

# An isometric representation problem in quantum multimolecular polyhedra and similarity: (2) synisometry

Ramon Carbó-Dorca<sup>1,2</sup>

Received: 27 April 2015 / Accepted: 20 June 2015 / Published online: 30 June 2015  
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**Abstract** Collective distances in quantum multimolecular polyhedra (QMP), which can be set as a scalar indices associated to the QMP variance vector, enhance the role of the pair density similarity matrix. This paper describes a simplified efficient algorithm to compute triple, quadruple or higher order density similarity hypermatrices via an approximate isometry: a *synisometric* decomposition of the pair similarity matrix. Synisometries pretend to avoid the use of Minkowski metrics in QMP description problems, where the double density similarity matrix possesses negative eigenvalues. The synisometric decomposition of the similarity matrix opens the way to the general use of higher order approximate similarity elements in quantum QSAR and in the construction of scalar condensed vector statistical-like indices, for instance skewness and kurtosis. This might lead the way to describe, without excessive complication and within a real field computational framework, the collective structure of quantum multimolecular polyhedra.

**Keywords** Quantum molecular similarity · Quantum multimolecular polyhedra · Quantum object sets · Density functions discrete isometric and Synisometric representation · Collective distances · Collective similarity indices

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✉ Ramon Carbó-Dorca  
ramoncarbodorca@gmail.com

<sup>1</sup> Institut de Química Computacional i Catàlisi, Universitat de Girona, 17071 Girona, Catalonia, Spain

<sup>2</sup> Departamento de Química, Universidad Técnica Particular de Loja, 1101608 Loja, Ecuador

## 1 Introduction: isometric transformation problem of the pair density function quantum similarity matrix

Two of the many possible ways to obtain a set of discrete column or row vectors, which reproduce the structure of the double density function (DF) similarity matrix have been previously discussed, see reference [1], which constitutes a first paper of this series, useful as a previous introduction to the problem which will be discussed here.

The precise aim of such earlier procedures as described in [1] was the ability to discretely describe the set of any quantum multimolecular polyhedron (QMP) continuous DF vertices, see for more details references [2–9]. One can now propose to find out, whenever this QMP DF vertex discretization can be alternatively set up more accurately than the possibilities provided throughout, for example, by any even power of the similarity matrix, as it is discussed at the end of the present paper.

The isometry concept, which might be interesting as a starting point for the present purposes, could be described in such a way that the structure of the dual DF similarity matrix, which acts, in turn, as a metric matrix of the space generated by the QMP DF vertices, see for example reference [6], could be preserved as much as possible. A résumé of such a method will be described next and the possible application procedures and alternatives described in detail afterwards.

Without doubt, this reasoning contains the same purpose as the former double DF similarity matrix manipulations can claim [1]. Yet the present discussion appears to possess a deeper insight about the nature of the discrete representation of QMP DF vertices and their final Gram matrix.

### 1.1 The definition of an isometric set of column vectors based on the double DF similarity matrix

Suppose known a  $(M \times M)$  double density quantum similarity matrix:  $\mathbf{Z}$ , say. Suppose that a matrix  $\mathbf{A}$ , whose column set:  $\{\mathbf{a}_I \mid I = 1, M\}$  will correspond to a set of isometric vectors to the QMP DF vertices, is sought such that the following equality holds:

$$\mathbf{Z} = \mathbf{A}^T \mathbf{A}. \quad (1)$$

The present discussion might be fully justified just indicating that, after knowing a matrix like  $\mathbf{A}$  in Eq. (1), the main purpose of such a simple theoretical development aims to the possibility of computing the higher order similarity matrices, like those entering the QMP skewness and kurtosis condensed indices, see for example reference [7], without need of evaluating triple and quadruple DF integrals [1].

