}$ set, can be considered as an initial departure frame for a time device or to represent the time evolution of the simplex vertices. This has already been proposed in a large body of studies, with the hypercubic structures as protagonists, promoted in this laboratory [1–10].

Such a transformation from a Born-Oppenheimer frozen-vertex structure to a time-dependent mobile framework can also be applied to simplices. One just needs to replace the $\{0,1\}$ set of the simplex's original vertices with the set of non-negative functions: $\{\mathrm{S}(t),\mathrm{C}(t)\}$, which can be associated with the trigonometric squared functions: $\{s^2(t),c^2(t)\}$. Then the actual values of the simplices discussed here correspond to the values:

$$t = 0 \rightarrow \{\mathrm{S}(0),\mathrm{C}(0)\} \equiv \{0,1\} \tag{53}$$

More than this, according to the discussion performed in [20,22], the previous definition corresponds to a synchronous variation of the simplex vertices, but one can define for each vertex the $\{0,1\}$ set substituted by:

$$\forall I = 1, N : \langle \mathbf{e}_I | = \left(\mathrm{S}_{KI}(t_I)\delta(K \neq I) + \mathrm{C}_{KI}(t_I)\delta(K = I) \middle| K = 1, N \right) \tag{54}$$

and

$$\langle \mathbf{v}_P | = \lambda \langle \mathbf{1} | \rightarrow \langle \mathbf{v}_P(t_P) | = \lambda \mathrm{C}(t_P) \langle \mathbf{1} |, \tag{55}$$

These two equations provide an asynchronous description of the simplex vertices.

Therefore, the corresponding swarm integrals shall be transformed accordingly. Taking into account that the synchronous manner is equivalent to performing a simplex homothecy, while the asynchronous transformation, with time evolving independently on each vertex, will correspond to almost random transformations on each vertex. As a result of the asynchronous time evolution of the vertices' coordinates, the high symmetry discussed so far on simplices will be lost, as will the simplicity.

How to connect this time dependence, the previous properties, and information about simplices and particle swarms to a possible physical reality might be the question to be posed and answered elsewhere.

Preprints.org (www.preprints.org) | NOT PEER-REVIEWED | Posted: 29 January 2026 doi:10.20944/preprints202601.2273.v1

Perhaps an example that can be advanced is the connection of such a swarm, steady or evolving structure, with Bose-Einstein condensates [28], superconductivity and superfluidity [27], and similar phenomena such as superposition [29] could be made evident with further in-depth studies.

7.2. Time-Dependency as Simplex Homothecy and Translation

Alternatively, observing the equation **Error! Reference source not found.**, one can also write that:

$$\forall t : 1 = S(t) + C(t), \tag{56}$$

then at any time value, one can write the vertices of a simplex using the fact that $\{1\} \rightarrow \{C(t)\}$, the result if performed this substitution over the simplex $\mathbf{V}_N = \{\mathbf{C}_N ; |\mathbf{v}_P\rangle\}$, is equivalent to obtaining a homothetic simplex, with the homothetic parameter chosen as $C(t)$, one will then obtain a possible set of time-dependent homothetic simplices, which can be written as:

$$\mathbf{\Omega}_N \{C(t)\mathbf{C}_N ; C(t)|\mathbf{v}_P\rangle\} = C(t)\mathbf{V}_N \{\mathbf{C}_N ; |\mathbf{v}_P\rangle\} \tag{57}$$

Therefore, the equation **Error! Reference source not found.**, defines a *homothetic* simplex that depends only on the squared cosine. However, one can envisage *translating* the whole simplex by a homothecy of the unity vector, like: $|\mathbf{t}\rangle = S(t)|\mathbf{1}\rangle$, which symbolically transforms the already homothetic time-dependent simplex into:

$$\mathbf{\Omega}_N \{C(t)\mathbf{C}_N ; C(t)|\mathbf{v}_P\rangle\} + S(t)|\mathbf{1}\rangle = \mathbf{\Xi}_N \{\mathbf{C}_N ; |\mathbf{v}_P\rangle\}(t) \tag{58}$$

However, the simplices of type $\mathbf{\Xi}_N$, because of the relationship **Error! Reference source not found.**, will be equivalent to the transformation $\{0,1\} \Rightarrow \{S(t),1\}$. Then, the canonical basis set in full can be used to construct a square $(N \times N)$ matrix with the structure:

$$\mathbf{S}_N(t) = \mathbf{I}_N + S(t)\mathbf{T} \tag{59}$$

which corresponds to an infinite set of time-dependent matrices with a structure similar to the overlap matrix given by the equation **Error! Reference source not found.**.

The overlap is a number defined in the interval: $0 \le S \le 1$, and is coincident with every time in that interval, that is: $0 \le S(t) \le 1$.

Therefore, the behavior of the time-dependent shifted-translated simplex under the present rules yields a canonical basis set that behaves like an overlap matrix.

