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About some questions relative to the arbitrariness of signs: Their possible consequences in matrix signatures definition and quantum chemical applications

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The generalization of the arbitrary concept of sign to N-dimensional mathematical objects is discussed. Basically, the main argument employed here is founded in the previously described concepts of vector semispaces and their organization in shells. Usual operations in vector spaces are complemented by the inward matrix product, a matrix and vector product present within high level programming languages, as a sustentation of generalized signatures. It is shown how any vector space can be simply constructed from a simple set of convex positive definite mathematical objects. The sign generalization described here permits the definition of sign multiplets and signature support groups as a first step of deepening into the concept of general sign structures, which can be considered as possible conventions, situated far away from the classical Boolean sign structure. One can conclude that the study and use of sign generalization still is far to be complete. The theoretical set up developed in this way can be easily introduced in quantum chemistry wave function and density analysis.

KEY WORDS: sign extension and generalization, matrix and vector signatures, vector semispaces, inward matrix product, unit shell vector generation

1. Introduction

Curiously enough, the numerical structure of the mathematical objects, employed in computational exercise, appears to possess many aspects far to be exploited. It is a current practice the daily use of computational chemistry procedures in terms of prefabricated programs, dealing with the main algorithms set up in order to solve Schrödinger equation and, thus, allowing the calculation of atomic and molecular properties throughout the statistical concepts of density functions and expectation values. Such custom and the derivations of its use, appears to be a great obstacle in order to deepen in the problems, derived of the quantum chemical developed algorithms large utilization. As a consequence, the subject of attempting to understand the interesting puzzles encountered in everyday quantum chemical practice, becomes increasingly abandoned in the literature. To try to overcome this tendency as much as possible constitutes the conducting thread of this study.

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The basic mathematical properties of wave and density functions numerical representation, as used in the computational implementation of quantum chemical lore, have still quite a large set of aspects waiting to be well understood. This is the reason why, with a stepwise pace, during a span of several years, it has been studied in this laboratory a good deal of subjects pointing to the direction on how to find the way to define new theoretical elements in order to understand the chemical application of quantum theory as a whole, which appears to be not an easy task whatsoever.

From the early development of these mentioned studies, a good deal of new concepts has emerged. Among other minor descriptions, it can be quoted the structure of *tagged sets* [1,2], as a background to find out a generalization of *fuzzy sets* [3] and leading, in turn, to a non ambiguous description of a new category of mathematical elements based on old concepts, the *quantum objects* [4,5], which have the possibility to unequivocally connect, by means of theoretical definitions, submicroscopic systems of physical or chemical interest with their quantum mechanical statistical description in terms of density functions. Also, under the same working philosophy, the problem of the density function structure and its construction has been studied in the same general background [6], conducting to the definitions of several alternative concepts like those of *vector semispaces*. In the progress of the mentioned work, some symbolic devices had been put forward, as the so called *density generators* and *convex conditions* symbols, allowing to understand the connection of infinite dimensional functional spaces with N-dimensional ones [2], when the construction of probability distributions is needed.

Generalization of the concept of wave function has been put forward using the definition of *extended* wave functions and, thus, the relationship of these new mathematical structures with the ideas set up around density functions, has been conducted and employed for several purposes too [7]. One of them has been the set up of a way to construct extended and nonlinear Schrödinger equations [5], while another is being constituted by building up a broad point of view to expose the theoretical basis of the techniques, associated to the so called *quantum quantitative structure-properties relationships* (QSPR) [8–10]. These problems lead to the study in deep, as an ancillary but successful idea, of a new operation, which was partly originally set by Hadamard (see, for example, the definitions in [11], the origins in [12]) but not well studied until now, an easily programmable operation, which was named as *inward matrix product* (IMP) [13]. Such a product has presented great advantages at the moment of describing the connection of density functions with wave functions [14] and the associated problems.

Along these studies, the concept of *matrix signature* as well as the possibility to generalize the nature of sign in numerical fields has been already described [9] primarily in a very schematic manner. As the conceptualization of *metric vector semispaces* has been recently put forward [15], and in this previous work the leading role of signatures naturally appeared, then it seems, as a consequence, that it is already time to study the possibility of systematically using generalized signs and signatures. This will constitute the main task which this work will deal with.

2. Vector semispaces and shell structure

2.1. Vector semispaces

Vector *semispaces* are quite interesting and straightforward derivations of the usual concepts, which can be easily understood and deduced from the axiomatic definition of vector space structure. Indeed, in vector semispaces the original vector space *Abelian additive group*, associated to vector summation, is transformed into a *semigroup* [16, p. 249]. A semigroup, then, is a group without reciprocal elements, so in semispaces no *negative vectors* are present. Thus, in this way, semispaces even can be worked out without the neutral additive element, the *null* or *zero vectors*. Vector semispaces possess almost the same properties of vector spaces and, so, the same symbols for noting them can be used. However, it must be taken into account and stressed, that one of the vector semispace main features consists on the presence of the positive real half line, in substitution of the space reference real or complex field. Scalar reference fields in vector semispaces are made by the positive definite real numbers, alternatively by the rational numbers, in case one wants to point out the intrinsic nature of the computational environment in practical terms.

