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LETTER TO THE EDITOR

Quantum similarity matrices column set as holograms of DF molecular point clouds

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Abstract A simple argument proves that quantum similarity measures, performed on any density function (DF) tag set of a given quantum object set, create a hologram of such DF tag set.

Keywords Quantum similarity · Quantum point clouds · Quantum similarity measures · Quantum similarity matrices · Holographic isomorphism of quantum object sets · Holographic electron density theorem

Sir,

Quantum similarity (QS) Measures (QSM) have been described since the first paper on this subject [1], setting the initial background and applications as a way to obtain relations between members of some quantum object set[1] (QOS) [2–7]. In fact, when known a set of molecular structures and the attached set of electronic density functions (DF): $P = \{\rho_I | I = 1, N\}$, acting as tags, the theoretical most simplified background of QS corresponds to compute a set of simple QSM which can be formulated like the DF scalar products [1,7,11–17]:

$$\forall \rho_I, \rho_J \in P : Z_{IJ} = \langle \rho_I \rho_J \rangle = \int_D \rho_I \rho_J dV. \quad (1)$$

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[1] A quantum object set (QOS): Q is a Cartesian product composite set constructed by submicroscopic objects or states of an object O and the attached quantum density functions set P: Q = O × P. The density function set P is called the *tag set*.

So, a QS matrix (QSMx) $\mathbf{Z} = \{Z_{IJ}\}$ can be constructed. The diagonal elements of the QSMx: $\mathbf{Z}$, that is: $Diag(\mathbf{Z}) = \{Z_{II}\}$, are the quantum selfsimilarity measures of the elements of the QOS. The QSMx is positive and symmetrical: $\forall I, J : Z_{IJ} \in \mathbf{R}^+ \wedge Z_{IJ} = Z_{JI} \leftrightarrow \mathbf{Z} = \mathbf{Z}^T$.

The elements of the QSMx can be ordered by columns (or rows) in the following way:

$$\mathbf{Z} = (|\mathbf{z}_1\rangle, |\mathbf{z}_2\rangle, \ldots |\mathbf{z}_I\rangle, \ldots |\mathbf{z}_N\rangle) \leftrightarrow |\mathbf{z}_I\rangle = \{Z_{JI} \,|J = 1, N\}.$$

Due to the equation (1), each column (or row), the I-th say, of the QSMx is formed by the scalar products of the whole DF tag set specifically by the I-th DF. Thus, a one to one correspondence can be built, connecting any QOS elements with the columns (or rows) of the QSMx in the following way:

$$\forall I : \rho_I \leftrightarrow |\mathbf{z}_I\rangle.$$

Therefore, one might say that, as every element of the DF space present in the initial QOS belongs to an infinite dimensional function semispace, that is: $\forall I : \rho_I \in P_\infty$, then via the construction of the QSMx, every DF tag set corresponds to a unique vector, belonging to a N dimensional space made of column (or row) vectors, as one can write: $\forall I : |\mathbf{z}_I\rangle \in C_N$. The set of columns (or rows) of the QSMx considered as tags of the QO instead of the DF tags, constitute a discrete QOS (DQOS) [7,15].

Thus, a QSMx construct can be considered as some kind of transformation of a DF set into some N dimensional column (or row) vector space subset, which if the DF set P is linearly independent, then if the QSMx $\mathbf{Z}$ is properly constructed, the columns (or rows) of such a matrix are also linearly independent [14,16]. The set of QSMx columns (or rows) also represents an isomorphic set to the DF tag set. From this point of view, the construction of the QSMx corresponds to the transformation of a set of infinite dimensional vectors into a finite dimensional space. The set of column (or row) vectors being isomorphic to the DF QOS tag set, possess the same mathematical properties than the DF set. For instance: a) linear combinations are equivalent in both sets, b) translation of origin is reproduced in both sets, see for instance [20,21], c) homothetic transformations leave the similarity index structure invariant [10,18], d) Minkowski normalization of the DF QOS tag set [12,13], originating the so-called shape functions, corresponds to the same operation in the QSMx column (or row) set originating stochastic QSMx [8,9], ... When considering a QOS formed by the DF tags, attached to a n-fold degenerate state, it has been recently proved [21] that the emerging DQOS picture, obtained via a QSMx isomorphism, corresponds to a $(n-1)$-dimensional simplex. For instance, the DQOS of a triple degenerate state corresponds to an equilateral triangle, the one of a quadruple degenerate state to a tetrahedron, and so on.

