

***n*-Dimensional Euclidean space Gaussian enfoldment**

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Abstract In this study Euclidean space is enfolded with Gaussian functions of various orders. A simple analysis of the properties of such a functional enclosing of *n*-dimensional space is performed. In this way, once more Gaussian functions appear to have some interesting not yet fully described mathematical properties, some of which are disclosed and discussed here. The quantum chemical application of such an *n*-dimensional Euclidean space enfoldment is developed as an example.

Keywords Multivariate Gaussian functions · *n*-Dimensional Euclidean space Gaussian enfoldment · Quantum chemistry in ∞ -dimensional LCAO MO framework · Generalized harmonic oscillator wave functions

1 Introduction

The present authors have chosen to look at the usual, simple and well-known spherical Gaussian functions and their linear combinations from different points of view. Such kind of studies started with the definition of the Atomic Shell Approximation [1–7], to continue with the Gaussian function relationship with quantum similarity and Mezey's [8] holographic theorem [9–11] and other various properties [12–14]. Gaussian functions possess aspects which were not apparently noticed beforehand and the present work has evolved following the search path of more facets from such quantum chemical ubiquitous functions.

The fact that Cartesian space can be associated perhaps to other kinds of structures than the usual tridimensional one we live in, it is a well-known idea since the initial evolution of relativity and quantum mechanics; see references [15, 16] for a

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comprehensive review of one of such important aspects of rethinking space-time, related to the so called Kaluza-Klein theory. References [17, 18] correspond to another recent point of view, which prove the interest of one of the present authors about unusual space-time properties enhancement. Such papers are related to an old idea about distinct time associated to every particle [19]; although, they obviously constitute a naïve framework, compared with the previous Kaluza-Klein theoretical development.

This paper pretends to present another vision of Euclidean space, where every n -dimensional point contains attached an infinite dimensional vector structure in the form of a Gaussian function or even better: to a wave function of a generalized harmonic oscillator. As a result of this functional construction, the Euclidean space can be seen as appearing enclosed, surrounded or embedded within an infinite number of Gaussian functions.

With such an image in mind, here will be briefly developed the practical properties one can consider from a simple point of view of such a spatial *enfoldment*¹ structure made by means of the simplest Gaussian function structure. Some possible extensions to higher order Gaussian functions will be suggested afterwards. The present work will therefore be organized as follows: first the n -dimensional Euclidean space enfoldment by a Gaussian function will be described with some extended characteristics like the possibility that the Gaussian exponent becomes a function, then the unnormalized and normalized linear combinations of Gaussian enfoldments will be presented, followed by a study of the enfoldment attached kinetic energy, Coulomb potential and virial coefficient; finally a discussion about the possible general structure of Gaussian enfoldments will close the present study.

2 n -Dimensional Euclidean space Gaussian enfoldment

To obtain the first image of what can be called a Gaussian enfoldment, one can start with the definition of a classical Gaussian function, which can be written like:

$$\gamma_0(\mathbf{r} - \mathbf{R}|\alpha) = \exp\left(-\alpha|\mathbf{r} - \mathbf{R}|^2\right), \quad (1)$$

where \mathbf{r} corresponds to n -dimensional Euclidean coordinates acting as variables, \mathbf{R} is any position within this n -dimensional space, which acts as a center or origin of the Gaussian function, finally α in principle² is a positive definite real constant scalar.

¹ The word *enfoldment* or the action of *enfoldment*, of surrounding something with a covering, has been chosen according to the authors' criterion, and used as the reasonable descriptor of the mathematical idea, which will be developed along the present paper. The plural: *enfoldments* will be also employed. The verb to *enfold*, (*enfolds*, *enfolded*, *enfoldment*) can also appear.

² In Eq. (1) the parameter α and the Euclidean norm of the shifted variable vector can be substituted by a diagonal matrix: $\mathbf{A} = \text{Diag}(a_{II} | I = 1, N)$ and a weighted scalar product: $\langle \mathbf{r} - \mathbf{R} | \mathbf{A} | \mathbf{r} - \mathbf{R} \rangle = \sum_{I=1}^n a_{II} (r_I - R_I)^2$. In this way can be taken in consideration a possible anisotropic influence over every space direction. However, this refinement will complicate the whole description of the present Gaussian enfoldment and therefore has not been considered here. Instead, it has been used the usual GTO simpler scalar matrix feature: $\alpha \in \mathbf{R}^+ : \mathbf{A} = \alpha \mathbf{I}_n$.