The following definition of N-dimensional vector semispaces $V_N(\mathbf{R}^+)$ applies:

$$V_N(\mathbf{R}^+) \subset V_N(\mathbf{R}) \quad \rightarrow \quad \forall \mathbf{x}, \mathbf{y} \in V_N(\mathbf{R}^+) \wedge \alpha, \beta \in \mathbf{R}^+ \colon \alpha\mathbf{x} + \beta\mathbf{y} \in V_N(\mathbf{R}^+).$$

Vector semispace basic structure definition, thus, is the same as the vector space one, except for the *absence* of negative scalars and reciprocal vectors.

2.2. Minkowski norms

The semispace definition as given above can be applied to matrices, column or row vectors, or over the elements of any other vector spaces, with the appropriate restrictions. Due to the special structure of vector semispaces a natural norm, which can be attached to every vector element $\mathbf{x} \in V_N(\mathbf{R}^+)$, can be associated, in turn, to a *Minkowski norm* and noted by means of the symbol $\langle\mathbf{x}\rangle$ (see, for example, [17]). The main property of this norm can be expressed in such a way like:

$$\forall \mathbf{x} \in V_N(\mathbf{R}^+) \quad \rightarrow \quad \exists \langle\mathbf{x}\rangle \in \mathbf{R}^+.$$

Minkowski norms can be submitted to the following linear properties, besides its positive definite nature:

1. $\forall \mathbf{x}, \mathbf{y} \in V_N(\mathbf{R}^+) \colon \langle\mathbf{x} + \mathbf{y}\rangle = \langle\mathbf{x}\rangle + \langle\mathbf{y}\rangle$.
2. $\forall \mathbf{x} \in V_N(\mathbf{R}^+) \wedge \forall \alpha \in \mathbf{R}^+ \colon \langle\alpha\mathbf{x}\rangle = \alpha\langle\mathbf{x}\rangle$.

The above properties of Minkowski norms prove without doubt that the norm symbol $\langle\mathbf{x}\rangle$, when applied to vector space or semispace elements, can be considered as a linear operator. In the vector or matrix semispaces the Minkowski norm is coincident with the sum of the whole vector or matrix elements. Due to this reason the symbol adopted (see, for example, [17]) for the matrix elements sum algorithm has been also adopted in this case. That is, whenever an N-dimensional column vector semispace is defined, then it can be also set the following procedure:

$$\forall \mathbf{c} \in C_N(\mathbf{R}^+) \quad \rightarrow \quad \mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \wedge \langle \mathbf{c} \rangle = \sum_{I=1}^{N} c_I \in \mathbf{R}^+.$$

2.3. *Shell structure in semispaces*

Once written in this classical way, then, Minkowski norms can be employed to classify vector semispaces into subsets, which have been called σ-*shells* [15]. A vector semispace σ-shell, $S(\sigma)$ is made by the set of all semispace vectors, whose Minkowski norm has a unique definite *shell character* value σ. That is the same as to set:

$$\forall \mathbf{x} \in S(\sigma) \subset V_N(\mathbf{R}^+) \quad \rightarrow \quad \langle \mathbf{x} \rangle = \sigma.$$

Among all the σ-shells the *unit shell*, $S(1)$, shall be noted as a fundamental background tool by which all the other shells can be made. Indeed, any semispace σ-shell can be constructed from the unit shell, simply taking into account that:

$$\forall \mathbf{z} \in S(\sigma) \quad \rightarrow \quad \mathbf{z} = \sigma \mathbf{x} \wedge \mathbf{x} \in S(1): \langle \mathbf{z} \rangle = \langle \sigma \mathbf{x} \rangle = \sigma \langle \mathbf{x} \rangle = \sigma.$$

Conversely, any unit shell vector can be obtained by multiplying a σ-shell vector by the scalar factor: σ^{-1}. Thus, a vector semispace is nothing else but the set of *homothetic shells* associated to the unit shell. Any vector semispace is *covered* by its σ-shell partition in the sense:

$$V_N(\mathbf{R}^+) = \bigcup_{\sigma \in \mathbf{R}^+} S(\sigma) \wedge \forall \lambda \neq \sigma: S(\sigma) \cap S(\lambda) = \emptyset.$$

Other properties of the shell structure are so obvious which will not be given here, except for enhancing the fact that the vectors sum, belonging to different σ-shells, produces a vector of a new shell, whose shell character is the sum of the intervening shell characters.

The unit shell corresponds to the whole set of N-dimensional vectors, which present or fulfil *convex conditions* [2], which can be symbolized by

$$K_N(\mathbf{x}) = \{\mathbf{x} \in S(1) \subset V_N(\mathbf{R}^+)\},$$

although for arrays made of real numbers the convex condition symbol can be written explicitly as follows:

$$K_N(\mathbf{x}) = \left\{ \mathbf{x} = \{x_I\} \,\middle|\, \forall I: x_I \in \mathbf{R}^+ \wedge \langle \mathbf{x} \rangle = \sum_{I=1}^{N} x_I = 1 \right\}.$$

When considering column or row vector semispaces, then the corresponding elements of the unit shell in this special case can be also observed as representing the set of all N-dimensional *discrete* probability distributions. Infinite dimensional unit shells represent, in this way, continuous probability distributions, probability density functions.

