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ORIGINAL PAPER

A Gaussian holographic theorem and the projection of electronic density functions into the surface of a sphere

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Abstract A theorem, associated to the holographic nature of general Gaussian functions, is employed to describe holographic projections of electronic density model functions, both in position and momentum spaces, over the surface of a sphere.

Keywords Gaussian holographic theorem · Electronic density functions (EDF) · Projection of EDF into spherical surfaces · ASA density functions

1 Introduction

Gaussian functions (GFs), since the modern development of quantum chemistry, had and still have an overwhelming influence in the everyday computational practice of this discipline and other fields of interest. Indeed, since the first papers of Boys [1] and Shavitt [2] on the use of GFs as basis set orbitals, several studies have developed the necessary formulations of molecular integrals [3,4] to be employed in practical quantum computational chemistry. Besides the historical development of the theoretical background of GFs, it has also been research on precise and exhaustive atomic calculations (see reference [5] for instance, as a single but quite complete specimen of the large amount of literature generated in this field). The accurate computation of AO based on GFs permitted to furnish with Gaussian basis sets the basis set AO for the contemporary routine molecular quantum computations of MO within the widespread LCAO MO theory.

In this paper it will be shown a simple theorem associated to GFs and their possible holographic representation into the surface of a sphere. In this way quantum chemistry may appear as to be also furnished of a similar property, like the one related to the

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so-called holographic principle which has been postulated in quantum gravity [6] and string theories [7], see also reference [8] for more details.

The results of the development of the present paper can be seen as an autonomous particular but practical case, a clear consequence of the so-called holographic electronic density theorem of (HEDT)first described by Mezey [9]. In order to distinguish the present development from HEDT, in this paper one can say that here it will be studied the *Gaussian holographic theorem* (GHT).

The present paper will first study the position space GF holography, propose the GHT afterwards and then use it in the ASA density environment and in the momentum space GF Fourier transforms as well.

2 The Gaussian holographic theorem

2.1 A two-dimensional example

In order to start the present study, a simplified quite particular case will be first discussed in order to present with sheer clarity the holographic capabilities of GFs. Suppose one aims to see how behaves, when projected into a circumference, a two-dimensional variable GF collection. Such a function assembly can be written like:

$$\gamma_2\left(\alpha\left|\mathbf{r}\right.\right)=\gamma_1\left(\alpha\left|x\right.\right)\gamma_1\left(\alpha\left|y\right.\right)=\exp\left(-\alpha\left(x^2+y^2\right)\right)=\exp\left(-\alpha\left|\mathbf{r}\right|^2\right)$$

with: $\alpha\in\mathbf{R}^+\wedge\mathbf{r}=(x;y)$.

Such a function when projected into a circumference of radius $R:R^2=x^2+y^2=|\mathbf{r}|^2=\langle\mathbf{r}|\mathbf{r}\rangle=\langle\mathbf{r}^*\mathbf{r}\rangle$, corresponds to the infinitely degenerate function value collection:

$$\gamma_1\left(\alpha\left|R\right.\right)=\exp\left(-\alpha R^2\right).$$

2.2 *N*-dimensional general result

The previous consideration on two-dimensional variable GFs precludes a far reaching general result.This can be easily seen when considering the projection involving a generic GF:

$$\gamma_N\left(\alpha\left|\mathbf{r}\right.\right)=\exp\left(-\alpha\left\langle\mathbf{r}^*\mathbf{r}\right\rangle\right)$$

of a N-dimensional variable vector: $\mathbf{r}=(x_1;x_2;\ldots x_N)=\{x_I\,|I=1,N\}$ into the surface of a N-dimensional sphere of radius R:

$$R^2=\sum_{I=1}^{N}x_I^2=\left\langle\mathbf{r}^*\mathbf{r}\right\rangle$$

Such a projection obviously corresponds to the infinitely degenerate collection of GFs:

$$\gamma_1(\alpha\,|R) = \exp\left(-\alpha R^2\right).$$

Thus, it seems that the one-dimensional values of the function collection: $\Gamma = \left\{\exp\left(-\alpha R^2\right)\,\middle|\forall\alpha \in \mathbf{R}^+ \wedge R \in [0,+\infty]\right\}$, within the points of the N-dimensional sphere,contains information overall the N-dimensional function values.