As a consequence, the set of columns (or rows) of the QSMx can be considered a *hologram* of the set of DF; that is: a set of finite dimension objects carrying the information of an infinite dimensional set of DF.

Recently, a review on the QS mathematical formalism has been published [7,15,19]. The set of molecules described as a QOS, from the geometrical point of view can be called a molecular point cloud (MPC). The set of the QOS tag set DF in QS language can be named as a function MPC, while the set of columns (or rows) of the QSMx might be named as a column (or row) MPC.

Accordingly, it can be said that: a) QSM transforms a function MPC into a column (or row) MPC and b) a column (or row) MPC acts as a hologram of the function MPC.

Perhaps such a holographic property of the MPC can be considered in close connection with Mezey's holographic electron density theorem [22].

References

1. R. Carbó, L. Leyda, M. Arnau, Int. J. Quantum Chem. **17**, 1185 (1980)
2. R. Carbó, B. Calabuig, J. Mol. Struct. (Theochem) **254**, 517 (1992)
3. R. Carbó, B. Calabuig, J. Chem. Inf. Comput. Sci. **32**, 600 (1992)
4. R. Carbó-Dorca, J. Math. Chem. **23**, 353 (1998)
5. R. Carbó-Dorca, *Advances in Molecular Similarity*, vol. 2. (JAI Press Inc., Greenwich (Conn.), 1998), p. 43
6. R. Carbó-Dorca, J. Math. Chem. **23**, 365 (1998)
7. R. Carbó-Dorca, E. Besalú, J. Mol. Struct. (Theochem) **451**, 11 (1998)
8. R. Carbó-Dorca, Int. J. Quantum Chem. **79**, 163 (2000)
9. R. Carbó-Dorca, J. Math. Chem. **27**, 357 (2000)
10. P. Bultinck, R. Carbó-Dorca, J. Math. Chem. **36**, 191 (2004)
11. P. Bultinck, X. Gironés, R. Carbó-Dorca, In: *Review Computer Chemistry*, vol. 21, eds. by K.B. Lipkowitz, R. Larter, T. Cundari, (Wiley, Hoboken, 2005), pp. 127–207
12. R. Carbó-Dorca, J. Math. Chem. **39**, 551 (2006)
13. R. Carbó-Dorca, J. Math. Chem. **44**, 628 (2008)
14. R. Carbó-Dorca, J. Math. Chem. **44**, 228 (2008)
15. R. Carbó-Dorca, A. Gallegos, Quantum similarity and quantum QSPR (QQSPR) entry: 176. In: *Encyclopedia of Complexity and Systems Science*, vol 8, ed. by M. Robert (Springer, New York, 2009), pp. 7422–7480. ISBN: 978-0-387-75888-6
16. R. Carbó-Dorca, E. Besalú, L.D. Mercado, J. Comput. Chem. **32**, 582 (2011)
17. L.D. Mercado, R. Carbó-Dorca, J. Math. Chem. **49**, 1558 (2011)
18. R. Carbó-Dorca, J. Math. Chem. **49**, 2109 (2011)
19. R. Carbó-Dorca, E. Besalú, J. Math. Chem. **50**, 210 (2012)
20. R. Carbó-Dorca, E. Besalú, *Centroid Origin Shift of Quantum Object Sets and Molecular Point Clouds: Description and Element Comparisons. IQC Technical Report TR-2011-11*. J. Math. Chem. (2011). doi:10.1007/s10910-011-9960-y
21. R. Carbó-Dorca, Quantum similarity. In: *Concepts and Methods in Modern Theoretical Chemistry*, vol. 1, eds. by S.K. Ghosh, P.K. Chattaraj (Taylor & Francis, London, 2012). To be published
22. P.G. Mezey, Mol. Phys. **96**, 169 (1999)