2.4. Generating symbols

Still more interesting is the fact that unit shell vectors can be constructed from normalized vectors, extracted, in turn, from arbitrary metric vector spaces. In order to grasp this construction possibility, which generalizes and extends the quantum mechanical relationship between wave functions and density functions, in any metric vector space it must be defined the following auxiliary operation, symbolized by a so called *generating symbol* [2]:

$$R(\mathbf{v} \ \rightarrow \ \mathbf{x}) = \left\{\forall \mathbf{v} \in V_N(\mathbf{C}) \ \rightarrow \ \mathbf{x} = \mathbf{v}^* * \mathbf{v} \in V_N\left(\mathbf{R}^+\right) \wedge \langle \mathbf{v}|\mathbf{v}\rangle \equiv \left\langle \mathbf{v}^* * \mathbf{v}\right\rangle = \langle \mathbf{x}\rangle\right\},$$

where the vector $\mathbf{v}^*$ can be taken in a general manner as the complex conjugate of the original chosen vector $\mathbf{v}$. In the generating symbol body, it is supposed that some product can be also defined, involving the vectors of the initial vector space, and resulting into another real and positive definite vector of an attached semispace. Then, in case that this kind of operations are feasible, like it occurs in Hilbert spaces, Minkowski norms in the semispace will become equivalent to a typical *Euclidean norm* in the attached *origin* vector space. Therefore, the set of all normalized vectors in the origin space can be considered as generating the attached semispace unit shell. Construction of any density function ρ by means of a wave function Ψ, can be symbolically expressed by means of the generating symbol $R(\Psi \rightarrow \rho)$, just taking into account that in functional semispaces the Minkowski norm has to be associated to an integral, approximately an infinite sum like:

$$\forall \rho(\mathbf{r}) \in V_\infty\left(\mathbf{R}^+\right) \colon \langle \rho \rangle = \int_D \rho(\mathbf{r})\,\mathrm{d}\mathbf{r}.$$

This definition also constitutes the usual statistical concept of a probability distribution norm.

3. Inward matrix products

The best way to grasp the interest of *inward matrix products* consists in the possibility to connect such a vector space internal operation with the so called *Hadamard product* [11,12]. Hadamard products have been initially described to deal with products performed over series, for instance as:

$$\left(\sum_\mu a_\mu\right) * \left(\sum_\mu b_\mu\right) = \sum_\mu a_\mu b_\mu.$$

The definition above, which uses for the final product expression just the diagonal terms of a classical product, has been written in a form that no indication is made about the initial and final subindex values. However, for the Hadamard product to be *feasible*, both sums must have the same number of terms, providing as the Hadamard product result an object with the same characteristics as the factors involved into the same Hadamard product.

Thus, one of the characteristics of Hadamard products is to produce results belonging to the same set as the involved active factors. Thus, for example, in vector or matrix spaces the resultant Hadamard product object is an element of the same space with the dimension of the two involved factors. The term *inward matrix product* was coined for such a multiplicative closed composition rule.

Inward matrix product definition [13], added to the matrix sum rules, makes easy to describe its properties, this is so because it induces, within the matrix space possessing such product, a structure, a formalism which allows matrices to resemble the scalar field elements behaviour. Except for the general existence of inward product inverses, which are not directly allowed in matrices with null elements, all the general properties of the definition fields can be extended to matrices in this way [18]. With some extra definition extension, even general inward matrix product inverses can be constructed, as will be later discussed. Also, inward matrix product is a commutative operation, which can be distributive respect the addition, possessing a neutral element in the form of the so called unity matrix: **1**, whose elements are all, without exceptions, the scalar neutral multiplicative element. All these properties can be immediately deduced from the following definition:

$$\forall \mathbf{A} = \{a_{IJ}\} \wedge \mathbf{B} = \{b_{IJ}\} \in M_{(M\times N)} \quad \rightarrow \quad \mathbf{A} * \mathbf{B} = \mathbf{P} = \{p_{IJ} = a_{IJ} b_{IJ}\} \in M_{(M\times N)}$$

and supposing the usual properties, attached to both vector space definition as well as the scalar reference field, hold. The definition has been given here within a usual matrix space, but it is obvious that can be immediately extended to any hypermatrix space.

When describing the generating symbol, an internal vector space operation, such as the inward matrix product, was essential in order to connect vector norms, based in scalar products, and Minkowski norms in vector semispaces. Then, the inward matrix product constitutes an adequate operation in order to perform this task. Indeed, suppose the connection between a vector space and a semispace is made using the inward matrix product in the following way:

$$R(\mathbf{x} \rightarrow \mathbf{y}) = \left\{\forall \mathbf{x} = \{x_I\} \in M(\mathbf{C})\colon \mathbf{y} = \mathbf{x}^* * \mathbf{x} = \left\{y_I = |x_I|^2\right\} \ \rightarrow\ \mathbf{y} \in M\left(\mathbf{R}^+\right)\right\},$$

then, as a consequence the manner vector spaces and semispaces are associated is well defined without ambiguities.

