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ORIGINAL PAPER

Function extended spaces

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Abstract Extended function spaces defined over the real field are defined as vector spaces made by the Cartesian product of a real Euclidian space and a real function space. This construct is related to the Holographic Electronic Density Theorem and to the stereographic projection of quantum chemically related and well behaved functions in general. It permits to establish the basis for the Holographic General Function Theorem.

Keywords Density function (DF) · Holographic electronic density theorem (HEDT) · Holographic general function theorem (HGFT) · Function extended spaces (FES) · Stereographic projection of quantum chemical functions · Molecular fields · Quantum similarity

1 Introduction

Recently, it has been published some work on the stereographic projection of density functions (DF) [1]. The present study pretends to enlarge and provide more information about some of the ideas employed in this previously mentioned paper. Essentially, the aim of the present theoretical development is to describe the structure and properties of a new kind of vector spaces, which were named *function extended spaces* (FES) in the article of reference.

FES were just loosely described in reference [1] because the aim of this previous paper was to demonstrate the possibility to represent quantum mechanical functions of chemical interest, like density functions or electrostatic potential maps (EMP) [2], within a stereographic projection point of view, allowing in this manner the

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representation of such function fields in a potential dynamical way, among other possibilities. Stereographic projections, for instance, are well adapted to any molecular shape, including the quasi spherical structures associated to buckminsterfullerene.

In order to accomplish the indicated task of extending and clarifying the concept of FES, the present paper will be organized in the following way. First, a brief description of those spaces will be given adapted to quantum mechanical DF, then a simple example of such FES structure will precede the axiomatic description of FES. Then, gradient spaces will be taken as an application of the powerful FES description and this step will be followed by the connection between FES, stereographic projections and the holographic features which can be in general attached to well-behaved functions as an extension of Mezey's holographic DF theorem [3–5]. Finally, after some remarks one can provide on FES practical applications, a conclusion section will be given.

2 Function extended spaces (FES) of quantum chemical interest involving density functions (DF) and shape functions (ShF)

2.1 Density and Shape functions

In order to define FES associated to quantum functions it is interesting to present the notation which will be employed here. Then a few words about density functions (DF) and shape functions (ShF) will be firstly given. In fact, a ShF: $\sigma(\mathbf{r})$ is simply defined from any arbitrary one-electron DF: $\rho(\mathbf{r})$, according to the next algorithm, which can be written in several ways, but here is chosen as follows:

$$\forall \rho(\mathbf{r}) : \langle \rho \rangle = \int_D \rho(\mathbf{r})\, d\mathbf{r} = N \rightarrow \ \sigma(\mathbf{r}) = N^{-1}\rho(\mathbf{r}) = \langle \rho \rangle^{-1} \rho(\mathbf{r}), \tag{1}$$

where N is the number of electrons and the integral represented by the symbol $\langle \rho \rangle$ is the Minkowski norm of the DF $\rho(\mathbf{r})$.

Moreover it is easy to see ShF can be interpreted as the probability distribution for the location of an electron in a volume element of the position space. ShF can be generalized into volume functions within the scope of quantum similarity measures [6], also they can be straightforwardly extended in connection with higher order DF.

2.2 DF and ShF extended spaces

The ordered couple made by a three dimensional Euclidean space position vectors $\mathbf{r}, \mathbf{s} \in E_3(\mathbf{R})$ and the value of a known DF or ShF at this point:

$$|\mathbf{p}\rangle = (\mathbf{r}, \rho(\mathbf{s})) \vee |\mathbf{q}\rangle = (\mathbf{r}, \sigma(\mathbf{s})) \in C_4(\mathbf{R}) \tag{2}$$

can be considered as a new point structure associated with some four dimensional real space: $C_4(\mathbf{R})$, where the fourth coordinate corresponds to the function value at the considered position provided by the first vector Euclidean part. The whole space

$C_4(\mathbf{R})$ can be thought as a hybrid Cartesian product of the three dimensional Euclidean space $\mathbf{R}^3$ with an infinite dimensional functional space, containing real valued functions of three real variables $F_\infty(\mathbf{R})$:

$$C_4(\mathbf{R}) = E_3(\mathbf{R}) \times F_\infty(\mathbf{R}).$$

Such composite sets possessing in addition a structure of vector space, as one can sum and multiply by a scalar the elements of $C_4(\mathbf{R})$ in the way which is explained in detail below. These hybrid vector spaces will be called FES. In the next paragraph discussion it is proved that arbitrary dimension similarly constructed mathematical structures comply with the associated usual properties of the two basic operations defining a vector space.