Indeed, there is only necessary to well-define such a one-dimensional variable function collection,in order to know the behavior of any N-dimensional function within every point of the whole position space.

2.3 The Gaussian holographic theorem (GHT)

Then, curiously enough, one can state the Gaussian holographic theorem is simple terms as follows:

Theorem 1 *Any Gaussian function of a N-dimensional variable vector:* $\mathbf{r} = (x_1; x_2; \ldots x_N)$*, which can be written as:* $\gamma_N(\alpha\,|\mathbf{r}) = \exp(-\alpha\,\langle\mathbf{r}^*\mathbf{r}\rangle)$*, behaves like the Gaussian function of a mono-dimensional variable:* $\gamma_1(\alpha\,|R) = \exp\left(-\alpha R^2\right)$*. At fixed R, the values of* $\gamma_1(\alpha\,|R)$ *are these of* $\gamma_N(\alpha\,|\mathbf{r})$ *computed within the spherical surface defined by the function:* $R^2 = \langle\mathbf{r}^*\mathbf{r}\rangle$.

Thus, the single variable GF $\gamma_1(\alpha\,|R)$ can be considered some kind of résumé about *all* the possible values of *any* arbitrary dimension variable GF with the same exponent. The function family: $\{\gamma_1(\alpha\,|R)\}$ can accordingly be considered as a generalized hologram, containing the *whole* information on any kind of variable GF. As a consequence, a function like: $\gamma_1(\alpha\,|R)$, with a fixed exponent, can be safely named a *Gaussian hologram*.

2.4 Gaussian holograms of GFs centered arbitrarily at any point in position space

In case the general GF is centered in a point of space different from the position space origin, it can be also written in the following fashion:

$$\gamma_N(\alpha\,|\mathbf{r}-\mathbf{A}) = \exp\left(-\alpha\left\langle(\mathbf{r}-\mathbf{A})^*(\mathbf{r}-\mathbf{A})\right\rangle\right)$$

and one can seek for the projection sphere surface definition, which can be redefined as:

$$R^2 = \left\langle(\mathbf{r}-\mathbf{A})^*(\mathbf{r}-\mathbf{A})\right\rangle;$$

thus, one arrives (in this even more general case)at the same Gaussian mono-dimensional holographic representation collection: $\gamma_1(\alpha\,|R)$. As a result, Theorem 1 above applies not only to any GF but to *any GF centered anywhere* in position space.

2.5 Projection of a linear combination of GFs

Having studied the Gaussian holograms of isolated GFs it is necessary to consider how one can define holograms of linear combinations of GFs.

A linear combination of two GFs, which one can write like:

$$\chi_N(\mathbf{r}) = w_a \gamma_N(\alpha\,|\mathbf{r}-\mathbf{A}) + w_b \gamma_N(\beta\,|\mathbf{r}-\mathbf{B})$$

where $\{w_a; w_b\}$ are a pair of coefficients, can be manipulated first in the following way in order to project the whole linear combination into a spherical surface with center at the point $\mathbf{A}$ and radius R:

$$\begin{aligned}
&\chi_N(\mathbf{r}) = w_a \gamma_N(\alpha\,|\mathbf{r}-\mathbf{A}) + w_b \gamma_N(\beta\,|\mathbf{r}-\mathbf{A}+(\mathbf{A}-\mathbf{B})) \\
\Rightarrow\ &\chi_N(\mathbf{r}) = w_a \exp\left(-\alpha R^2\right) + w_b \exp\left(-\beta\left(R^2 + R_{AB}^2 + 2\left\langle(\mathbf{r}-\mathbf{A})^*(\mathbf{A}-\mathbf{B})\right\rangle\right)\right) \\
&\qquad = w_a \exp\left(-\alpha R^2\right) \\
&\qquad\quad + \left[w_b \exp\left(-\beta R_{AB}^2\right) \exp\left(-2\beta\left\langle(\mathbf{r}-\mathbf{A})^*(\mathbf{A}-\mathbf{B})\right\rangle\right)\right] \exp\left(-\beta R^2\right)
\end{aligned}$$

where: $R_{AB}^2 = |\mathbf{A}-\mathbf{B}|^2 = \left\langle(\mathbf{A}-\mathbf{B})^*(\mathbf{A}-\mathbf{B})\right\rangle$.