4. Vector and matrix signature

4.1. Signatures

In general, vector or matrix space elements can be associated to field element arrays whose structure admits a sign in the real case and two in the general complex case. In order to obtain a not too cumbersome set of examples and definitions, there will be discussed the real field case, and the reader can simply develop the corresponding definition and properties for the complex field situation. Any vector or matrix of arbitrary dimensions, defined over the real field, can possess elements trivially associated to a positive or negative sign, multiplying a positive definite real number, as one can always write for an arbitrary two index array:

$$\mathbf{A} = \{a_{IJ}\} \quad \to \quad a_{IJ} = \sigma_{IJ}|a_{IJ}| \wedge \sigma_{IJ} \in \{+1, -1\}, \quad |a_{IJ}| \in \mathbf{R}^+.$$

Suppose that now both the signs and the positive definite elements are ordered in separate arrays, that is:

$$\mathbf{S} = \{\sigma_{IJ}\} \equiv \mathrm{Sign}(\mathbf{A}) \wedge |\mathbf{A}| = \left\{|a_{IJ}|\right\}$$

so, the inward matrix product previous definition can be invoked to write the initial array structure by means of the trivial algorithm:

$$\mathbf{A} = \mathbf{S} * |\mathbf{A}| \equiv \mathrm{Sign}(\mathbf{A}) * |\mathbf{A}|.$$

Then, the matrix $\mathbf{S} = \mathrm{Sign}(\mathbf{A})$, holding the signs of the initial matrix, can be named as a *matrix signature*.

4.2. Signature classes and tagged sets

Two points must be signalled here. In a first place, any matrix signature $\mathrm{Sign}(\mathbf{A})$ has a Boolean structure associated to its elements, in such a way that for an arbitrary matrix dimension $(N \times M)$, just a finite number of different signatures will exist, exactly, $2^{N \cdot M}$. In second term, the matrix absolute value $|\mathbf{A}|$, has to be necessarily an element of some vector semispace, possessing the same dimension as the one containing the original matrix:

$$\mathbf{A} \in V_{(N\times M)}(\mathbf{R}) \quad \to \quad |\mathbf{A}| \in V_{(N\times M)}\left(\mathbf{R}^+\right).$$

This situation is quite interesting as it also permits, through such signature decomposition, to associate every vector space element with a *tagged set* element [1,2]. In order to set this question in an easy way, suppose that the whole collection of matrix signatures associated to some N-dimensional matrix space are collected into a set $\Sigma = \{\mathbf{S}_I;\ (I = 1, 2^N)\}$. The cardinality of the signature set is necessarily well defined, and as it has already been commented has a specific value given by $\#(\Sigma) = 2^N$. The elements of the signature set can be employed, in turn, as a tag set, associated to the elements of some vector semispace of the same dimension. That is, the following tagged set T in terms of the ordered pairs of signatures as tags and semispace elements as objects is formed:

$$T = \left\{ \tau \in T \mid \mathbf{S} \in \Sigma \wedge \mathbf{A} \in V_N\left(\mathbf{R}^+\right): \tau = (\mathbf{S}, \mathbf{A}) \right\}.$$

This is equivalent to consider the signature tags as a way to classify matrices in exactly 2^N object classes.

Also, it can now be noted the fact that in vector spaces, when a basis set is known, then every vector in the space is spanned as a unique linear combination of the basis set vectors. Then, one can consider that the signature of an arbitrary vector in a given vector space is the signature of the array of its coefficient coordinates with respect some chosen basis set. The vector signature owing to the nature of these cases will obviously be basis set dependent. In this simple way and using the fundamental property of vector spaces, the signature concept can be extended to any kind of vector space made of arbitrary objects.

4.3. Basis sets constructed from unit shell elements and a signature subset

Another remark can be now discussed at this stage of the signature theoretical development. When constructing the binary signature sets of type Σ as defined above, the signature vectors $\{S_I\}$ can be considered a set from where a N-dimensional basis set can be chosen. In fact, the columns of the symmetrical $(N \times N)$ matrix

$$\mathbf{Z} = \mathbf{1} - 2\mathbf{I}$$

belong to the signature class set and also are in general such a basis set. The basis set matrix $\mathbf{Z}$ is made by subtracting from the already mentioned unity matrix: $\mathbf{1} = \{1_{IJ} = 1\}$, an $(N \times N)$-dimensional matrix in this case, whose elements are entirely composed by ones, minus twice the matrix multiplicative unit. Thus, one can easily see that: $\mathrm{Tr}(\mathbf{Z}) = -N$. The eigenvalues of this basis set matrix can be defined without great problems, as one of the eigenvectors is the unity vector: $|\mathbf{1}\rangle = \{1_I = 1\}$, constructed as the N-dimensional counterpart of the previously defined unity matrix, this is so because:

$$\mathbf{Z}|\mathbf{1}\rangle = \mathbf{1}|\mathbf{1}\rangle - 2\mathbf{I}|\mathbf{1}\rangle = (N-2)|\mathbf{1}\rangle.$$

Now choosing the whole set of $N-1$ linearly independent vectors orthogonal to the unity eigenvector $|\mathbf{1}\rangle$, and calling them generically $|x\rangle$, then, as one can also write $\mathbf{1} = |\mathbf{1}\rangle\langle\mathbf{1}|$, and because $\langle\mathbf{1}|x\rangle = 0$, it is straightforward to obtain:

$$\mathbf{Z}|x\rangle = |\mathbf{1}\rangle\langle\mathbf{1}|x\rangle - 2\mathbf{I}|x\rangle = -2|x\rangle.$$