Independently of the center \mathbf{R} , the Minkowski norm of the Gaussian (1) can be written as:

$$\langle \gamma_0 \rangle_{\mathbf{r}} = \int_{-\infty}^{+\infty} \gamma_0(\mathbf{r} - \mathbf{R} | \alpha) d\mathbf{r} = \left(\frac{\pi}{\alpha} \right)^{\frac{n}{2}}, \tag{2}$$

where the integration now and in forthcoming formulae has to be understood over the n -dimensional variable vector \mathbf{r} . Nevertheless, nothing opposes to consider the function (1) as being simultaneously a function of both the variable vector \mathbf{r} and the center vector \mathbf{R} .

That is, one can also define an alternative Minkowski norm, symmetrical to Eq. (2), with the obvious result:

$$\langle \gamma_0 \rangle_{\mathbf{R}} = \int_{-\infty}^{+\infty} \gamma_0(\mathbf{r} - \mathbf{R} | \alpha) d\mathbf{R} = \left(\frac{\pi}{\alpha} \right)^{\frac{n}{2}}. \tag{3}$$

Therefore, both variable and center vectors act interchangeably with respect to the Minkowski norm integration. The same can be said about Euclidean norms, as the equivalent equations to Minkowski's can be easily deduced:

$$\begin{aligned} \langle |\gamma_0|^2 \rangle_{\mathbf{r}} &= \int_{-\infty}^{+\infty} \gamma_0(\mathbf{r} - \mathbf{R} | 2\alpha) d\mathbf{r} = \left(\frac{\pi}{2\alpha} \right)^{\frac{n}{2}} \\ &= \int_{-\infty}^{+\infty} \gamma_0(\mathbf{r} - \mathbf{R} | 2\alpha) d\mathbf{R} = \langle |\gamma_0|^2 \rangle_{\mathbf{R}}. \end{aligned} \tag{4}$$

Thus, nothing opposes to define and observe any Euclidean n -dimensional space, enfolded with Gaussian functions, which can be in turn considered centered at each point of such Euclidean space.

In fact, in other words, the Gaussian function definition (1), when considering the center \mathbf{R} also as a variable n -dimensional vector, as it has been described here, simultaneously corresponds to a two faced mathematical object: a generalized Gaussian function and a n -dimensional Euclidean space enfoldment.

3 Exponent functionality

Yet, as shown in Eqs. (2) to (4), such a Gaussian enfoldment has a generic normalization property. That is, if the exponent α remains constant, the whole embedded space acts as a unique Gaussian function with respect to the normalization.

Depending on the kind of functionality one can assign to the exponent of the function (1), then the symmetry shown in Eqs. (2) and (3) or (4) will obviously no longer hold. For instance, one can suppose the exponent becomes a function of the Gaussian

centers: $\alpha(\mathbf{R})$, instead of the scalar used until now, then the Minkowski norm will be transformed into a function of the position vector:

$$\langle \gamma_0 \rangle_{\mathbf{r}}(\mathbf{R}) = \int_{-\infty}^{+\infty} \gamma_0(\mathbf{r} - \mathbf{R} | \alpha(\mathbf{R})) d\mathbf{r} = \left(\frac{\pi}{\alpha(\mathbf{R})} \right)^{\frac{n}{2}}. \quad (5)$$

Another possibility is to provide this exponent function with an explicit Gaussian structure too, like:

$$\alpha(\mathbf{R}) = \exp(\pm \theta |\mathbf{R}|^2)$$

which permits to rewrite the Minkowski norm (5) as:

$$\langle \gamma_0 \rangle_{\mathbf{r}}(\mathbf{R}) = \pi^{\frac{n}{2}} \exp\left(\mp \frac{n\theta}{2} |\mathbf{R}|^2\right).$$

4 Gaussian enfoldment linear combinations

In order to take advantage of the Gaussian enfoldment as earlier defined, one can build up an integral of the center variables involving the enfoldment, just writing the position vector function:

$$\phi_0(\mathbf{r}) = \int_{-\infty}^{+\infty} \kappa(\mathbf{R}) \gamma_0(\mathbf{r} - \mathbf{R} | \alpha) d\mathbf{R}. \quad (6)$$