Indicating in this way that the holographic spherical surface centered at the point $\mathbf{A}$ can be used when projecting *both* GFs entering the linear combination. However, in the projected linear combination function, the coefficient of the second Gaussian will depend, unless both centers are coincident, on the scalar product of the position variable vector and the center of the second function, both translated to the origin of the first function. Such translation and subsequent manipulation can be considered applicable in the same way to any extra additional GF forming part of the linear combination.

2.6 The nature of the scalar product $\left\langle(\mathbf{r}-\mathbf{A})^*(\mathbf{A}-\mathbf{B})\right\rangle$

In order to develop the projection of a GF centered at a point: $\mathbf{B}(\neq \mathbf{A})$, clearly distinct from where the receiving projection spherical surface has the center, one can write without problems:

$$\begin{aligned}
\left\langle(\mathbf{r}-\mathbf{A})^*(\mathbf{A}-\mathbf{B})\right\rangle &= \langle \mathbf{r}-\mathbf{A}|\mathbf{A}-\mathbf{B}\rangle = -\langle \mathbf{r}_A|\mathbf{B}_A\rangle \\
&= -|\mathbf{B}_A|\,|\mathbf{r}_A|\cos\psi = -R_{AB}R\cos\psi;
\end{aligned}$$

where the angle ψ corresponds to the one subtended between the position vector $\mathbf{r}$ and the vector of the second GF center $\mathbf{B}$. Both vectors are supposed to be translated where the origin $\mathbf{A}$ of the projection spherical surface is. The angle ψ is invariant upon translation.

Therefore, one easily arrives to express the linear combination $\chi_N(\mathbf{r})$ as another one made with the two mono-dimensional Gaussian holograms:

$$\chi_2(R;\psi) = w_a \exp\left(-\alpha R^2\right) + \left[w_b \exp\left(-\beta R_{AB}^2\right) \exp\left([2\beta R_{AB}]\, R\cos\psi\right)\right] \exp\left(-\beta R^2\right)$$

Afterwards, one can try to average the variable coefficient of the second function over the subtended angle: ψ. Such an average[1] can be obtained using the following integral, providing in turn a zero-th order modified Bessel function:

$$\frac{1}{\pi}\int_0^\pi \exp\left([2\beta R_{AB}]\, R\cos\psi\right) d\psi = I_0\left([2\beta R_{AB}]\, R\right).$$

A modified Bessel function of this order can be easily defined and expressed by a power series [10] as:

$$I_0(z) = \frac{1}{\pi}\int_0^\pi \exp\left(\pm z\cos\psi\right) d\psi = 1 + \sum_{k=1}^{\infty}\left(\frac{z^k}{2^k k!}\right)^2.$$

In fact, the averaged second coefficient of the linear combination depends on the radius of the sphere with origin at the point **A**, the same position site as the center of the first GF. The final projected and averaged linear combination can be written in terms of the zero-th order modified Bessel function:

$$\chi_1(R) = w_a \exp\left(-\alpha R^2\right) + \left[W_b \exp\left(-\beta R_{AB}^2\right) I_0\left([2\beta R_{AB}]\, R\right)\right] \exp\left(-\beta R^2\right);$$

where $W_b \leftarrow k w_b$ and the constant k takes into account a general angular average.

In the case of dealing with multiple GFs linear combinations, one can proceed in the same way as in the two term case, transforming independently every function element, after choosing coherently the appropriate projection sphere origin. This is so, because this two GF linear combination development is equivalent to project a unique GF centered at some point **B** into a sphere surface centered at another point (which can be coincident) **A**.

If both centers are the same, the distance is null: $R_{AB} = 0$, and the hologram of the linear combination will simply become a linear combination of Gaussian holograms:

$$\chi_1(R) = w_a \exp\left(-\alpha R^2\right) + w_b \exp\left(-\beta R^2\right).$$

[1] The average can be made over the whole angular part of some spherical coordinates and will thus contribute with a constant factor k to the integral; for instance, in the three-dimensional case a multiplicative factor 2π has to be taken into account on the definition of the modified Bessel function.