### 1.2 Using generalized scalar products of the isometric vectors to obtain higher order similarity integrals

Once obtained any isometric matrix, their columns can be employed to obtain the similarity matrix elements of any order. In fact, because Eq. (1) holds, then one can also write:

$$\forall I, J = 1, M : Z_{IJ} = \int_D \rho_I \rho_J d\mathbf{r} = \langle \mathbf{a}_I | \mathbf{a}_J \rangle = \sum_P a_{PI} a_{PJ} = \langle |\mathbf{a}_I \rangle * |\mathbf{a}_J \rangle \rangle. \quad (2)$$

The last equality is most interesting because, provided there an isometry exists, then a complete sum of an indefinite set of vector inward products, see for example reference [10], can be extended to the computation of any higher order similarity integral.

For instance, triple density similarity integrals [11–14], which are involved in the computation of the skewness vector condensed QMP indices [7], could be simply obtained by means of the straightforward algorithm:

$$\forall I, J, K = 1, M : Z_{IJK} = \int_D \rho_I \rho_J \rho_K d\mathbf{r} \equiv \langle |\mathbf{a}_I \rangle * |\mathbf{a}_J \rangle * |\mathbf{a}_K \rangle \rangle = \sum_P a_{PI} a_{PJ} a_{PK}. \quad (3)$$

Obviously enough, quadruple density similarity integrals, involved in turn with the kurtosis vector condensed QMP indices [7]:

$$\begin{aligned} \forall I, J, K, L = 1, M : Z_{IJKL} &= \int_D \rho_I \rho_J \rho_K \rho_L d\mathbf{r} \\ &\equiv \langle |\mathbf{a}_I \rangle * |\mathbf{a}_J \rangle * |\mathbf{a}_K \rangle * |\mathbf{a}_L \rangle \rangle = \sum_P a_{PI} a_{PJ} a_{PK} a_{PL} \end{aligned} \quad (4)$$

The general formulation in order to compute similarity integrals with an indefinite number of DF, which can be employed to build up the quantum QSPR fundamental Eq. [8] up to any order, can be thus straightforwardly designed.

### 1.3 Nature of the isometric decomposition based on the canonical decomposition of the double density similarity matrix

Then, among the collection of possible decompositions, see for example [15], which can be used to obtain a particular structure for the matrix  $\mathbf{A}$  in Eq. (1), some can be chosen, based on the canonical decomposition of  $\mathbf{Z}$ , provided by the matrix equality:

$$\mathbf{Z} = \mathbf{X} \Theta \mathbf{X}^T. \quad (5)$$

In the well-known Eq. (5) the eigenvector matrix  $\mathbf{X}$  is orthogonal:

$$\mathbf{X}^T \mathbf{X} = \mathbf{X} \mathbf{X}^T = \mathbf{I}$$

and the eigenvalue matrix corresponds to a diagonal structure, which can be defined like:

$$\Theta = \text{Diag} (\theta_I | I = 1, M). \quad (6)$$

Thus, after computing the square root of the diagonal matrix (6):

$$\Theta^{\frac{1}{2}} = \text{Diag} \left( \sqrt{\theta_I} | I = 1, M \right), \quad (7)$$

two possible solutions of the isometric decomposition (1) can be immediately obtained as follows:

$$1) \mathbf{A}_a = \Theta^{\frac{1}{2}} \mathbf{X}^T \leftrightarrow \mathbf{A}_a^T = \mathbf{X} \Theta^{\frac{1}{2}} \quad (8)$$

$$2) \mathbf{A}_s = \mathbf{X} \Theta^{\frac{1}{2}} \mathbf{X}^T = \mathbf{Z}^{\frac{1}{2}} \leftrightarrow \mathbf{A}_s^T = \left( \mathbf{X} \Theta^{\frac{1}{2}} \mathbf{X}^T \right)^T = \mathbf{X} \Theta^{\frac{1}{2}} \mathbf{X}^T = \mathbf{Z}^{\frac{1}{2}}. \quad (9)$$

The option (1) might be called asymmetrical, while the option (2) might be called the symmetrical one.

Both options rely upon the fact that the square root of the diagonal eigenvalues  $\Theta$  and the orthogonal eigenvector  $\mathbf{X}$  matrices are known. Careful observation of the two presented solutions (8) and (9) might produce the result consisting into that each one is just a slight variation of the other. Yet they indeed are different issues of the same isometric decomposition, allowing a discrete representation of the QMP DF vertex set.