Then, one can consider the function of the position vector (6) as some kind of linear combination, thus its Euclidean norm can be written as:

$$\begin{aligned} \langle \phi_0 | \phi_0 \rangle &= \langle |\phi_0|^2 \rangle \\ &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \kappa(\mathbf{R}_1) \kappa(\mathbf{R}_2) \gamma_0(\mathbf{r} - \mathbf{R}_1 | \alpha) \gamma_0(\mathbf{r} - \mathbf{R}_2 | \alpha) d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r} \\ &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \kappa(\mathbf{R}_1) \kappa(\mathbf{R}_2) s_{00}(\mathbf{R}_1; \mathbf{R}_2 | \alpha) d\mathbf{R}_1 d\mathbf{R}_2 = \langle \kappa | \mathbf{S}_{00} | \kappa \rangle \end{aligned} \quad (7)$$

where an infinite dimensional overlap matrix \mathbf{S}_{00} is defined:

$$\begin{aligned} s_{00}(\mathbf{R}_1; \mathbf{R}_2 | \alpha) &= \int_{-\infty}^{+\infty} \gamma_0(\mathbf{r} - \mathbf{R}_1 | \alpha) \gamma_0(\mathbf{r} - \mathbf{R}_2 | \alpha) d\mathbf{r} \\ &\rightarrow \mathbf{S}_{00} = \{s_{00}(\mathbf{R}_1; \mathbf{R}_2 | \alpha)\} \end{aligned} \quad (8)$$

the elements of it are immediately computed as Gaussian functions with the form:

$$s_{00}(\mathbf{R}_1; \mathbf{R}_2 | \alpha) = \left(\frac{\pi}{2\alpha}\right)^{\frac{n}{2}} \exp\left(-\frac{\alpha}{2} |\mathbf{R}_1 - \mathbf{R}_2|^2\right).$$

Whenever the set of linear coefficients-functions $K = \{\kappa(\mathbf{R})\}$ can be uniformly defined as Gaussian functions too, then the scalar product under the metric matrix \mathbf{S}_{00} can be written as a constant:

$$\begin{aligned} \langle \kappa | \mathbf{S}_{00} | \kappa \rangle &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \exp(-\lambda_1 |\mathbf{R}_1|^2) \exp(-\lambda_2 |\mathbf{R}_2|^2) s_{00}(\mathbf{R}_1; \mathbf{R}_2 | \alpha) d\mathbf{R}_1 d\mathbf{R}_2 \\ &= \left(\frac{\pi^3}{2\alpha(\lambda_1\lambda_2 + (\lambda_1 + \lambda_2)\frac{\alpha}{2})}\right)^{\frac{n}{2}}. \end{aligned} \tag{9}$$

5 Normalized linear combinations

Alternatively one can define the linear combination function (6) in the same fashion, yielding a position vector Gaussian with the structure:

$$\begin{aligned} \phi(\mathbf{r}) &= \int_{-\infty}^{+\infty} \exp(-\lambda |\mathbf{R}|^2) \exp(-\alpha |\mathbf{r} - \mathbf{R}|^2) d\mathbf{R} \\ &= \exp\left(-\frac{\gamma}{2} |\mathbf{r}|^2\right) \int_{-\infty}^{+\infty} \exp\left(-(\alpha + \lambda) \left|\mathbf{R} - \frac{\alpha\mathbf{r}}{\alpha + \lambda}\right|^2\right) d\mathbf{R} \\ &= \left(\frac{\pi}{\alpha + \lambda}\right)^{\frac{n}{2}} \exp\left(-\frac{\gamma}{2} |\mathbf{r}|^2\right) \end{aligned} \tag{10}$$

where, for further purposes, it has been defined the parameter

$$\gamma = \frac{2\alpha\lambda}{\alpha + \lambda}.$$

Curiously enough, as shown in Eq. (10), the integral combination produces a unique Gaussian function centered at the origin. Such a property proves that Gaussian functions, even present in an infinite number, behave in the same manner as in finite sets of them, see for example reference [14].