Moreover, both kinds of points $|\mathbf{p}\rangle$ and $|\mathbf{q}\rangle$, as defined in Eq. (2), are related by means of the homothetic relationship between DF and ShF. Such a relationship can be easily obtained by constructing a new four dimensional vector like: $\mathbf{h} = (\mathbf{1}, N)$, where the Euclidean three dimensional unity vector is customarily defined as: $\mathbf{1} = (1, 1, 1)$. Then, it is easy to see that the inward product of the vector $\mathbf{h}$ by the vector $|\mathbf{q}\rangle$ produces the vector $|\mathbf{p}\rangle$: $|\mathbf{p}\rangle = \mathbf{h}*|\mathbf{q}\rangle$, due to the definition of this kind of product[1] (see for example references [7–12]) and the relationship between DF and ShF (1). The transformation involving vectors $|\mathbf{p}\rangle$ and $|\mathbf{q}\rangle$ becomes obviously reversible, because using the vector: $\mathbf{w} = \mathbf{h}^{[-1]} = \left(\mathbf{1}, N^{-1}\right)$, then it can be also written: $|\mathbf{q}\rangle = \mathbf{w}*|\mathbf{p}\rangle$. The vector $\mathbf{w}$ acts as the inward inverse of $\mathbf{h}$, that is: $\mathbf{w}*\mathbf{h} = \mathbf{h}*\mathbf{w} = \mathbf{1}$.

2.3 General function extended spaces

In fact, the four dimensional FES, as the previously described ones, can be also constructed when considering any well-behaved function of the three dimensional Euclidean position coordinates, $\gamma(\mathbf{s})$ say; then, in general the function extended vector space $C_4(\mathbf{R})$ can be supposedly made of vectors like:

$$|\mathbf{g}\rangle = (\mathbf{r}, \gamma(\mathbf{s})) \in C_4(\mathbf{R}).$$

Furthermore, the non-negative nature of the DF and the associated ShF, makes non-negative the fourth vector coordinate, as it is defined in Eq. (2). However, with general functions of arbitrary definition type this fourth coordinate positive definiteness restriction has not to be compulsively present in FES. The only extra consideration on the coordinate function behavior has to be associated to the fact that the associated function must be continuous.

In addition, the position coordinates of FES do not need to be restrictedly associated with three dimensional Euclidean spaces; but obviously enough, if the well-behaved

[1] The *inward product* of two vectors of some vectorial space: $\mathbf{a}, \mathbf{b} \in V$, corresponds to another vector of the same space: $\mathbf{z} = \mathbf{a}*\mathbf{b} \in V$. Not all vectors possess necessarily an inward inverse. However, there exists the inward identity element, the *unity* vector: $\mathbf{1} \in V$, for which: $\forall \mathbf{a} \in V : \mathbf{1}*\mathbf{a} = \mathbf{a}*\mathbf{1} = \mathbf{a}$. Thus, vector spaces form a monoid under inward product and a commutative ring together with vector addition. The inward product constitutes a generalization of the so-called Hadamard or Schur products.

function terms in a given FES are constructed bearing n variables, the FES can be defined as $n + 1$ dimensional as well.

3 A simple example

The simplest practical example one can think about FES is: $C_2(\mathbf{R})$, where some of the elements will be generically made of vectors which can be written as: $|\mathbf{f}_d\rangle = (x; f(x))$, where $x \in \mathbf{R}$ and $f(x)$ is a continuous well-behaved real function. Constructed in this way the vector $|\mathbf{f}_d\rangle$ is nothing else than the function $f(x)$ map and it doesn't include all the two-dimensional $C_2(\mathbf{R})$ space coordinate values.