## 2 The nature of the vector space generated by the isometric column vectors

In both alternatives (8) and (9) to construct a set of isometric vectors to the QMP DF vertex set, leading to the similarity matrix computation, the generated column vector space has to be real. Therefore, in the previous discussion, the columns of the matrices  $\mathbf{A}_a$  or  $\mathbf{A}_s$  are supposed to be real.

However, the real nature of the two described options in Eqs. (8) and (9) becomes essentially associated to the signature of the elements of the eigenvector matrix:  $\Theta$ . Indeed, whenever the similarity matrix  $\mathbf{Z}$  bears positive definite real eigenvalues only, that is:  $\{\theta_l\} \subset \mathbf{R}^+$ , then the square root diagonal matrix:  $\Theta^{\frac{1}{2}}$ , as defined in Eq. (7), possess positive real elements too.

### 2.1 Definite positive nature and signature of the similarity matrix $\mathbf{Z}$

Such a property derives from the positive definite nature of the matrix elements, which, like those of the similarity matrix, are obtained from scalar products of a linearly independent set of vectors. It has been previously assumed in reference [1] that this is the case when obtaining both asymmetrical and symmetrical options, as described in Eqs. (8) and (9), of the isometric decomposition in Eq. (1).

In the usual construction of double density quantum similarity matrices it can happen that the positive definite nature of the matrix  $\mathbf{Z}$  is not fulfilled, as it has been commented in the literature [16]. Thus, in general the matrix  $\mathbf{Z}$  might be not a positive definite metric matrix, but could have a non-definite signature metric [17].

Such a problem appears mainly due to the scalar products involving two quantum DF, associated to a distinct molecular pair, which are used in turn to construct the elements of the matrix  $\mathbf{Z}$ . Optimization of the similarity matrix elements is usually performed by systematic translations and rotations of the molecular coordinate frames; see for example [17].

Under the Born–Oppenheimer approximation, it is well known that fixed molecular coordinate frames are involved in the calculation of the respective wave functions and therefore are parametrizing the attached DF. An optimal process involving seeking of the maximal value of the integral associated to the scalar product of two DF, such as the one above described in Eq. (2), corresponds to the maximal superposition of the pair of molecules involved into the computation of each quantum similarity matrix element. That is: every molecule in the QMP is located in a three dimensional space, facing every other DF vertex and superposed to them. However, in general this is not a process by which a given molecular frame remains in the same relative position in front of the remaining others.

Thus, optimal superposition of two molecules corresponds to superpose in some way molecular sets of coordinates, belonging to two different molecular structures, and involves the relative positioning of one coordinate molecular frame in front of the other. Therefore, the DF of each molecule when confronted to every other molecular DF forming part of the QMP remnant vertices, it can happen that in several similarity integrals the same DF could be referred to a different translated-rotated set of coordinates. This kind of different coordinate set connected with the same molecule, while leaving the associated DF invariant, produces an intrinsically different DF reference frame. This fact, when studying some concrete QMP cases, produces the non-definite structure of the similarity matrix  $\mathbf{Z}$ .

To attain a positive definite homogeneous result for the similarity matrix has been demonstrated to be quite difficult [16] and therefore, the usual superposition algorithms [17] try to obtain the best compromise between optimal molecular translations-rotations and double density similarity matrix structure. Because of this compromise, it might in some circumstances happen that some of the eigenvalues collected into the matrix  $\Theta$  present negative signatures.

Then, generally speaking the eigenvalue matrix  $\Theta$  has to be considered just real, that is:  $\{\theta_I | I = 1, M\} \subset \mathbf{R}$ . As a consequence of this fact, it has to be taken into account that the square root diagonal matrix  $\Theta^{\frac{1}{2}}$  could bear some imaginary elements, associated to the negative eigenvalues. Then, if this is the case, the columns of the matrix  $\mathbf{A}$  in both the asymmetric or symmetric isometric choices, in order to fulfill Eq. (1) should be associated to some Minkowski space algebra.