So, it is also easy to write:

$$\mathrm{Det}(\mathbf{Z}) = (N-2)(-2)^{(N-1)},$$

which tells that, for $N > 2$, the columns of the matrix $\mathbf{Z}$ are linearly independent. The same can be said of the complementary subset signature matrix $-\mathbf{Z}$. Thus, one can freely choose any vector of the unit shell, say, $|a\rangle = \{a_I\} \in S(1)$, then taking into account the columns of the matrix $\mathbf{Z} = \{|\mathbf{z}_I\rangle\}$ and defining the inward matrix products of these columns by the chosen unit shell vector, a new matrix can be constructed:

$$\mathbf{A} = \left\{|\mathbf{a}_I\rangle = |\mathbf{z}_I\rangle * |a\rangle\right\}.$$

The determinant of the matrix constructed in this way is easily determined employing the non-zero product of the elements of the unit shell vector:

$$\mathrm{Det}(\mathbf{A}) = \left(\prod_{I=1}^{N} a_I\right)\mathrm{Det}(\mathbf{Z}),$$

showing that the columns of the matrix **A** form a basis set too, provided that the elements of the chosen semispace vector are non-null.

Consequently, choosing the appropriate signature subset and an arbitrary element of the unit shell a basis set adapted to any vector space can be constructed.

4.4. Real field signature

Another question, which has been already published [9], consists in the fact that, from this point of view the real field can be divided into two classes. However, the number zero can be either attached to one or another, being irrelevant its sign. This was a typical situation encountered in practice, when in old generation computers the result of some operation could provide an answer with a signed zero result. This is no wonder, as computer numerical signs can be considered as bit tags, accompanying the rest of the mantissa. Thus, provided that one considers the possible appearance of signed zeros, the real field can be divided into two equivalent classes: as it was earlier pointed out [9], to each equivalent real class, could be considered attached a signed zero element.

5. Vector space generation through the unit shell

5.1. Vector spaces as unit shell homotheties

Moreover, another related question to all the previously developed analysis is basically connected to the possibility to write any matrix employing an inward matrix product of some signature and an element of a matrix semispace. However, this can be worked out in a much better way, even enhancing the role played by the unit shell structure in semispaces. As any semispace element can be deduced by means of a unit shell homothety, then this fact can tell us that any vector space element can be constructed from a parent unit shell element by means of an appropriate homothety and an *a posteriori* association of the final shell element with an appropriate signature. This is the same as to employ the following set of operations, initially:

$$\forall \mathbf{A} \in V_N(\mathbf{R}) \quad \rightarrow \quad \exists \mathbf{X} = \mathrm{Sign}(\mathbf{A}) \wedge \alpha = \left\langle|\mathbf{A}|\right\rangle,$$

then afterwards as:

$$|\mathbf{A}| \in S(\alpha) \subset V_N(\mathbf{R}^+) \quad \rightarrow \quad \mathbf{Z} = \alpha^{-\mathbf{1}}|\mathbf{A}| \in S(1)$$

and, so, the initial space element can be immediately written using the simple algorithm, involving an element of the unit shell, its product by an appropriate scalar and, finally, the inward matrix product of the scaled result by a chosen signature:

$$\mathbf{A} = \mathbf{X} * (\alpha \mathbf{Z}).$$

Besides, the previous algorithm set up tells that any matrix could be nothing else than some homothety of a unit shell vector inwardly multiplied by a signature class identifier, providing in this fashion the algebraic formalism of the tagged set structure discussed above. This is sufficient to prove the initial statement consisting in that any vector space element is expressible by means of some unit shell element. Thus, the unit shell becomes in this manner the core of any vector space construction. More than this can be said around this subject, because the algorithm above also tells that a unique unit shell homothety can produce as many matrices as signature classes are allowed by the vector space dimension.

5.2. Inward matrix product inverses

Such vector space fundamental property can also provide the general algorithm to compute inward matrix inverses, but poses another interesting problem, which has not been pointed out until the present discussion stage, although appeared as a consequence of the possibility to generate basis sets with chosen signature classes and unit shell vectors. Any element of a semispace can be considered constructed *without* zero elements, as every semispace feature can be attached to a strictly positive definite formalism. This semispace characteristic feature is transferred within the matrix or vector of the space, or alternatively in the coefficient array associated to any given vector, through the representation in a basis set linear combination. The elements of the unit shell are, thus, forming convex real sets and lacking, by construction, of null elements. Then, any matrix constructed by means of the unit shell homothety and the appropriate signature can be considered non singular from the inward matrix product point of view, the inward inverse being easily defined with the following algorithm:

$$\forall \mathbf{A} = \mathrm{Sign}(\mathbf{A}) * (\alpha \mathbf{Z}) \quad \rightarrow \quad \exists \mathbf{A}^{[-1]}\colon \mathbf{A}\mathbf{A}^{[-1]} = \mathbf{A}^{[-1]}\mathbf{A} = \mathbf{1}$$

and, thus:

$$\mathbf{A}^{[-1]} = \mathrm{Sign}(\mathbf{A}) * \left(\alpha^{-1}\mathbf{Z}^{[-1]}\right) \quad \rightarrow \quad \mathbf{Z}^{[-1]} = \left\{z_{IJ}^{-1}\right\}.$$

That is, the inward product inversion in the algorithm above defined is supposed to affect the semispace part of the matrix only. But such a trivial result, deduced from the construction of space elements from semispace ones, do not takes into account the possible occurrence of vector space matrix or vector representations bearing null elements. The problem can be solved as follows, by extending the signature concept.