Whenever the FES vector is written with the aid of two independent variables, using another form like: $|\mathbf{f}\rangle = (x_1; f(x_2))$, then the whole $C_2(\mathbf{R})$ space can be described. In fact both vectors $|\mathbf{f}_d\rangle$ and $|\mathbf{f}\rangle$ can be compared with an infinite dimensional matrix, whose diagonal elements could be represented by the vector: $|\mathbf{f}_d\rangle$.

In order to illustrate this picture, a particular case of this very particular example can be associated to the possibility to choose: $f(x) = x$. In this particular situation, one can write: $|\mathbf{f}_d\rangle = (x; x)$ which produces the bisection of the positive and negative quadrants. While the whole space can be, of course, written by the bi-dimensional vector: $|\mathbf{f}\rangle = (x_1; x_2)$. In this latest form, the vector $|\mathbf{f}\rangle$ can be easily seen as an infinite-dimensional two index hollow matrix, with indices which are coincident with the real coordinates of the $\mathbf{R}^2$ Euclidian space.

4 Axiomatic definition of FES

The structure of a FES possesses several distinctive traits, when compared with the usual vector space formalism. Here, the vector space definition field will be chosen as the real field: $\mathbf{R}$. Thus, as a first consideration, one must take into account that the functions: γ, entering the general definition of FES must be taken as well behaved real valued functions of n real variables, that is: $\gamma : \mathbf{R}^n \to \mathbf{R}$.

Then, generally speaking, a FES will be defined as containing elements formed by a couple constructed like a Cartesian product:

$$C_{n+1}(\mathbf{R}) = \mathbf{R}^n \times \Gamma_\infty(\mathbf{R}),$$

which can be made more explicit as a generalization of the previously defined bidimensional diagonal point of view as follows:

$$\forall \mathbf{r} : |\mathbf{g}_d\rangle = (\mathbf{r}, \gamma(\mathbf{r})) \in C_{n+1}(\mathbf{R}) \leftarrow \left\{\gamma(\mathbf{r}) \in \mathbf{R} \leftarrow \left\{\forall \mathbf{r} \in \mathbf{R}^n \wedge \gamma(\mathbf{r}) \in \Gamma_\infty(\mathbf{R})\right\}\right\}.$$

However, written in this way this corresponds just to the map of a function of n variables. To obtain a covering of all the $C_{n+1}(\mathbf{R})$ space there is need, as in the two-dimensional case example, of two generating Euclidian n-dimensional vectors $\{\mathbf{r}; \mathbf{s}\}$:

$$|\mathbf{g}\rangle = (\mathbf{r}, \gamma(\mathbf{s})) \in C_{n+1}(\mathbf{R}) \leftarrow \left\{\gamma(\mathbf{s}) \in \mathbf{R} \leftarrow \left\{\forall \mathbf{r}, \mathbf{s} \in \mathbf{R}^n \wedge \gamma(\mathbf{s}) \in \Gamma_\infty(\mathbf{R})\right\}\right\}.$$

In fact, the vectors of the type $|\mathbf{g}_d\rangle$ correspond to the hyperdiagonal elements of some hypermatrix indices properly defined by the vector: $|\mathbf{g}\rangle$.

Vectors in a FES can be seen as Euclidian vectors extended with an extra Riemannian coordinate.

4.1 Axioms

Then, one can propose the following axioms, which are necessary to properly build any FES structure:

A) The *addition* over the FES can be defined as:

Assuming that: $|\mathbf{g}\rangle = (\mathbf{r}_1, \gamma(\mathbf{r}_2))$ and $|\mathbf{h}\rangle = (\mathbf{r}_1, \eta(\mathbf{r}_2))$

$$\forall \{|\mathbf{g}\rangle, |\mathbf{h}\rangle\} \in C_{n+1} : |\mathbf{g}\rangle + |\mathbf{h}\rangle = (\mathbf{r}_1 + \mathbf{r}_2, \gamma(\mathbf{s}_1) + \eta(\mathbf{s}_2))$$

Then, one can also design the following axioms with respect to addition:

1A) Commutability:

$$\begin{aligned}&\forall |\mathbf{g}\rangle, |\mathbf{h}\rangle \in C_{n+1}(\mathbf{R}) :\\ &|\mathbf{g}\rangle + |\mathbf{h}\rangle = (\mathbf{r}_1 + \mathbf{r}_2, \gamma(\mathbf{s}_1) + \eta(\mathbf{s}_2)) = (\mathbf{r}_2 + \mathbf{r}_1, \eta(\mathbf{s}_2) + \gamma(\mathbf{s}_1)) = |\mathbf{h}\rangle + |\mathbf{g}\rangle\end{aligned}$$

2A) Associativity:

$$\forall |\mathbf{g}\rangle, |\mathbf{h}\rangle, |\mathbf{j}\rangle \in C_{n+1}(\mathbf{R}) : |\mathbf{g}\rangle + (|\mathbf{h}\rangle + |\mathbf{j}\rangle) = (|\mathbf{g}\rangle + |\mathbf{h}\rangle) + |\mathbf{j}\rangle$$

Because it can be written, for instance:

$$\begin{aligned}|\mathbf{g}\rangle + |\mathbf{h}\rangle + |\mathbf{j}\rangle &= (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3, \gamma(\mathbf{s}_1) + \eta(\mathbf{s}_2) + \mu(\mathbf{s}_3))\\ &= (\mathbf{r}_1, \gamma(\mathbf{s}_1)) + (\mathbf{r}_2 + \mathbf{r}_3, \eta(\mathbf{s}_2) + \mu(\mathbf{s}_3))\end{aligned}$$

3A) Existence of a neutral element with respect to the addition:

$$\exists |\mathbf{0}\rangle \in C_{n+1} \to \forall |\mathbf{g}\rangle \in C_{n+1} : |\mathbf{0}\rangle + |\mathbf{g}\rangle = |\mathbf{g}\rangle + |\mathbf{0}\rangle = |\mathbf{g}\rangle$$

Such an element has to be defined along the existence in the associated function space of the null function: $\exists 0(\mathbf{s}) \in F_\infty(\mathbf{R}) \to \forall \mathbf{s} \in \mathbf{R}^n : 0(\mathbf{s}) = 0$, thus forming a FES zero element like: $|\mathbf{0}\rangle = (\mathbf{0}, 0(\mathbf{s}))$.

4A) Existence of a reciprocal element with respect to the addition for each FES element:

$$\forall |\mathbf{g}\rangle \in C_{n+1} : \exists -|\mathbf{g}\rangle \to |\mathbf{g}\rangle + (-|\mathbf{g}\rangle) = |\mathbf{0}\rangle$$

Construction of such an element can be achieved defining:

$$\forall |\mathbf{g}\rangle = (\mathbf{r}, \gamma(\mathbf{s})) \in C_{n+1} : \exists - |\mathbf{g}\rangle = -(\mathbf{r}, \gamma(\mathbf{s})) = (-\mathbf{r}, -\gamma(\mathbf{s})) \in C_{n+1}$$

In this way: $\forall \mathbf{s} : \gamma(\mathbf{s}) + (-\gamma(\mathbf{s})) = 0(\mathbf{s})$.

B) The *product of a vector by a scalar* can be constructed in a similar manner as one has proceeded with the addition:

$$\forall \lambda \in \mathbf{R} \wedge \forall |\mathbf{g}\rangle = (\mathbf{r}, \gamma(\mathbf{s})) \in C_{n+1} : \lambda |\mathbf{g}\rangle = (\lambda \mathbf{r}, \lambda \gamma(\mathbf{s}))$$

and axiomatized accordingly as follows:

1B) Distributivity with respect scalar addition:

$$\forall \lambda, \mu \in \mathbf{R} \wedge \forall |\mathbf{g}\rangle \in C_{n+1} : (\lambda + \mu) |\mathbf{g}\rangle = \lambda |\mathbf{g}\rangle + \mu |\mathbf{g}\rangle$$