It must be finally remarked that due to the equation **Error! Reference source not found.**, the $\{1\}$ within the original vertices of the simplex remain invariant in the transformed structure, and as a consequence, while the canonical basis set varies upon the time-transformation described in this section as to be constructed with the overlap-like matrix **Error! Reference source not found.**, the rotor vertex $|\mathbf{v}_P\rangle$ remains invariant.

7.3. Hyperbolic Functions as Time-Dependent Coordinate Generators

 doi:10.20944/preprints202601.2273.v1

Because some hyperbolic functions, such as the hyperbolic tangent and secant [30], can be associated with a relation similar to the equation **Error! Reference source not found.**, it is possible to use such hyperbolic functions to transform the simplex coordinates, making them time-dependent, in ways similar to the previously described trigonometric options.

As noted elsewhere in this article, the possibility will be kept open, leaving for further development to introduce this extension into the scientific lore of simplices and hypercubes applied to the physical sciences.

8. Final Remarks and Conclusions

The canonical simplex vertex structure can be used to discuss the behavior of highly symmetric particle swarms. Yielding an interesting picture of the possible features associated with this simple N-dimensional geometry.

While the simplex description of three-dimensional particles allows four particle geometries of this kind, once the swarm reaches a particle number $P > 4$, then the theoretical treatment requires that particles be located in extra dimensions.

However, it is shown here, at least in a very schematic manner (by the way, allowed by the highly symmetric nature of the simplices), that this does not pose any further problem in considering particle swarms described in any dimension extension.

Thus, the paradox that particle swarms in the simplex topology cannot be studied because particles in three-dimensional space cannot reach higher numbers is resolved by the possibility of studying particles within higher-dimensional simplex swarms.

Still, it is shown here that even within a simple quantum-mechanical scheme, the usual integrals can be computed, yielding the particle swarm simplex energy. With more details, the overlap matrix is analyzed, connecting its form with the previous topological simplex formalism and precluding a time-dependent structure of any simplex.

Simplex homotheties and synchronous simplex coordinates time dependency become the same problem. Asynchronous time-vertex coordinate dependencies destroy the simplex's high symmetry and transform the problem into one different from the one discussed here. Time-dependent synchronous homothecies followed by a time translation, using the squared sine function, yield a time-dependent canonical basis set that shares the overlap matrix structure.

This simple work on simplices and their possible roles in theoretical and quantum chemistry concludes that swarms of particles, located in a simplex's vertices, can be elegantly described in appropriate multiple dimensions, without any more problems than the usual ones appearing in the three-dimensional framework.

Due to the high symmetry involving simplices, the matricial descriptions of the swarm's mathematical structure at various levels appear as having a well-defined formalism, including at most two different parameters.

Finally, one must remark the persistence along this study of the matrices $\mathbf{I}$ and $\mathbf{T}$, related to the canonical and reciprocal basis sets, with which the simplex matrices are adapted to the various theoretical circumstances in which simplices (and hypercubes) are present.

Both matrices are related to the unity matrix $\mathbf{1}$ in *any* dimension, so this simple matrix trio can serve as a valuable asset throughout the theoretical development of useful and interesting features of simplices.

Acknowledgments: The author wants to acknowledge the invaluable help provided by Blanca Cercas, MP. Without it, this work couldn't have been written.

References

1. R. Carbó-Dorca; "Natural Vector Spaces, (Inward Power and Minkowski Norm of a Natural Vector, Natural Boolean Hypercubes) and Fermat's Last Theorem"; J. Math. Chem. **55** (2017) 914-940.

