J Math Chem (2013) 51:420–426
DOI 10.1007/s10910-012-0094-7

BRIEF COMMUNICATION

# Position-momentum Heisenberg uncertainty in Gaussian enfoldments of Euclidian space

**Ramon Carbó-Dorca**

Received: 10 April 2012 / Accepted: 21 September 2012 / Published online: 29 September 2012


**Abstract** Gaussian enfoldments have been derived from the form of general Gaussian functions centered at arbitrary positions in Euclidian space. Every point of Euclidian space acts in this way as the center of a Gaussian function defined in position space. Using the position-momentum Fourier transform in the quantum mechanical way and applied into the position functions of the Gaussian Euclidian enfoldment, the transform result provides a unique momentum Gaussian function, centered at the origin. In this way, the Euclidian enfoldment disappears in momentum space. Further analysis of the position-momentum relationship indicates that the product of the variances of the enfoldment in position and the corresponding momentum Fourier transform produces some kind of Heisenberg's uncertainty relation.

**Keywords** Gaussian enfoldments in Euclidian spaces · Heisenberg position-momentum uncertainty · Position-momentum Fourier transform · Gaussian functions · Density functions

## 1 Introduction

Not long ago, the concept of Gaussian enfoldment in $N$-dimensional Euclidian space and its geometrical structure was studied [1,2]. Such a previous research was associated to Gaussian functions, because they are everywhere present in modern quantum chemistry, successfully employed mainly as GTO basis functions, since Boys [3] proposed them and Shavitt [4] backed them up 10 years later. Later on GTO basis sets have been submitted to an ever growing interest which still is not decaying in present times. Also, since the starting point of quantum similarity [5], in current studies, see

R. Carbó-Dorca (✉)
Institut de Química Computacional, Univ. de Girona, 17071 Girona, Catalonia, Spain
e-mail: quantumqsar@hotmail.com

for example [6–8], the approximate density functions are obtained basically via the atomic shell approximation (ASA) framework [9–13] developed in our laboratory and essentially relying on linear combinations of 1s type GTO. On the other hand, the vast presence of Gaussian functions in computational quantum chemistry stimulated the interest of my laboratory, and recently produced a line of several related studies about characteristic properties of Gaussian functions [14–18]. The enfoldment concept [1] was a consequence of this line of work.

Following such Gaussian functions research path, it appeared interesting to consider the possibility to apply Fourier transforms to the position enfoldment framework, in order to arrive from a quantum mechanical point of view to a corresponding momentum panorama. While structuring the task of transforming position enfoldments to momentum space, it appeared in the author's mind the possibility of obtaining an enfoldment position-momentum uncertainty relation. These research options constitute the basic scheme and objective of the present study.

Furthermore, as presented here, this kind of research leading to a particular scheme of position-momentum uncertainty, can be also connected with previous studies performed on basic quantum mechanical elements of knowledge, based on employing specific simple geometrical conceptions of space. These studies lead to the description of Heisenberg uncertainty [19,20], the setup of the Schrödinger equation [20] and the analysis of the Einstein-Podolsky-Rosen paradox [21,22]. Considering this alternative line of work on basic concepts deduced from space geometry properties, one can say that the present paper objective can be also partially connected to this specific line of thought.

Finally, it can be said that the unpretentious mathematical development of this work can be used as to illustrate with a practical simple case the position-momentum interchangeable descriptions and the Heisenberg uncertainty principle as well. In this manner both concepts might be also taught without effort to quantum chemistry students.

## 2 Heisenberg uncertainty in a simple Gaussian picture

Using the ideas of the enfoldment structure earlier described [1], one can start with a Minkowski normalized position GTO, centered at an arbitrary three dimensional Euclidian point $\mathbf{R}$:

$$\gamma_{S3}(\mathbf{r}) = \left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} \exp\left(-\alpha\left|\mathbf{r}-\mathbf{R}\right|^2\right) \rightarrow \langle\gamma_{S3}(\mathbf{r})\rangle = \int_D \gamma_{S3}(\mathbf{r})\, d\mathbf{r} = 1. \tag{1}$$

The Minkowski normalized Fourier transform [23] of the function (1), following a suggestion of Messiah to include the Planck constant [24], can be written as, see for more details Appendix 1:

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

The momentum enfoldment (2) appears to be independent of the previous Gaussian centers of the corresponding position enfoldment. This is a typical characteristic of the quantum mechanical description in momentum space, see for example [25,26], where functions attached to molecular structures loose the atomic centers, at least under the usual Born-Oppenheimer approach. On the other hand, the Gaussian functions (1) and (2) appearing in this work, being Minkowski normalized, might also be associated to probability density distributions.