2B) Distributivity with respect FES vector sum:

$$\forall \lambda \in \mathbf{R} \wedge \forall |\mathbf{g}\rangle, |\mathbf{h}\rangle \in C_{n+1} : \lambda (|\mathbf{g}\rangle + |\mathbf{h}\rangle) = \lambda |\mathbf{g}\rangle + \lambda |\mathbf{h}\rangle$$

3B) Associativity with respect the product of scalars:

$$\forall \lambda, \mu \in \mathbf{R} \wedge \forall |\mathbf{g}\rangle \in C_{n+1} : \lambda (\mu |\mathbf{g}\rangle) = (\lambda \mu) |\mathbf{g}\rangle$$

4B) Existence of a neutral element with respect of the product by a scalar:

$$\exists 1 \in \mathbf{R} \wedge \forall |\mathbf{g}\rangle \in C_{n+1} \to 1 |\mathbf{g}\rangle = |\mathbf{g}\rangle$$

Therefore, the reciprocal element with respect to the addition in FES can be redefined as it is also usual in vector spaces:$- |\mathbf{g}\rangle = (-1) |\mathbf{g}\rangle$.

Taking into account all these axioms as defined above, FES can be considered as having a vector space structure possessing all the associated properties of such constructs.

5 Special characteristics of FES

FES can be also associated to unconventional properties, which are not necessarily to be found in usual vector spaces; for instance, just to mention some assorted examples of them:

1) Because of the hybrid construction of FES, there could be defined *Euclidian zeros* like: $(\mathbf{0}, \gamma(\mathbf{0})) \in G_{n+1}$; of course, such elements cannot be confused with the FES zero vector: $|\mathbf{0}\rangle$. However, for the same FES hybrid definition reason, there can also exist *function extended zeros* like: $(\mathbf{r}_0, \gamma(\mathbf{s}_0)) = (\mathbf{r}_0, 0)$, obviously appearing whenever: $\exists \mathbf{s}_0 \neq \mathbf{0} : \gamma(\mathbf{s}_0) = 0$.

2) It can be considered a *Euclidian addition*, which implies the Euclidian part of any FES vector and which can be defined as:

$$(\mathbf{r}_1, \gamma(\mathbf{s})) \dot{+} (\mathbf{r}_2, \gamma(\mathbf{s})) = (\mathbf{r}_1 + \mathbf{r}_2, \gamma(\mathbf{s}))$$

3) In the same way one can define a *function extended vector addition*:

$$(\mathbf{r}, \gamma(\mathbf{s})) \ddot{+} (\mathbf{r}, \eta(\mathbf{s})) = (\mathbf{r}, \gamma(\mathbf{s}) + \eta(\mathbf{s}))$$

4) Several kinds of Banach and pre-Hilbert FES can be easily defined:
   4.1) Provided that the functions of the space $F_\infty(\mathbf{R})$ are square summable, that is: $\forall\gamma(\mathbf{s}) \in F_\infty(\mathbf{R}) : \exists \int_D |\gamma(\mathbf{s})|^2 d\mathbf{s} \in \mathbf{R}^+$, then an Euclidian norm of a FES vector can be easily constructed as:

$$\langle \mathbf{g}|\mathbf{g}\rangle = |\mathbf{r}|^2 + \langle\gamma|\gamma\rangle = |\mathbf{r}|^2 + \int_D |\gamma(\mathbf{s})|^2 d\mathbf{s}.$$

   4.2) A scalar product can be also easily defined between two FES elements:

$$\langle \mathbf{g}|\mathbf{h}\rangle = \langle \mathbf{r}_1|\mathbf{r}_2\rangle + \int_D \int_D \gamma(\mathbf{s}_1)\,\delta(\mathbf{s}_1 - \mathbf{s}_2)\,\eta(\mathbf{s}_2)\,d\mathbf{s}_1 d\mathbf{s}_2$$

   However, a variant associated to a Euclidian norm and a function extended scalar product, can be also contemplated for some specific kind of FES vectors:

$$\langle (\mathbf{r}, \gamma(\mathbf{s}))|(\mathbf{r}, \eta(\mathbf{s}))\rangle = |\mathbf{r}|^2 + \int_D \gamma(\mathbf{s})\,\eta(\mathbf{s})\,d\mathbf{s}.$$

   One can grasp in this way how rich in operation possibilities are FES when compared with classical vector spaces.