As such, the function (10) can be easily normalized both in Minkowski stile:

$$\langle \phi(\mathbf{r}) \rangle = \left(\frac{\pi}{\alpha + \lambda}\right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \exp\left(-\frac{\gamma}{2} |\mathbf{r}|^2\right) d\mathbf{r} = \left(\frac{\pi^2}{\alpha\lambda}\right)^{\frac{n}{2}}$$

or in the Euclidean way:

$$\langle |\phi(\mathbf{r})|^2 \rangle = \left(\frac{\pi}{\alpha + \lambda} \right)^n \int_{-\infty}^{+\infty} \exp(-\gamma |\mathbf{r}|^2) d\mathbf{r} = \left(\frac{\pi^3}{2\alpha\lambda(\alpha + \lambda)} \right)^{\frac{n}{2}}$$

in this way, the Euclidean normalization factor can be easily written and included into the linear combination (10) producing the function:

$$\phi_E(\mathbf{r}) = \left(\frac{\gamma}{\pi} \right)^{\frac{n}{4}} \exp\left(-\frac{\gamma}{2} |\mathbf{r}|^2\right). \quad (11)$$

6 Dirac function enfoldment

For the sake of completeness it is instructive to briefly review the previous results when the Gaussian function (1) is substituted with a Dirac function. Such functions can be individually considered the limit of the zeroth order enfoldment Gaussian, when the exponent becomes infinite. Equation (6) can be written in this case as:

$$\kappa_\delta(\mathbf{r}) = \int_{-\infty}^{+\infty} \kappa(\mathbf{R}) \delta(\mathbf{r} - \mathbf{R}) d\mathbf{R}. \quad (12)$$

One can consider the function of the position vector (12) also as some kind of linear combination; thus its Euclidean norm can be written as:

$$\begin{aligned} \langle \kappa_\delta | \kappa_\delta \rangle &= \langle |\kappa_\delta|^2 \rangle \\ &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \kappa(\mathbf{R}_1) \kappa(\mathbf{R}_2) \delta(\mathbf{r} - \mathbf{R}_1) \delta(\mathbf{r} - \mathbf{R}_2) d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r} \\ &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \kappa(\mathbf{R}_1) \kappa(\mathbf{R}_2) \delta(\mathbf{R}_1 - \mathbf{R}_2) d\mathbf{R}_1 d\mathbf{R}_2 \\ &= \int_{-\infty}^{+\infty} \kappa_\delta(\mathbf{R}_1) \kappa_\delta(\mathbf{R}_1) d\mathbf{R}_1 \end{aligned} \quad (13)$$

which yields an easier structure than in the zeroth order Gaussian case, as the infinite dimensional metric matrix (8) can be supposed now to be equivalent to an infinite dimensional unit matrix.

7 Kinetic energy

The same analytical structure, as the one employed in the normalization of the infinite dimensional linear combination (6) of the preceding paragraph, can be used subjected to the effect of the quantum mechanical kinetic energy operator in the form of a position gradient.

Thus, in order to obtain the expectation value of the kinetic energy under a Gaussian enfoldment, one needs to know the gradient of the function (11) with respect to the position vector first. The result of such a gradient operation can be written as a scaled n -dimensional position vector multiplied by a Gaussian function:

$$\begin{aligned}\frac{\partial \phi_E(\mathbf{r})}{\partial \mathbf{r}} &= \left(\frac{\gamma}{\pi}\right)^{\frac{n}{4}} \frac{\partial}{\partial \mathbf{r}} \exp\left(-\frac{\gamma}{2} |\mathbf{r}|^2\right) \\ &= -\left(\frac{\gamma}{\pi}\right)^{\frac{n}{4}} \gamma \mathbf{r} \exp\left(-\frac{\gamma}{2} |\mathbf{r}|^2\right)\end{aligned}$$

From this resultant expression, the quantum mechanical kinetic energy can be easily written in terms of the two involved exponents as the simple integral scalar:

$$\frac{1}{2} \left\langle \left| \frac{\partial \phi_E(\mathbf{r})}{\partial \mathbf{r}} \right|^2 \right\rangle = \frac{n}{2} \frac{\alpha \lambda}{(\alpha + \lambda)} = \frac{n}{4} \gamma. \quad (14)$$