 doi:10.20944/preprints202601.2273.v1

2. R. Carbó-Dorca; "Boolean Hypercubes as Time Representation Holders"; J. Math. Chem. **56** (2018) 1349-1352.
3. R. Carbó-Dorca; "DNA, Unnatural Base Pairs and Hypercubes"; J. Math. Chem. **56** (2018) 1353-1356.
4. R. Carbó-Dorca; "Boolean Hypercubes and the Structure of Vector Spaces"; Journal of Mathematical Sciences and Modelling (JMSM) **1** (2018) 1-14.
5. R. Carbó-Dorca; "Cantor-like Infinity Sequences and Gödel-like Incompleteness Revealed by means of Mersenne Infinite Dimensional Boolean Hypercube Concatenation"; J. Math. Chem. **58** (2020) 1-5.
6. R. Carbó-Dorca; "About the Construction of Probability Hypercubes"; J. Math. Chem. **59** (2021) 1151-1154.
7. R. Carbó-Dorca; "Boolean Hypercubes: The Origin of a Tagged Recursive Logic and the Limits of Artificial Intelligence"; Universal Journal of Mathematics and Applications **4** (2021) 41-49.
8. R. Carbó-Dorca; "Shadows' Hypercube, Vector Spaces, and Non-Linear Optimization of QSPR Procedures"; J. Math. Chem **60** (2022) 283–310.
9. R. Carbó-Dorca, T. Chakraborty; "Chemical and Molecular Spaces, QSPR, Boolean Hypercubes, Algorithmic Intelligence and Gödel's Incompleteness Theorems" In Chemical Reactivity (Volume **1** Theories & Principles) S. Kaya, L. von Szentpaly, G. Serdaroglu, L. Guo (Editors); Chapter **18**. pp. 505-573. Elsevier (Amsterdam), The Netherlands (2023); ISBN: 978-0-323-90257-1.
10. R. Carbó-Dorca, D. Nath; "Fermat surfaces and Hypercubes"; Mathematics and Systems Science **2** (2024) 2490-2498.
11. R. Carbó-Dorca; "Fuzzy sets and Boolean Tagged sets"; J. Math. Chem. **22** (1997) 143-147.
12. R. Carbó-Dorca; "Tagged sets, convex sets, and QS measures"; J. Math. Chem. **23** (1998) 353-364.
13. R. Carbó-Dorca; "Fuzzy sets and Boolean tagged sets, vector semispaces and convex sets, QSM and ASA density functions, diagonal vector spaces and quantum chemistry"; Adv. Molec. Simil. Vol. **2** pg. 43-72. JAI Press, (1998) ISBN: 0-7623-0258-5.
14. R. Carbó-Dorca; "About some questions relative to the arbitrariness of signs: Their possible consequences in matrix signatures definition and quantum chemical applications"; J. Math. Chem. **33** (2003) 227-244.
15. R. Carbó-Dorca; "A Theorem on the Gram matrix of a Polyhedron"; J. Math. Chem. **55** (2017) 79-97.
16. E. Besalú, R. Carbó-Dorca; "N-dimensional Euclidean Space enfoldment"; J. Math. Chem. (2011) 49, 2231-2243.
17. R. Carbó-Dorca, E. Besalú; "Geometry of N-dimensional Euclidean Space enfoldments"; J. Math. Chem. 49 (2011) 2244-2249.
18. R. Carbó-Dorca; "Enfolded conformational spaces: definition of the chemical quantum mechanical multiverse under Born-Oppenheimer approximation"; J. Math. Chem. **51** (2013) 1092–1098.
19. R. Carbó-Dorca; "Position-momentum Heisenberg uncertainty in Gaussian enfoldments of Euclidean space"; J. Math. Chem. **51** (2013) 420-426.
20. R. Carbó-Dorca; "Time Vectors and Particle Swarms Defined as Polyhedra in Spherically Enfolded Spaces"; J. Math. Chem. **54** (2016) 1751–1757.
21. J. Chang, R. Carbó-Dorca; "A Quantum Similarity Discussion about Einstein-Podolsky-Rosen (EPR) Paradox in Gaussian Enfolded Spaces"; J. Math. Chem. **58** (2020)1815-1827.
22. R. Carbó-Dorca; "Enfolding *N*-dimensional Euclidean Spaces with *N*-dimensional Spheres as a Framework to Define the Structure of Time Foam"; J. Math. Chem. **59** (2021) 1450-1455.
23. R. Carbó-Dorca, T. Chakraborty; "On the Nature of Chemical Bond: Space Enfoldings, Density Bond Matrices, Quantum Molecular Polyhedra, and a Collective Bond Description Proposal"; Sci. Insights **1** (2025) 1-22.
24. Zheng-Hao Liu, Yu Meng, Yu-Ze Wu, Ze-Yan Hao, Zhen-Peng Xu, Cheng-Jun Ai, Hai Wei, Kai Wen, Jing-Ling Chen, Jie Ma, Jin-Shi Xu, Chuan-Feng Li, Guang-Can Guo; "Exploring the boundary of quantum correlations with a time-domain optical processor"; Sci. Adv. **11** (2025) eabd8080:1-12.
25. H. Taketa, S. Huzinaga, K. O-ohata; "Gaussian-Expansion Methods for Molecular Integrals"; J. Phys. Soc. (Japan) **21** (11) (1966) 2313-2324.

 doi:10.20944/preprints202601.2273.v1

26. V. R. Sanders; "An introduction to molecular integral evaluation" in Dircksen et al. (eds.) "Computational Techniques in Quantum Chemistry and Molecular Physics" (1975) 347-424; D. Reidel Pub. Co.; Dordrecht-Holland.
27. R. P. Feynman; "Superconductivity and Superfluidity"; Revs. Mod. Phys. **29** (1957) 205-212.
28. E. A. Cornell, J. R. Ensher, C. E. Wieman; "Experiments in Dilute Atomic Bose-Einstein Condensation"; arXiv: cond-mat/9903109v1 5 Mar (1999); and https://en.wikipedia.org/wiki/Bose-Einstein_condensate.
29. Sebastian Pedalino, Bruno E. Ramírez-Galindo, Richard Ferstl, Klaus Hornberger, Markus Arndt, Stefan Gerlich; "Probing quantum mechanics with nanoparticle matter-wave interferometry"; Nature **649** (2026) 866–870.
30. M. Abramowitz, I. Stegun; "Handbook of Mathematical Functions"; Dover Publications, New York (1972).