6 Gradient extended spaces (GES)

In order to show other possible forms of the previously defined FES, one can recall a recent study about the possibility to use the DF gradients as some kind of molecular Riemannian coordinates [13]. Also it is worthwhile to remember previous work on the use of DF derivatives in quantum similarity theory and applications [14].

The gradient of a DF will be noted by means of the following conventions:

$$\langle \mathbf{d}| = \langle \partial_{\mathbf{r}}\rho(\mathbf{r})| = \left(\partial_x\rho(\mathbf{r}); \partial_y\rho(\mathbf{r}); \partial_z\rho(\mathbf{r})\right).$$

The vector $\langle \mathbf{d}|$ can be trivially written by means of the operator acting on the DF, for which one can choose any of the notations like:

$$\nabla^T \rho(\mathbf{r}) = \langle \partial_{\mathbf{r}}| \rho(\mathbf{r}) = \left(\partial_x; \partial_y; \partial_z\right) \rho(\mathbf{r}).$$

This formalism allows writing a four dimensional FES vector with the generic form described before, where the coordinate Euclidian part is made of the gradient elements computed at the point **r,** as:

$$(\langle \mathbf{d}| ; \rho(\mathbf{s})) = \langle \partial_{\mathbf{r}} \rho(\mathbf{r}); \rho(\mathbf{s})| = \left(\partial_x \rho(\mathbf{r}); \partial_y \rho(\mathbf{r}); \partial_z \rho(\mathbf{r}); \rho(\mathbf{s})\right)$$

In turn, the diagonal part of this particular FES can be rewritten using several alternative notations with an extended operator vector definition:

$$\Theta^T [\rho(\mathbf{r})] = \left(\nabla^T; 1\right) \rho(\mathbf{r}) = \langle \partial_{\mathbf{r}}; 1| \rho(\mathbf{r}) = \left(\partial_x; \partial_y; \partial_z; 1\right) \rho(\mathbf{r}). \tag{3}$$

Such a process can be structured in general for an arbitrary dimension and then applied to any well behaved function of an arbitrary number of variables. Such functions must possess, at least, adequate continuous first partial derivatives. The appropriate definition of such vector is just a matter to define an extended operator vector over the complete number of involved variables. Such a FES construct can be called gradient extended spaces (GES).

6.1 A spherical Gaussian function example

As an illustrative example of GES, it is interesting to study the structure this Riemann extended vector acquires, when applied to a spherical Gaussian function of an arbitrary number of variables n, that is: $\mathbf{r} \in \mathbf{R}^n$. Such Minkowski normalized function can be defined as:

$$\gamma(\alpha|\mathbf{r}) = \left(\frac{\alpha}{\pi}\right)^{\frac{n}{2}} \exp\left(-\alpha|\mathbf{r}|^2\right). \tag{4}$$

In this simple example the gradient elements can be also written as:

$$\partial_{\mathbf{r}} \gamma(\alpha|\mathbf{r}) = -2\alpha \left(\frac{\alpha}{\pi}\right)^{\frac{n}{2}} \exp\left(-\alpha|\mathbf{r}|^2\right) \mathbf{r} = -2\alpha\gamma(\alpha|\mathbf{r})\mathbf{r},$$

therefore the diagonal part of the extended gradient vector, defined like in Eq. (3), can be written in this case with the form:

$$\langle \mathbf{d}(\mathbf{r})| = (\partial_{\mathbf{r}} \gamma(\alpha|\mathbf{r}); \gamma(\alpha|\mathbf{r})) = (-2\alpha\mathbf{r}; 1)\gamma(\alpha|\mathbf{r}),$$

which yields an extended vector of the type: $(-2\alpha\mathbf{r}; 1)$ with a constant unit in the function position. The original Gaussian function acts as a variable scalar factor of any vector in the position space. It is interesting to note that, at the extremum: $\mathbf{r} = \mathbf{0}$, the gradient is null and the GES vector can be written at this position as an Euclidian zero FES vector:

$$\langle \mathbf{d}\,(\mathbf{0})| = \left(\partial_{\mathbf{r}}\gamma\,(\alpha\,|\mathbf{0})\,;\,\gamma\,(\alpha\,|\mathbf{0})\right) = (\mathbf{0};\,1)\,\gamma\,(\alpha\,|\mathbf{0}) = \left(\frac{\alpha}{\pi}\right)^{\frac{n}{2}}(\mathbf{0};\,1)\,.$$