### 3 Synisometry as the art of avoiding Minkowski metrics

However, if the whole QMP potential algorithmic structure, to exactly evaluate high order density similarity integrals, becomes a collection of mathematical procedures defined in Minkowski space, that is: based on the particular complex algebra of such space, then perhaps some inconsistencies will appear when isometric matrices, defined as in Eq. (1), are employed. Inconsistencies might appear not only to reproduce the double density similarity matrix, but in order to evaluate in a similar way, without algebraic problems, higher order scalar products involving any number of molecular DF.

How to evaluate similarity integrals, involving several DF have been already discussed here. They do appear in the evaluation of the condensed QMP indices involving

skewness and kurtosis vectors; see for example reference [7]. Multiple density similarity integrals can be associated to a set of generalized Euclidian scalar products [18–20]. Such generalized scalar products between DF will produce, in any case when exactly computed, results which are real and positive definite, generally speaking as a consequence of the DF nature associated to real definite non-negative functions.

Using the possibility that such kind of high order similarity integrals can be computed with condensed products of isometric column vectors, associated to the described similarity matrix decomposition (1), the algorithms cannot be therefore based into Minkowski space algebra. This statement follows from the fact that in Minkowski algebra, some products could become negative, imaginary or complex. Then, such not-real similarity integral values might create an inconsistent quantum similarity tensorial framework, which could be cumbersome within the application of the QMP collective structure theory into quantum QSPR [8].

In order to circumvent such a drawback, there can be redefined in a simple manner the description of the eigenvalue matrix square root as described in Eq. (7). Such a solution to the complex similarity integrals problem can be based on transforming the previously described isometry into a slightly different (or a nearby kind of) isometry, which might be called *synisometry*.

The procedure to obtain such a synisometry might be based in constructing a modified eigenvalue diagonal matrix, which can be expressed writing it like:

$$|\Theta|^{1/2} = \text{Diag} \left( \sqrt{|\theta_I|} \mid I = 1, M \right). \quad (10)$$

Such small difference between isometric and synisometric eigenvalues means also that, when dealing with positive definite similarity matrices, the decomposition (1) will become an exact isometry.

While in the cases where negative eigenvalues do appear, the resultant synisometry will be of course just approximate. It will hold the obvious advantage consistent into the fact that by means of the synisometry computed via the matrix in Eq. (10), the generated similarity matrix, while approximate, will become certainly positive definite. Of course, then, higher order synisometric scalar products associated to higher order similarity integrals, for instance: using Eqs. (3) and (4), will be well defined and real.

This is the way the calculations of variance, skewness and kurtosis have been designed in this work and in further studies.

### 3.1 Difference between the original similarity matrix and the resultant of a synisometric procedure

It is interesting to know the differences one can encounter between the original double density similarity matrix  $\mathbf{Z}$  and the synisometric resultant matrix:  $|\mathbf{Z}|$  say, obtained with the same eigenvectors but with the forced positive definite eigenvalues, as defined in Eq. (10).

It is easy to write the synisometric similarity matrix as:

$$|\mathbf{Z}| = \mathbf{X} |\Theta| \mathbf{X}^T, \quad (11)$$

and decomposing the eigenvector matrix into its columns:

$$\mathbf{X} = (|\mathbf{x}_1\rangle, |\mathbf{x}_2\rangle, \dots, |\mathbf{x}_M\rangle)$$

or rows:

$$\mathbf{X}^T = \begin{pmatrix} \langle \mathbf{x}_1 | \\ \langle \mathbf{x}_2 | \\ \vdots \\ \langle \mathbf{x}_M | \end{pmatrix}$$