3 The GHT and the ASA approximation

The results obtained above are general and can be applied into any GF environment. One of these Gaussian complicated combinations is associated to the so-called atomic shell approximation (ASA), see for example references [11–14].

The ASA approach idea is simple though: the electronic density of any atom can be represented, approximately but with high accuracy, as a linear combination of GFs, whose coefficients and exponents have been fitted to the *ab initio* atomic electronic density functions, computed at some basis set level. Apart of the papers commented before, one can download ASA functions for different background atomic basis sets from a public web depository, see reference [15]. Thus, one can write for a given atom an approximate shape function like:

$$\sigma_A(\mathbf{r}) = \sum_I w_I^A \gamma_I^A \left(\alpha_I^A \,|\mathbf{r}\right)$$

with the property: $\langle \sigma_A \rangle = \int_D \sigma_A(\mathbf{r}) dr = 1$. The coefficient set $\left\{w_I^A\right\} \subset \mathbf{R}^+$, by construction has been chosen positive definite.

Since the ASA atomic functions have diverse GFs centered at the same origin, it is obvious that the corresponding Gaussian hologram is just the linear combination of the individual GFs forming the ASA functions for every atomic center A. Such ASA hologram can be represented as:

$$\sigma_A(R) = \sum_{I \in A} w_I^A \gamma_{1;I}^A \left(\alpha_I^A \,|R\right)$$

However, the ASA functions are not the unique step in the context of such theoretical development, as the ASA shape functions can be employed in order to construct approximate electronic density functions for molecules under the so-called promolecular approximation. See, for instance, references [16–18] for a set modern application examples of such an approach. Thus, the ASA based promolecular functions can be written in general as:

$$\rho_M(\mathbf{r}) = \sum_{I \in M} Q_I^M \sigma_I \left(\mathbf{r} - \mathbf{A}_I\right)$$

where, the set $\{\mathbf{A}_I\}$ corresponds to the atomic Cartesian coordinates associated to molecule M; also calling N_M the number of electrons within the molecule M. The coefficients in the promolecular electronic density expression fulfill: $\left\{Q_I^M\right\} \subset \mathbf{R}^+ \wedge \sum_{I \in M} Q_I^M = N_M$. The coefficient set of the promolecular ASA density function can be chosen as the atomic numbers of the involved molecular atoms or alternatively, in a slightly sophisticated description they can be taken as atomic populations of arbitrary origin. In any of these circumstances, one has:

$$\langle \rho_M \rangle = N_M.$$

Thus, it is obvious that the promolecular ASA density holograms, once the projection sphere origin is chosen, will be easily obtained in terms quite similar to the one previously discussed, when a two term linear combination has been analyzed.

As the projections affect every GF entering the promolecular approach and can be considered independent one from another, accordingly the ASA in every atomic representation will appear with modified coefficients. To see this, suppose that the K-th atom has been chosen as origin for the hologram projection. Then, any of the ASA atomic contributions will become modified in the following sense:

$$\forall L \neq K : \sigma_L(R) = \sum_{I \in L} \left[w_I^L \exp\left(-\alpha_I^A R_{KL}^2\right) I_0\left(\left[2\alpha_I^L R_{KL}\right] R\right)\right] \exp\left(-\alpha_I^L R^2\right)$$

where R_{KL} is the distance between atoms K and L. The holographic promolecular contribution of the K-th atom has exactly the same form as the linear combination of two GF hologram previously presented.

4 Gaussian holograms in momentum space

Until this moment, the Gaussian holograms have been studied from a position space point of view. It is quite instructive to look at another simple example of the theoretical power present within Gaussian holography based on momentum space. Momentum space wave functions are scarcely used in quantum chemistry, but there exist quite well documented and excellent work on them, see for instance references [19,20].