6. Extended signatures

Despite that the solution of the zero bearing matrix elements precludes the appearance of a highly redundant information structure, the zero elements problem, already discussed with respect the real numbers signatures may be also solved considering another new situation.

Suppose that along with the signature binary set: $S_2 = \{-1, +1\}$, one can consider that nothing opposes to the definition a ternary signature basic set too, adding a zero element to the usual Boolean situation: $S_3 = \{-1, 0, +1\}$. Then, obviously three real classes will appear, the former couple of positive and negative half lines, plus a highly degenerate one formed by zero. The problem of zero signatures will disappear in this way, but a highly redundant situation will appear on the contrary, produced by multiplying by the signature zero every unsigned real number. However, in vector space representation the zero augmented signature classes permit to really consider the semispace unit shell as a kind of universal vector core, able to be employed in order to build up any vector in the original parent vector space, including the matrix or vector zero. The actual ternary number of signature classes will augment accordingly for N-dimensional vector spaces and be raised up to a cardinality 3^N, but, then, the definition of any matrix from the unit shell construct will be as a result completely general. A most interesting consequence can be associated to the fact that, both previously described algorithms, the one constructing any vector space matrix or the builder of inward product inverses are applicable within the triadic signature set without modification.

It may be now worthwhile to somehow consider the geometric implications of the structure of the Boolean or triadic signature tags, which can be constructed with S_2 and S_3 signature sets, respectively. The Boolean tags have been discussed and employed in an earlier paper [2], dealing with this kind of theoretical discussion, as a basic device to construct Boolean tagged sets. It is straightforward to realize that the generated tags using the binary set: S_2, can be considered the set of vertices associated to an N-dimensional hypercube, H_N, with a side length of 2, and centred at the origin of coordinates. While the use of the triadic signature set provides the same N-dimensional figure, but including not only the hypercube vertex coordinates, but also adding to these dyadic points the collection of all the points representing the centres of sides and faces, as well as including the origin itself, which was not present in the Boolean H_N.

Moreover, nothing opposes to consider other kinds of extended signature sets, as it will be discussed in the next section.

7. Signature multiplets and the support signature group

The augmented triadic signature set S_3 can open the way to consider other kinds of *signature multiplets*, as one can call these basic signature elements, whose set can be plausibly described by the symbol S_P, where P will stand for the cardinality of the basic signature set. Of course, given such a set, the number of N-dimensional signature tags will be raised to P^N.

An immediate option, serving as an example of signature extension, is to add to the set S_3, two more elements consisting in the imaginary unit with positive and negative signs. It is obvious that the set $S_5 = \{-\mathrm{i}, -1, 0, +1, +\mathrm{i}\}$, forms a multiplicative Abelian group, and has the power to generate an N-dimensional signature set of 5^N elements. In this sense, the so called Pauli matrices [19,20] can be considered as three of the possible signature tags, defined in a (2×2)-dimensional matrix space using the quintuplet signature set S_5, as defined above.

Obviously the $(N \times N)$-dimensional multiplicative unit matrix $\mathbf{I}_N = \{\delta_{IJ}\}$, whose elements are the Kronecker's delta symbols, is one of such signature matrices, as well as the unity matrix, $\mathbf{1} = \{1_{IJ} = 1\}$, with all the elements equal to the real multiplicative unit, already employed in inward matrix product inversion, constitutes another example of the general form such signature matrices can take when constructed by S_3 or S_5. Precisely, the unity matrix signature has to be attached forcibly to the whole elements of any semispace.

The extension of basic signature sets to any cardinality, has probably to contain some essential classical elements; that is, those contained in S_3, most probably, but can be adequately chosen as forming an Abelian group, even more generally relaxing some group properties, and collected within a basic set $S_P = \{\sigma_I;\ (I = 1, P)\}$. Still, the unit shell construction algorithms will continue to remain fixed up as those defined above.

8. Fuzzy signature functions

When facing the possibility to construct any vector or matrix from the semispace unit shell by means of homothetic transforms plus the inward matrix product by a signature, which shall be classically constructed with the basic signature set S_3, in order to allow the possible appearance of null elements in the final array structure, one is also facing the problem of infinite-dimensional spaces and the possible definition of well-designed signatures in these cases.