Then Eqs. (5) or (11) could be written also as:

$$\mathbf{Z} = \sum_I \theta_I |\mathbf{x}_I\rangle \langle \mathbf{x}_I|$$

and

$$|\mathbf{Z}| = \sum_I |\theta_I| |\mathbf{x}_I\rangle \langle \mathbf{x}_I|;$$

therefore one can easily write:

$$|\mathbf{Z}| - \mathbf{Z} = 2 \sum_I \delta[\theta_I < 0] |\theta_I| |\mathbf{x}_I\rangle \langle \mathbf{x}_I|, \quad (12)$$

where  $\delta[\theta_I < 0]$  is a logical Kronecker's delta, see for example reference [21]. Computational tests performed while this paper was written revealed that the difference represented by Eq. (12), do not distort in a great manner the second order characteristics of QMP, like the condensed collective indices associated to the variance vector, see for example references [6] and [7].

#### 4 Isometric vector sets using: $\mathbf{Z}^2$ , the similarity matrix squared

It is not very difficult to see this above defined isometric or synisometric decomposition technique, as related to the former direct use of the columns of the same similarity matrix  $\mathbf{Z}$ , which can be considered as a source of information in order to discretize the QMP set of DF vertices.

In this manner one can obtain a set of isometric or synisometric vectors acting as a discrete description of the QMP DF vertices. This possibility has been discussed in many ways along the development of quantum similarity theory and practice; see for example references [22, 23].

Accepting this theoretical thinking and practical proceeding, one can arrive to construct a new metric matrix, which according to Eq. (1) corresponds to the squared similarity matrix:  $\mathbf{Z}^2$ .

In the same line of thought, it can be now remembered that in general any power of a Hermitian matrix possesses the same eigenvector set as the original matrix, but has to be associated to the corresponding power of the diagonal eigenvalue matrix.

Then, it is obvious that both  $\mathbf{Z}$  and  $\mathbf{Z}^2$  matrices possess the same eigenvector matrix, whereas the eigenvalues of the squared matrix are made with the squares of the initial eigenvalues. Consequently, the equivalent expression written in the Eq. (5) can be now written in this case as:

$$\mathbf{Z}^2 = \mathbf{X}\Theta^2\mathbf{X}^T \leftarrow \Theta^2 = \text{Diag}(\theta_I^2 | I = 1, M).$$

Thus, as an alternative to the isometric decomposition developed beforehand in reference [1], another synisometry can be described via the decomposition of the squared similarity matrix instead. This procedure yielding another pair of matrices, which in close similarity with these described in Eqs. (8) and (9) can be easily written by means of the following pair of matrix definitions:

$$\begin{aligned} 1') \quad \mathbf{A}_{2a} &= \Theta\mathbf{X}^T \leftrightarrow \mathbf{A}_{2a}^T = \mathbf{X}\Theta \\ 2') \quad \mathbf{A}_{2s} &= \mathbf{X}\Theta\mathbf{X}^T = \mathbf{Z} \leftrightarrow \mathbf{A}_{2s}^T = \mathbf{Z}^T = \mathbf{Z} \end{aligned}$$

The asymmetrical decomposition 1') might appear perhaps as a real isometric alternative to the direct one represented by Eqs. (8) and (9), which as it has earlier commented, possess the drawback of having the possible appearance of square roots of negative numbers.

Therefore, the use of the absolute value of the  $\mathbf{Z}$  eigenvalues as described in Eq. (10), and thus, as it has been also commented, defining a synisometry, might correspond to a compromise between forcing the problem in one hand to overcome a case of Minkowski space algebra, and on the other hand using the similarity matrix squared as a Gram matrix to solve the isometry problem.

## 5 Conclusions

In order to avoid Minkowski space complex algebra, the isometric problem is transformed into a synisometric procedure, where the similarity matrix potential negative eigenvalues are transformed into a set of positive definite ones. Synisometric computations of higher order similarity integrals are feasible in this way. The approximate collective structure of QMP can be easily and efficiently reached. Numerical systematic results will be published elsewhere.

**Acknowledgments** The author wishes to specify that this work has been developed under a Prometeo fellowship, and acknowledges the SENESCYT, Government of Ecuador, for granting it.

**Conflict of interest** The author confirms that this paper contents have no conflict of interest.



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