## 2.1 Position and momentum variances

Hence, both functions can be used to represent quantum particles in a quite simplified way. Then, it is sound to use them as such to obtain expectation values in the usual statistical point of view. The variance of position and momentum, associated to both Gaussian functions can be easily written via the expectation value integrals, attached to position and momentum mean values:

$$\left\langle |\mathbf{r}-\mathbf{R}|^2 \right\rangle = \left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} \int_D |\mathbf{r}-\mathbf{R}|^2 \exp\left(-\alpha\, |\mathbf{r}-\mathbf{R}|^2\right) \mathrm{d}\mathbf{r} \tag{3}$$

and

$$\left\langle |\mathbf{p}|^2 \right\rangle = \left(\frac{1}{4\hbar\alpha\pi}\right)^{\frac{3}{2}} \int_D |\mathbf{p}|^2 \exp\left(-\frac{1}{4\hbar\alpha}\, |\mathbf{p}|^2\right) \mathrm{d}\mathbf{p} \tag{4}$$

both expectation values (3) and (4) being related to products of the monovariate integral:

$$\int_{-\infty}^{+\infty} x^2 e^{-ax^2} dx = \frac{1}{2a}\left(\frac{\pi}{a}\right)^{\frac{1}{2}}.$$

Taking this into account, the expectation values (3) and (4) can be easily written as:

$$\left\langle |\mathbf{r}-\mathbf{R}|^2 \right\rangle = \frac{3}{2\alpha}$$

For position variance and therefore in the same way for momentum variance:

$$\left\langle |\mathbf{p}|^2 \right\rangle = 6\hbar\alpha.$$

### 2.2 Heisenberg uncertainty and the product of position-momentum variances

Consequently, the product of both variances permits to finally write the relation:

$$\left\langle |\mathbf{r}-\mathbf{R}|^2 \right\rangle \left\langle |\mathbf{p}|^2 \right\rangle = 9\hbar, \tag{5}$$

which corresponds somehow to a Heisenberg uncertainty principle for a particle described in a Gaussian three-dimensional Euclidian enfoldment. The factor 9 affecting the Planck constant has to be associated to the square of the attached working spaces dimension. It will transform into $N^2$ if the space dimension was modified into a $N$th dimension.

The meaning of this result as appearing in Eq. (5) might be understood as follows. When it is wanted a sharper[1] particle density description, associated to the position Gaussian function, then it can be taken into account that as $\alpha \to \infty$ the particle sharpness will grow, until being transformed into a completely localized point-like one, defined by a pulse function, as reaching this situation, the Gaussian function will become a Dirac function as well. However, as sharper becomes the particle in position space, softer becomes the particle in momentum space as: $\alpha \to \infty \Rightarrow \alpha^{-1} \to 0$, and at this situation the momentum Gaussian function transforms into a flat uniform distribution function. The product (5) of the respective position-momentum variances becomes indefinite, when the particle is confined into a precise space position **R**, in agreement with the position-momentum Heisenberg indetermination principle.

### 2.3 Kinetic energy of an enfolded particle

Moreover, the integral result of the position-momentum variances, taking into account different factors, can be associated to the kinetic energy of a particle, described by the density function, represented in turn both by the Gaussian enfoldment (1) or the Fourier transform (2). Then, one can write in atomic units:

$$K = 2\alpha^2 \left\langle |\mathbf{r}-\mathbf{R}|^2 \right\rangle = \frac{1}{2} \left\langle |\mathbf{p}|^2 \right\rangle = 3\alpha. \tag{6}$$

It is interesting to note that sharper the position function will be, larger will grow the kinetic energy computed with the above resultant expression (6), in either position or momentum spaces. Again, the factor 3 corresponds to the considered space dimension and will become $N$ in case of $N$-dimensional spaces.