The signature set S_3 seems to mark some kind of classical pattern, in order to find out a similar structure in a general case. In the restricted situation, where the basic signature set S_3 marks the limits and elements, which one can associate to signatures, then it can be designed some of the possible continuous forms signatures can have. Indeed, S_3 and the parent basic signature extensions discussed before, correspond to discrete signature structures and in functional spaces may be interesting to try continuous forms instead. The typical functions having an adequate range, containing the S_3 set, can be chosen immediately within the trigonometric function set. The cosine and sine functions possess such a nature, as, for example, within the variable domain $x \in [0, \pi]$, then the function acquires a suitable range $\cos(x) \in [+1, -1]$. Thus, the cosine function can be employed to conveniently provide functions, constructed within some functional semispace unit shell, with an appropriate range of continuous signatures, encompassing the discrete S_3 set and all the intermediate values. This example constitutes not only a quite obvious way to generalize signatures into continuous structures, but indicates that signatures can be extended in such a way that they arrive to possess a *fuzzy structure*. That is, instead of a classical set of triadic S_3 values, intermediate interval signature figures, like $\pm 1/2$, can be also accepted in a fuzzy signature environment. In the same way as classical binary ownership functions can be supposedly transformed into N-dimensional fuzzy ones and, thus, by taking a possible limit, into infinite-dimensional ownership relationships, like those provided by cosine and sine functions. Also, other fuzzy signature candidates can possess a structure similarly constructed to the trigonometric defined functions, like the hyperbolic tangent, which for the even more convenient variable domain, $x \in [-\infty, +\infty]$, varies within the adequate S_3 range as it is well known that $\tanh(x) \in [-1, +1]$.

9. Quantum mechanical applications of the signature concept

Some chosen application examples of the signature extension possibility will be now given in the quantum chemical environment.

9.1. Phase functions

In this way, the well-known quantum mechanical phase functions, which leaves the wave function module invariant, and which can be considered as a linear combination of cosine and sine functions with signature coefficients belonging to S_5 are a good example of the flexibility and general use of the signature concept.

Another possibility of sign generalization can be found in the Bohm treatise [19] and concerns the way one can suppose that can be written a wave function Ψ as a linear combination of a known set of state wave functions $\{\psi_I\}$, in terms of some set of phase factors $\{e^{i\alpha_I}\}$, acting as linear coefficients:

$$\Psi = \sum_I e^{i\alpha_I} \psi_I.$$

The set of phase factors can be described as complex numbers, which using Euler's formula can be written as [21]:

$$e^{i\alpha_I} = \cos(\alpha_I) + i \sin(\alpha_I),$$

that is, every phase factor is just a combination of two fuzzy sign conventions, as previously described.

9.2. Density functions

A recent study about the nature and properties of density functions [14] has put forward the first ideas about the possibility to use density functions, with appropriate signatures, to construct attached wavelike functions of the same order. Indeed, in MO theory a first order density function can always be expressed in terms of the MO set $\{\psi_I(\mathbf{r})\}$, considered as monoelectronic normalized functions in the Euclidean norm sense:

$$\langle \psi_I | \psi_I \rangle = \int_D |\psi_I|^2 \, d\mathbf{r} = 1.$$

The first order density function may be described with the linear combination

$$\rho(\mathbf{r}) = \sum_I \omega_I |\psi_I|^2,$$

where the coefficient set $\{\omega_I\}$ constitutes the occupation numbers of the MO set. Nothing opposes to consider that a convexity condition [2] holds for the occupation number set $K(\{\omega_I\})$, in this fashion the first order density could be considered a member of the unit shell:

$$\langle\rho\rangle = \int_D \rho(\mathbf{r})\,\mathrm{d}\mathbf{r} = \sum_I \omega_I \int_D |\psi_I|^2\,\mathrm{d}\mathbf{r} = \sum_I \omega_I = 1.$$

The squared modules of the MO set can be considered too as first order density functions, belonging to the same unit shell, and thus forming a basis set in a way to express first order density functions as convex linear combinations. Forming the occupation numbers a convex set, they then are real numbers and so can be expressed by squared modules of real, even complex, numbers: $\forall I\colon \omega_I = |c_I|^2$. Also, owing to this last property, the density expression can be rewritten like:

$$\rho(\mathbf{r}) = \sum_I |c_I\psi_I|^2,$$

an expression, which can be taken as an Hadamard product in the way:

$$\rho(\mathbf{r}) = \left(\sum_I c_I\psi_I\right)^* * \left(\sum_I c_I\psi_I\right) = \left|\sum_I c_I\psi_I\right|^{[2]},$$

which has been expressed in the inward matrix product fashion. Thus, an inward square root of the density function seems plausible to be defined, and can be expressed as

$$\phi(\mathbf{r}) = \bigl(\rho(\mathbf{r})\bigr)^{[1/2]} = \sum_I (s_I c_I)\psi_I,$$

where the set $\{s_I\}$ corresponds to the MO coefficient signatures. In this manner, one can see how a first order wavelike function $\phi(\mathbf{r})$ can be deduced from MO first order density functions. However, a signature set has to be present, as the signs of the square roots of the occupation numbers remain underdetermined by a choice of the 2^N signature set combinations, if the number of used MO's is N.