4.1 Fourier transform

Before going deeper in the simple ideas which will be developed here, some fundamental and basic elements will be shown; in order that the readers could have fresh images and also that the notation used here could be set. It is well known that the Fourier integral transform procedure [21] within a three dimensional variable function set can be defined within a quantum mechanical scope [4,22] by means of:

$$F(\mathbf{p}) = (2\pi)^{-\frac{3}{2}} \int_D f(\mathbf{r}) \exp\left(-i \left\langle \mathbf{r}^* \mathbf{p} \right\rangle\right) d\mathbf{r},$$

where in this case: $\mathbf{r}$ and $\mathbf{p}$ are three-dimensional position and momentum vectors respectively; also i is the imaginary unit and D corresponds to the whole space three-dimensional domain.

4.2 Fourier transform of a normalized GF

When the function to be transformed via the Fourier transform above defined corresponds to a Minkowski normalized (or Euclidian normalized, which amounts the

same except for an exponent scale factor as it will be discussed later on) spherical GF centered at the point **A**, which can be written like:

$$\gamma_{M3}(\mathbf{r}) = \left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} \exp\left(-\alpha\left|\mathbf{r}-\mathbf{A}\right|^2\right) \rightarrow \left\langle \gamma_{M3}\left(\mathbf{r}\right)\right\rangle = \int\limits_D \gamma_{M3}(\mathbf{r})d\mathbf{r} = 1,$$

while the Euclidian normalized GF will be written as:

$$\gamma_{E3}(\mathbf{r}) = \left(\frac{2\alpha}{\pi}\right)^{\frac{3}{4}} \exp\left(-\alpha\left|\mathbf{r}-\mathbf{A}\right|^2\right) \rightarrow \left\langle \left|\gamma_{E3}\left(\mathbf{r}\right)\right|^2\right\rangle = \int\limits_D \left|\gamma_{E3}(\mathbf{r})\right|^2 d\mathbf{r} = 1$$

In the deductions given above, the inverse third power of the following well known integral [23]:

$$\iota_0(\alpha) = \int\limits_{-\infty}^{+\infty} \exp\left(-\alpha u^2\right)du = \left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}}$$

has been used in both Minkowski and Euclidian normalization cases.

Then, the Fourier transform of the Minkowski normalized GF above defined can be written in turn as:

$$\Gamma_{M3}(\mathbf{p}) = \left(\frac{\alpha}{2\pi^2}\right)^{\frac{3}{2}} \int\limits_D \exp\left(-\alpha\left[\left|\mathbf{r}-\mathbf{A}\right|^2 + \frac{i}{\alpha}\left\langle(\mathbf{r}-\mathbf{A})^*\,\mathbf{p}\right\rangle\right]\right)d\mathbf{r}$$

and can be furthermore rearranged (see, for example reference [24]) in order to yield:

$$\Gamma_{M3}(\mathbf{p}) = \left(\frac{\alpha}{2\pi^2}\right)^{\frac{3}{2}} \exp\left(-\frac{1}{4\alpha}\left|\mathbf{p}\right|^2\right) \int\limits_D \exp\left(-\alpha\left|(\mathbf{r}-\mathbf{A}) + \frac{i}{2\alpha}\mathbf{p}\right|^2\right)d\mathbf{r}.$$

The integral in the above equation, can be expressed [23] in turn as the third power of an integral like the used in the GF Minkowski norm above defined,using the triviality:

$$\int\limits_{-\infty}^{+\infty} \exp\left(-\alpha\left|x - A_x + \frac{i}{2\alpha}p_x\right|^2\right)dx \equiv \iota_0(\alpha)$$

and for the reason that the same result will be obtained for the pair of remaining coordinates y and z. Therefore, the Fourier transform of any spherical GF centered arbitrarily anywhere in space can be finally written as:

$$\Gamma_{M3}(\mathbf{p}) = \left(\frac{\alpha}{2\pi^2}\right)^{\frac{3}{2}} \exp\left(-\frac{1}{4\alpha}|\mathbf{p}|^2\right)\left(\frac{\pi}{\alpha}\right)^{\frac{3}{2}} = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \exp\left(-\frac{1}{4\alpha}|\mathbf{p}|^2\right),$$

$$\rightarrow \langle \Gamma_{M3}(\mathbf{p}) \rangle = \int_D \Gamma_{M3}(\mathbf{p}) d\mathbf{p} = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} (4\alpha\pi)^{\frac{3}{2}} = (2\alpha)^{\frac{3}{2}}$$

which conveniently divided by the above norm turns to be another Minkowski normalized momentum dependent GF, possessing a different exponent, which obviously is coincident with the scaled inverse of the original space defined GF:

$${}^{N}\Gamma_{M3}(\mathbf{p}) = \left(\frac{1}{4\alpha\pi}\right)^{\frac{3}{2}} \exp\left(-\frac{1}{4\alpha}|\mathbf{p}|^2\right)$$