From the enfoldment kinetic energy computed as above, by taking into account the Boltzmann energy of N particles:

$$E_K = \frac{3}{2} N k T,$$

and equalizing both results, one can easily obtain:

$$\frac{3}{2} N k T = \frac{3N}{2} \frac{\alpha \lambda}{(\alpha + \lambda)} \rightarrow k T = \frac{\alpha \lambda}{(\alpha + \lambda)},$$

which can be finally expressed as a simple relationship between the inverses of the involved elements:

$$(kT)^{-1} = \alpha^{-1} + \lambda^{-1}.$$

Also, supposing both exponents equal to a unique parameter a , say, one obtains:

$$2kT = a.$$

Thus, in this case, the condensed enfoldment function appearing in Eq. (11) can be written in terms of the absolute temperature as:

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

8 An origin centered Coulomb potential

It will be interesting and illustrative to know the enfoldment expectation value result, which can be obtained when an origin centered one-particle three-dimensional Coulomb potential is associated to the uniform function (10), and normalized as in Eq. (11). To deal with this case one needs to compute the integral³:

$$\langle |\mathbf{r}_3|^{-1} \rangle = \int_{-\infty}^{+\infty} |\mathbf{r}_3|^{-1} |\phi_E(\mathbf{r})|^2 d\mathbf{r} = \left(\frac{\gamma}{\pi}\right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} |\mathbf{r}_3|^{-1} \exp(-\gamma |\mathbf{r}|^2) d\mathbf{r}.$$

Essentially, the above integral has been described by Saunders [20] and based in the Laplace transform of $|\mathbf{r}_3|^{-1}$:

$$|\mathbf{r}_3|^{-1} = \pi^{-\frac{1}{2}} \int_0^{\infty} s^{-\frac{1}{2}} \exp(-s |\mathbf{r}_3|^2) ds,$$

which produces:

$$\langle |\mathbf{r}_3|^{-1} \rangle = \pi^{-\frac{1}{2}} \gamma^{\frac{3}{2}} \int_0^{\infty} s^{-\frac{1}{2}} (s + \gamma)^{-\frac{3}{2}} ds.$$

Now, taking:

$$t^2 = \frac{s}{\gamma + s}$$

one finds:

$$ds = \frac{2}{\gamma} s^{\frac{1}{2}} (s + \gamma)^{\frac{3}{2}} dt$$

and thus:

$$\langle |\mathbf{r}_3|^{-1} \rangle = 2\pi^{-\frac{1}{2}} \gamma^{\frac{1}{2}}, \quad (15)$$

yielding a reasonable value, which can be also associated to the previously described kinetic energy expression (14). However, the expression (15) corresponds to the Coulomb interaction of one of the particles, but considering all of them interacting in

³ The Coulomb operator is considered here as a three dimensional one particle operator and noted as: $|\mathbf{r}_3|^{-1}$, the subindex indicating the dimension of the position vector. Therefore, the total Euclidian dimension n has to be considered equal to the triple of the number of particles: $n = 3N$. This is chosen in this way in order to have a coherent description as the one employed in the previous kinetic energy discussion.

turn (but not among themselves), one is forced in this circumstance to write the total Coulomb energy of the N particles as:

$$C_N = N \langle |\mathbf{r}_3|^{-1} \rangle = 2N\pi^{-\frac{1}{2}} \gamma^{\frac{1}{2}}.$$

Of course, the same result for the expected value can be obtained by means of considering the Gaussian transform:

$$|\mathbf{r}_3|^{-1} = 2\pi^{-\frac{1}{2}} \int_0^\infty \exp(-t^2 |\mathbf{r}_3|^2) dt \tag{16}$$

which in this case needs the following integral result:

$$\int_0^\infty (t^2 + \gamma)^{-\frac{3}{2}} dt = \gamma^{-1}.$$

This formulation admits various alternative interpretations. An interesting one may consist to attach the normalized Gaussian function $\phi_E(\mathbf{r})$ to a unique particle within a space of dimension n . Then, in this case the repulsion operator can be assumed to be of dimension $2 \leq r \leq n$. The expected value for the operator defined in this way is:

$$\langle |\mathbf{r}_r|^{-1} \rangle = \int_{-\infty}^{+\infty} |\mathbf{r}_r|^{-1} |\phi_E(\mathbf{r})|^2 d\mathbf{r} = \left(\frac{\gamma}{\pi}\right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} |\mathbf{r}_r|^{-1} \exp(-\gamma |\mathbf{r}|^2) d\mathbf{r}.$$