9.3. Unit shell monoelectronic density functions

A related problem can be found in the definition of the unit shell monoelectronic MO density functions $\forall I\colon \pi_I(\mathbf{r}) = |\psi_I|^2$. The set $\Pi = \{\pi_I\}$, is a subset of the unit shell, where the first order density function, a convex linear combination of the set Π, also belongs. More interesting is the fact that these MO density functions are obtained in the same way as Fukui was describing the *frontier orbital* densities [22], and earlier Mulliken used the same idea to construct a molecular electron partition, leading to the well-known *orbital population* analysis [20]. In case that MO's are supposed to be expressed as linear combinations of an AO orthogonal basis set $X = \{\chi_\mu(\mathbf{r})\}$, then, the MO densities could be expressed in the same way as the global density, as

$$\psi_I = \sum_\mu x_{\mu I}\chi_\mu \quad \rightarrow \quad \pi_I = \sum_\mu |x_{\mu I}\chi_\mu|^2 = \sum_\mu \theta_{\mu I}|\chi_\mu|^2,$$

where the convex coefficient set $K(\{\theta_{\mu I}\})$ is constituted by the square modules of the AO coefficients, set up to express the MO's in LCAO MO theory. Thus the global first order density can be written as

$$\rho(\mathbf{r}) = \sum_I \omega_I \pi_I(\mathbf{r}) = \sum_I \sum_\mu \omega_I \theta_{\mu I}|\chi_\mu|^2.$$

In this special case, the sum over MO can be performed, resulting on a set of coefficients just depending on the orthogonal MO's:

$$\forall\mu\colon \gamma_\mu = \sum_I \omega_I \theta_{\mu I} \quad \rightarrow \quad \sum_\mu \gamma_\mu = 1,$$

but the new coefficient set can be defined fulfilling $\Gamma = \{\gamma_\mu\} \subset S(1)$. That is, it forms part of the appropriate dimension unit shell and is convex $K(\{\gamma_\mu\})$. This is coherent with the fact that the global first order density can be now written as

$$\rho(\mathbf{r}) = \sum_\mu \gamma_\mu |\chi_\mu|^2.$$

9.4. *Density-generated wavelike functions*

One can conclude that in LCAO MO theory the first order density can generate a wavelike function at the orthogonal AO level, possessing the same characteristics and signature indefiniteness as the ones deduced in the MO frame global density expression. The appropriate wavelike AO first order global function is now expressible as

$$\phi(\mathbf{r}) = \big(\rho(\mathbf{r})\big)^{[1/2]} = \sum_\mu \big(s_\mu \gamma_\mu^{1/2}\big)\chi_\mu,$$

with the set $\{s_\mu\}$ becoming in this AO frame the suitable signature.

9.5. *Matrix wavefunctions and spin*

In the same track, a recent study over the possible matrix expression of wave functions [23] within MO theory has used the signature concept, in order to identify the phenomenological spin function part of spin orbital construction as a signature, attached to the space part of the orbital matrix wave function. It will be here just schematically expressed the underlying idea. Supposing a Slater determinant [19,20] expressed in terms of spinorbitals, there can be constructed an $(N \times N)$-square matrix, from where the determinant will produce the N-electron Slater wave function. Let $\{\varphi_I\}$ be the set of spinorbitals, and $\{\psi_I\}, \{\sigma_I\}$, the sets of the spatial MO and the spin functions, respectively. Then, as usual $\forall I\colon \varphi_I(\mathbf{r}; s) = \psi_I(\mathbf{r})\sigma_I(s)$, with explicit use of the electron space and spin coordinates. Adopting the notation $\forall I\colon \varphi_I(J) = \psi_I(J)\sigma_I(J)$ for the representation of the Ith spinorbital associated to the Jth particle space-spin coordinates, then the following matrix can be set, providing the Slater determinant when such operation is made over it:

$$\begin{aligned}
&\left|\Phi(1,2,\dots,N)\right\rangle \\
&\quad = \begin{pmatrix} \varphi_1(1) & \varphi_1(2) & \dots & \varphi_1(N) \\ \varphi_2(1) & \varphi_2(2) & \dots & \varphi_2(N) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_N(1) & \varphi_N(2) & \dots & \varphi_N(N) \end{pmatrix} = \left|\Psi(1,2,\dots,N)\right\rangle * \left|\Sigma(1,2,\dots,N)\right\rangle \\
&\quad = \begin{pmatrix} \psi_1(1) & \psi_1(2) & \dots & \psi_1(N) \\ \psi_2(1) & \psi_2(2) & \dots & \psi_2(N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N(1) & \psi_N(2) & \dots & \psi_N(N) \end{pmatrix} * \begin{pmatrix} \sigma_1(1) & \sigma_1(2) & \dots & \sigma_1(N) \\ \sigma_2(1) & \sigma_2(2) & \dots & \sigma_2(N) \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_N(1) & \sigma_N(2) & \dots & \sigma_N(N) \end{pmatrix}.
\end{aligned}$$

This last expression shows how the set of spin functions can be observed as a signature of the MO matrix wave function.

10. Conclusions

The shell structure of semispaces attached to the Minkowski norm values can be well defined. Among all the possible shells must be noted the unit shell, the set of all semispace vectors with unit Minkowski norm. A general algorithmic structure permits to show that all elements in a vector space can be constructed by means of the attached semispace unit shell components. In order to perform such a space–semispace connection, which shows the extreme importance of the semispace unit shell, just a simple homothetic transformation, followed by an inward matrix product by a chosen signature, constitutes all the needed operations. Signatures on the other hand, appear to be easily generalized, from the classical binary basic set up to the triadic set formed by the binary signs plus zero, taken as another signature. Extended basic signature sets, associated to Abelian multiplicative groups, can be easily described. A fuzzy extension of the signature concept has been finally set, with useful properties to be used in functional spaces. Applications within the quantum chemical description of both density functions and wave functions can be easily imagined.

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