4.3 Euclidean normalized Fourier transform

Alternatively, one can seek for the Euclidian normalized Fourier transform:

$$\Gamma_{E3}(\mathbf{p}) = \left(\frac{\alpha}{2\pi^3}\right)^{\frac{3}{4}} \int_D \exp\left(-\alpha\left[|\mathbf{r}-\mathbf{A}|^2 + \frac{i}{\alpha}(\mathbf{r}-\mathbf{A})\cdot\mathbf{p}\right]\right) d\mathbf{r}$$

which can be transformed into

$$\Gamma_{E3}(\mathbf{p}) = \left(\frac{\alpha}{2\pi^3}\right)^{\frac{3}{4}} \exp\left(-\frac{1}{4\alpha^2}|\mathbf{p}|^2\right)\left(\frac{\pi}{\alpha}\right)^{\frac{3}{2}} = \left(\frac{1}{2\alpha\pi}\right)^{\frac{3}{4}} \exp\left(-\frac{1}{4\alpha}|\mathbf{p}|^2\right)$$

$$\rightarrow \left\langle |\Gamma_{E3}(\mathbf{p})|^2 \right\rangle = \int_D |\Gamma_{E3}(\mathbf{p})|^2 d\mathbf{p} = \left(\frac{1}{2\alpha\pi}\right)^{\frac{3}{2}} (2\alpha\pi)^{\frac{3}{2}} = 1$$

$$\rightarrow {}^{N}\Gamma_{E3}(\mathbf{p}) = \left(\frac{1}{2\alpha\pi}\right)^{\frac{3}{4}} \exp\left(-\frac{1}{4\alpha}|\mathbf{p}|^2\right)$$

Then, the ratio between Minkowski and Euclidian normalized Fourier transforms of a GF correspond to a simple constant factor such that one can write:

$${}^{N}\Gamma_{M3} = \left(\frac{1}{8\alpha\pi}\right)^{\frac{3}{4}} {}^{N}\Gamma_{E3} \leftrightarrow {}^{N}\Gamma_{E3} = (8\alpha\pi)^{\frac{3}{4}} {}^{N}\Gamma_{M3}$$

4.4 Gaussian holograms in momentum space

After this simple introduction to GFs Fourier transforms from position to momentum space, one can say not very much about the result. Both GF kinds of space-momentum functions possess formally the same structure and just differ on the exponent and the normalization factor. The meaning of this situation is such that the Gaussian

holograms in momentum space can be easily obtained in a general fashion; being momentum space GFs origin centered Gaussian functions. Therefore, the ideas used in position space can be blueprinted in momentum space in a simpler manner. As GFs in momentum space turn to be origin centered GFs, thus, one can project them into a spherical surface, which can be *always* chosen centered at the origin independently of the associated quantum object being studied. Contrarily to position space, where the linear combinations of GFs centered at distinct points, when projected into the spherical surfaces turn to be with modified coefficients implying modified Bessel functions, in momentum space being all the Fourier transforms origin centered, linear combinations projected into a spherical surface centered at the origin will remain with invariant coefficients.

One can say that, complicated linear relationships of GFs in momentum space acquire simplest holographic forms than their position space counterparts.

Perhaps this means that momentum space wave and density functions based on GFs have a full holographic power, which is more difficult to construct in position space. Momentum wave or density functions can be considered in this manner prepared to become holograms.

5 Conclusions

As a consequence of the GHT described in this paper, it has been made evident that GFs both in position or momentum space can be easily projected into a spherical surface and can be thus transformed into Gaussian holograms. That is: simpler monodimensional variable GFs, which in turn contain information on any N-dimensional imaginable GF. Perhaps such a Gaussian holographic behavior may be interpreted as a general picture, indicating the existence of an intrinsic property associable to all submicroscopic systems.

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