By application of the Gaussian transform (16) the previous expectation value can be expressed as:

$$\langle |\mathbf{r}_r|^{-1} \rangle = 2\pi^{-\frac{1}{2}} \gamma^{\frac{r}{2}} I_r$$

being the integral

$$I_r = \int_0^\infty (t^2 + \gamma)^{-\frac{r}{2}} dt$$

convergent for $r > 1$.

After some straightforward algebra, the following final result, bearing one or another structure according to the parity of r , can be easily obtained:

$$\forall r > 1 : \langle |\mathbf{r}_r|^{-1} \rangle = 2\pi^{-\frac{1}{2}} \gamma^{\frac{r-2}{2}} \frac{(r-3)!!}{(r-2)!!} \left[\delta(r \neq 2) + \frac{\pi}{4} \gamma^{-\frac{1}{2}} \delta(r = 2) \right]; \tag{17}$$

where it is assumed that $0!! = (-1)!! = 1$ and the delta symbol stands for a logical Kronecker delta [21–23].⁴ It can now be mentioned that, as a particular case, for $r = 3$, the previous formula in Eq. (17) becomes the one attached to the $\langle |\mathbf{r}_3|^{-1} \rangle$ integral, as obtained in Eq. (15).

9 Virial coefficient

By means to the previously computed kinetic and Coulomb energies, it can be obtained a virial coefficient, which can be expressed as:

$$\eta = \frac{2E_K}{C_N} = \frac{2E_K}{N \langle |\mathbf{r}_3|^{-1} \rangle} = \frac{\frac{n}{2}\gamma}{2N\pi^{\frac{-1}{2}}\gamma^{\frac{1}{2}}} = \frac{n\pi^{\frac{1}{2}}}{4N}\gamma^{\frac{1}{2}} = \frac{3N\pi^{\frac{1}{2}}}{4N}\gamma^{\frac{1}{2}} = \frac{3\pi^{\frac{1}{2}}}{4}\gamma^{\frac{1}{2}}$$

by employing a unique parameter:

$$a = \alpha = \lambda = \gamma,$$

as done before in the kinetic energy case. Then, the previous virial coefficient expression can be reduced to:

$$\eta = \frac{3\pi^{\frac{1}{2}}}{4}a^{\frac{1}{2}} \rightarrow 1 = \frac{3\pi^{\frac{1}{2}}}{4}a^{\frac{1}{2}} \rightarrow a = \frac{16}{9\pi} = \left(\frac{4}{3}\right)^2 \frac{1}{\pi}$$

constituting an interesting result, which in order to obtain a perfect virial coefficient value, constructs the unique Gaussian enfoldment exponent as independent of the number of particles.

10 Linear, quadratic and higher order Gaussian space enfoldments

The previous discussion has been performed over the simplest structure of a zeroth order Gaussian enfoldment. Nothing opposes to consider higher order Gaussian enfoldments though. In fact, in order to guess how a possible general enfoldment can be, it is just necessary to consider higher order Gaussian or other kinds of enfoldments, based on the basic features associated to the already analyzed one.

Whenever one can consider any function with scalar values, which upon interchange of the position and center coordinates can behave in a symmetric or antisymmetric manner:

$$\pm\psi(\mathbf{r} - \mathbf{R}) = \psi(\mathbf{R} - \mathbf{r}),$$

then there can be defined a corresponding enfoldment.

⁴ The value of a logical Kronecker's delta is one, if the logical condition acting as an argument is true, and zero otherwise.