6.2 Sobolev spaces and gradient extended spaces

For adequate functions, the GES can generate an appropriate Euclidian norm, which can be written as:

$$\forall \mathbf{r},\mathbf{s}:\langle \mathbf{g}| = \left(\langle \mathbf{d}|\,\gamma\,(\mathbf{r})\,;\,\gamma\,(\mathbf{s})\right) \in G_{n+1} \rightarrow \langle \mathbf{g}|\mathbf{g}\rangle = \sum_{I=1}^{n}\int_{D}|\partial_I\gamma\,(\mathbf{r})|^2 d\mathbf{r} + \int_{D}|\gamma\,(\mathbf{s})|^2 d\mathbf{s}$$

Acquiring in this way the structure of a Sobolev space [15]. Sobolev spaces have been employed in order to describe in a new way Schrödinger equation [16,17] and to generalize several aspects of molecular similarity measures [18].

7 Stereographic projections in FES and a holographic general functions theorem (HGFT)

Function extended spaces like $C_4\,(\mathbf{R})$ can be considered as a particular form of a general $C_{n+1}\,(\mathbf{R})$ vectorial structure, which can be constructed in turn as the hybrid Cartesian product of an Euclidian n-dimensional space with a function space containing vectors, constructed by functions of n-dimensional variables.

Thus, it is elementary to generalize stereographic projections from a function extended space of $(n + 1)$ dimensions, using the same symbols as the used ones for FES in the stereographic projection equations, taking into account that the original position vectors belong to some Euclidean n-dimensional space, that is: $\mathbf{r} \in E_n\,(\mathbf{R})$.

It is well-known [19–21] that the stereographic projection of a point vector belonging to a diagonal vector set, defined into the FES and written as: $\mathbf{p} = (\mathbf{r}, \gamma\,(\mathbf{r})) \in C_{n+1}\,(\mathbf{R})$, can be associated to a new scaled vector:

$$\mathrm{P}_S\,(\mathbf{p}) = \mathbf{P} = (R - \gamma\,(\mathbf{r}))^{-1}\,\mathbf{r} \in E_n \tag{5}$$

of the Euclidean space, where R is a parameter, which usually is chosen as the unit and can be defined as the radius of the sphere:

$$|\mathbf{r}|^2 + |\gamma\,(\mathbf{r})|^2 = R^2. \tag{6}$$

Therefore the stereographic projection can be written as:

$$\mathbf{P} = (R - \gamma\,(\mathbf{r}))^{-1}\,\mathbf{r} = \lambda^{-1}\mathbf{r} = \left\{\lambda^{-1}r_I\,|I = 1, n\right\} = \{P_I\,|I = 1, n\} \tag{7}$$

and the expression can be reversed, that is: one can try to obtain the original coordinates from the stereographic ones by using Eq. (6) and the inverse relationship of Eq. (7), which can be written as:

$$\mathbf{r} = \lambda\mathbf{P} = (R - \gamma(\mathbf{r}))\,\mathbf{P}, \tag{8}$$

thus, from knowing the stereographic projected coordinates one can recover the initial coordinates following the simple general algorithm:

$$\forall I = 1, n : r_I = \frac{2RP_I}{|\mathbf{P}|^2 + 1} \wedge \rho(\mathbf{r}) = \frac{R\left(|\mathbf{P}|^2 - 1\right)}{|\mathbf{P}|^2 + 1}, \tag{9}$$

where the Euclidean norm of the projected position vector written in the usual way as:

$$|\mathbf{P}|^2 = \langle \mathbf{P} * \mathbf{P} \rangle = \sum_{I=1}^{n} P_I^2$$

has an obvious fundamental role.