The most immediate functions of this type can be found in a kind of sequence of Gaussian function enfoldments. In this way, they can be chosen as constituted in their first terms by the linear and quadratic Gaussian enfoldments, which can be respectively defined as:

(1)

$$\gamma_1(\mathbf{r} - \mathbf{R}|\alpha) = \langle \mathbf{a}|\mathbf{r} - \mathbf{R} \rangle \gamma_0(\mathbf{r} - \mathbf{R}|\alpha) \quad (18)$$

and

(2)

$$\gamma_2(\mathbf{r} - \mathbf{R}|\alpha) = \langle \mathbf{r} - \mathbf{R}|\mathbf{A}|\mathbf{r} - \mathbf{R} \rangle \gamma_0(\mathbf{r} - \mathbf{R}|\alpha) \quad (19)$$

It is immediate to grasp that the first order function (18) will be antisymmetric with respect to the interchange position-center while the second order companion (19), as the zeroth order one in Eq. (1), will behave symmetrically upon such an interchange. The $(n \times n)$ matrix \mathbf{A} appearing in the second order enfoldment, can be considered diagonal, in the same way as it was considered in the footnote 2, when dealing with a quadratic form entering the Gaussian exponents. Therefore, both enfoldment equations can be more explicitly rewritten by means of the expressions⁵:

(1)

$$\gamma_1(\mathbf{r} - \mathbf{R}|\alpha) = \left(\sum_I a_I (r_I - R_I) \right) \gamma_0(\mathbf{r} - \mathbf{R}|\alpha)$$

and

(2)

$$\gamma_2(\mathbf{r} - \mathbf{R}|\alpha) = \left(\sum_I a_{II} |r_I - R_I|^2 \right) \gamma_0(\mathbf{r} - \mathbf{R}|\alpha)$$

Both linear and quadratic enfoldments can be designed in order to yield isotropic enfoldments whenever: $\forall I : a_I = a \wedge a_{II} = \alpha$, for instance. However, the structure of the specific elements of the vector in the linear case or the diagonal matrix in the quadratic situation can be employed to tune an infinite anisotropic space family of Gaussian enfoldments up.

Higher order Gaussian enfoldments can be also easily considered. Odd order ones will become antisymmetric, while even order are symmetric upon exchange of position-center variables.

While the zeroth order enfoldment may be seen imaginatively as a sponge of Gaussian spikes surrounding Euclidean space, a linear enfoldment can be seen as

⁵ In the summations below, each term represents a coordinate, so one can consider the same Euclidean dimension convention as in the preceding discussion about the zeroth order Gaussian enfoldment.

formed by layers or sheets filling up space. Finally, quadratic enfoldment can be imagined as spheres or spheroids filling Euclidean space by point by point elements, which in turn can be collected along arbitrary constructed backbone lines, like cylinders or distorted tubes filling all the space.

10.1 Higher order enfoldments

Nothing opposes to perform with both the higher order previous enfoldments the operations already described at zeroth order. The resultant structures, discussed beforehand at the zeroth order will be obtained in the same mechanical manner; so, the present authors for the sake of simplicity consider that it is not necessary to insist in this direction.

It can be also said that, in this way, one can define Gaussian enfoldments, which seem to correspond to a sequence, starting from the ground state of a generalized harmonic oscillator and can follow to its higher excited states, alternating the symmetry with the antisymmetry, using the structure of even and odd functions respectively. Such a description reminds of the even-odd behavior, which bosonic and fermionic wave functions must have to correctly describe such particle kinds.

10.2 Tensorial enfoldments

But this it is not the least, nor the last way enfoldments can be constructed. The previously described ones are scalar in the sense that at each n -dimensional Euclidean point, there a scalar function is centered. Nothing opposes to the fact that the vector bearing the variable and the center information: $|\mathbf{v}\rangle = \mathbf{r} - \mathbf{R}$ and its tensorial products: $\otimes_{I=1}^t |\mathbf{v}\rangle$ can be used as the elements of the enfoldment, providing in this way of a tensorial enfoldment sequence of order t , which can be as high as the tensor rank to be employed. But to enter into the in deep description of this kind of general enfoldments will mask up the naïve beauty of the present preliminary enfoldment ideas. In this sense, it is better to leave the study of such enfoldment higher structures for the future, if necessary.

11 Conclusions

General n -dimensional Euclidean space Gaussian enfoldments can be easily defined up to any arbitrary order. At a first glance, they constitute a set of interesting simple pathways to describe a gas of particles from ground state to higher excited states, by means of generalized harmonic oscillator wave functions, enfolding the n -dimensional Euclidean space. However, in addition they can be observed as a simple way to enrich the inmost structure of the ordinary n -dimensional Euclidean spaces.

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