Equations (7), (8) and (9) constitute quite a general framework, which permits to state that: "every well behaved function of an arbitrary number of variables n can be subject to a reversible stereographic projection into the surface of an n-dimensional sphere of arbitrary radius".

The sentence above declared is nothing else than the enunciation of a *holographic general function theorem* (HGFT), which holds for well-behaved functions of any number of variables, in particular including DF and ShF of first and higher arbitrary orders.

8 Some remarks on stereographic projection in FES

1) A possible problem, which can be encountered when applying Eq. (7), is associated with the factor: $\lambda^{-1} = (R - \gamma(\mathbf{r}))^{-1}$, which under determinate circumstances can introduce the presence of an infinite value into the stereographic transformation grid. This possibility has to be taken into account when programming the stereographic projection and within subsequent practical computations. However, theoretically one can invoke the Alexandrov one-point compactification, as Mezey [3] did when establishing the HEDT. In fact, in the present case one can avoid computationally the possible infinite values by choosing an appropriate radius R of the sphere (6), which can provide the following property fulfillment: $\forall \mathbf{r} : R - \gamma(\mathbf{r}) \neq 0$.
   This becomes a sensitive procedure when full EMPs are considered, as they become infinite at atomic positions. One can observe EMP stereographic projections from the point of view of any atom in a molecule, provided that the sphere centered at this atom do not includes another atom lying on the spherical surface. Such a caution will prevent the issue of representing infinite function values in a

given EMP snapshot. In a similar way, recently the present authors have developed based on previous EMP experience [22] the softened EMP (SEMP) [23], where the generated EMP using a hard original point charge, has been simply substituted by a soft density charge distribution, permitting to avoid the infinity poles at the atomic positions, thus easing the automatic drawing, while preserving the original shape of such an interesting molecular feature.

2) The stereographic transformation can be used to reduce an initial problem from C_{n+1} to E_n as explained, but one can iterate further on, for instance from E_n to E_{n-1} and so on, taking into account that the stereographic projection sequence is reversible from lower dimensions to upper ones by the provided algorithm in Eq. (9).

3) Equation (6) defining a sphere in C_{n+1} can be easily transformed into a unit radius structure, as one can also write:

$$\left|R^{-1}\mathbf{r}\right|^2 + \left|R^{-1}\gamma\left(\mathbf{r}\right)\right|^2 = 1. \tag{10}$$

However, this result permits to take into account the feasibility of stereographic projection not only into a sphere, as it has been previously described, but into a spheroid, whose principal axis can be gathered into a vector of C_{n+1}, with a constant in the function position, like:

$$\mathbf{A} = \{a_I, \alpha \,|I = 1, n\} = (\mathbf{a}, \alpha) \tag{11}$$

and possessing an inward inverse, which can be defined at once as:

$$\mathbf{A}^{[-1]} = \left\{a_I^{-1}, \alpha^{-1} \,|I = 1, n+1\right\} = \left(\mathbf{a}^{[-1]}, \alpha^{-1}\right),$$

and which can be used over the function extended vector $\mathbf{p}$ in order to define the general spheroidal structure:

$$\mathbf{q} = \mathbf{A}^{[-1]}\mathbf{p} = \left(\mathbf{a}^{[-1]}\mathbf{r}, \alpha^{-1}\gamma\left(\mathbf{r}\right)\right) \to |\mathbf{q}|^2 = \sum_{I=1}^{n}\left(\frac{r_I}{a_I}\right)^2 + \left(\frac{\gamma\left(\mathbf{r}\right)}{\alpha}\right)^2 = 1.$$

The unit spherical form as shown in Eq. (10) corresponds to the well-defined vector: $\mathbf{A} = R\left(\mathbf{1}_n, 1\right) = R\mathbf{1}_{n+1}$.

9 Conclusions

FES and well-known stereographic projections of multivariate functions can be considered as the mathematical basis to represent in a graphical way such mathematical objects in general. Particularly, when associated to quantum mechanical submicroscopic systems they can constitute quite adequate means to dynamically visualize relevant quantum molecular functions. Finally both FES and stereographic representations can be the basis to formalize a general holographic theorem, involving any kind of multivariate function.

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