[1] *Sharper* is used here in the sense of the particle being more localized around the Euclidean point, associated to the position **R**. The possible particle position delocalization will be referred as producing a *softer* particle.

## 3 Gaussian enfoldment and uncertainty

The Minkowski normalized Gaussian function (1) employed as starting point for this discussion has been also employed to define a Euclidian enfoldment space [1], where at every point $\mathbf{R}$ a well-defined Gaussian function of type (1) is centered. The interesting consequence within this geometrical picture contains the fact that the above proposed Fourier transform in the form of the Gaussian function embodied in Eq. (2), also represents the whole enfoldment structure which becomes transformed into a unique function in momentum space. The Fourier transform process provides a unique Gaussian function of the kind (2) as a result, where the enfoldment structure which can be observed in position space is lost. The result resembles the linear combination of the enfoldment functions studied in reference [1], providing a unique Gaussian centered at the position origin, instead of the momentum origin as the function (2) appears to be. Such a situation is clearly associated to the position-momentum uncertainty.

A position three-dimensional enfoldment provided by the Gaussian function (1) corresponds to a completely soft position description of a particle, as any center $\mathbf{R}$ can be chosen to consider the particle centered at the same footing, being Euclidian spaces isotropic. However, the associated Fourier transform momentum Gaussian function (2) of the enfoldment, corresponds to a unique precise origin centered momentum location, at $\mathbf{P} = \mathbf{0}$, say.

A momentum enfoldment might be also defined in the same way as has been done in position space. As a result, the associated position space Fourier transform will provide a unique Gaussian function centered at $\mathbf{R} = \mathbf{0}$. To see how such a reverse situation appears, one only needs to consider the inverse Fourier transform, for example defined according to Messiah [24] as:

$$f(\mathbf{r}) = (2\pi\hbar)^{-\frac{3}{2}} \int_D F(\mathbf{p}) \exp\left(+i\hbar^{-1} \langle \mathbf{r} * \mathbf{p} \rangle\right) d\mathbf{p}$$

which can be performed over a momentum Euclidian space enfoldment, defined like:

$$\gamma_{M3}(\mathbf{p}) = \left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} \exp\left(-\alpha\,|\mathbf{p} - \mathbf{P}|^2\right) \rightarrow \langle \gamma_{M3}(\mathbf{p}) \rangle = \int_D \gamma_{M3}(\mathbf{p})\, d\mathbf{p} = 1,$$

yielding an origin centered position space unique Gaussian function.

## 4 Conclusions

Fourier transform of the Gaussian enfoldment in Euclidian spaces furnish the possibility to describe some kind of Heisenberg uncertainty relation. It can be taken as a simple consequence of the geometry of enfolded space and yet as some application of the simple statistical concept of variance obtained as an expectation value.

**Appendix 1:**

Fourier transforms of position-momentum Gaussian functions.

It is well known that the Fourier integral transform procedure [23], within a three dimensional variable function set, can be defined under a quantum mechanical scope by means of including the Planck constant $\hbar$ as Messiah suggested [24]:

$$F(\mathbf{p}) = (2\pi\hbar)^{-\frac{3}{2}} \int_D f(\mathbf{r}) \exp\left(-i\hbar^{-1} \langle \mathbf{r} * \mathbf{p} \rangle\right) d\mathbf{r},$$

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

Fourier transform of a Minkowski normalized Gaussian function

When the function to be transformed via the Fourier transform, corresponds to a Minkowski normalized spherical Gaussian function centered at the point $\mathbf{R}$, which can be written like:

$$\gamma_{S3}(\mathbf{r}) = \left(\frac{\alpha}{\pi}\right)^{\frac{3}{2}} \exp\left(-\alpha |\mathbf{r} - \mathbf{R}|^2\right) \rightarrow \langle \gamma_{S3}(\mathbf{r}) \rangle = \int_D \gamma_{S3}(\mathbf{r})\, d\mathbf{r} = 1,$$

then, the above defined Fourier transform of the Minkowski normalized Gaussian function can be alternatively written as:

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

The integral in the above equation, can be expressed in turn as the third power of an integral like the used in the Gaussian function Minkowski norm also above defined. Therefore, the Fourier transform of any spherical Gaussian function centered arbitrarily anywhere in space can be finally written as:

$$\begin{gathered}\Gamma_{M3}(\mathbf{p}) = \left(\tfrac{\alpha}{2\hbar\pi^2}\right)^{\frac{3}{2}} \exp\left(-\tfrac{1}{4\hbar\alpha} |\mathbf{p}|^2\right) \left(\tfrac{\pi}{\alpha}\right)^{\frac{3}{2}} = \left(\tfrac{1}{2\hbar\pi}\right)^{\frac{3}{2}} \exp\left(-\tfrac{1}{4\hbar\alpha} |\mathbf{p}|^2\right) \\ \rightarrow \langle \Gamma_{M3}(\mathbf{p}) \rangle = \int_D \Gamma_{M3}(\mathbf{p})\, d\mathbf{p} = \left(\tfrac{1}{2\hbar\pi}\right)^{\frac{3}{2}} (4\hbar\alpha\pi)^{\frac{3}{2}} = (2\alpha)^{\frac{3}{2}}\end{gathered},$$

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

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

## References

1. E. Besalú, R. Carbó-Dorca, J. Math. Chem. **49**, 2231 (2011)
2. R. Carbó-Dorca, E. Besalú, J. Math. Chem. **49**, 2244 (2011)
3. S.F. Boys, Proc. R. Soc. (Lond.) A **200**, 542 (1950)
4. I. Shavitt, Method Comput. Phys. **2**, 1 (1963)
5. R. Carbó, L. Leyda, M. Arnau, Int. J. Quant. Chem. **17**, 1185 (1980)
6. P. Bultinck, X. Gironés, R. Carbó-Dorca, in *Rev. Comput. Chem.*, vol. 21, eds. by K.B. Lipkowitz, R. Larter, T. Cundari (Wiley, Hoboken, USA, 2005), pp. 127–207
7. R. Carbó-Dorca, A. Gallegos, in *Quantum Similarity and Quantum QSPR (QQSPR) Entry: 176*, vol. 8, eds. by Meyers, R. Encyclopedia of complexity and systems science (Springer, New York, 2009), pp. 7422–7480
8. R. Carbó-Dorca, E. Besalú, L.D. Mercado, J. Comput. Chem. **32**, 582 (2011)
9. P. Constans, R. Carbó, J. Chem. Inf. Comput. Sci. **35**, 1046 (1995)
10. P. Constans, X. Fradera, Ll. Amat, R. Carbó, in *Quantum Molecular Similarity Measures (QMSM) and the Atomic Shell Approximation (ASA) in Proceedings of the 2nd. Girona Seminar on Molecular Similarity*. July 1995. Advances in Molecular Similarity, vol. 1 (JAI PRESS INC., Greenwich (Conn.), 1996), p. 187.
11. Ll. Amat, R. Carbó-Dorca, J. Comput. Chem. **18**, 2023 (1997)
12. Ll. Amat, R. Carbó-Dorca, J. Comput. Chem. **20**, 911 (1999)
13. R. Carbó-Dorca, E. Besalú, J. Math. Chem. **50**, 981 (2012)
14. R. Carbó-Dorca, E. Besalú, J. Math. Chem. **48**, 914 (2010)
15. R. Carbó-Dorca, E. Besalú, J. Comput. Chem. **31**, 2452 (2010)
16. R. Carbó-Dorca, E. Besalú, J. Math. Chem. **49**, 836 (2011)
17. E. Besalú, R. Carbó-Dorca, J. Math. Chem. **49**, 1769 (2011)
18. R. Carbó-Dorca, E. Besalú, EMP as a similarity measure: a geometric point of view. IQC technical report TR-2012-9, J. Math. Chem. doi:10.1007/s10910-012-0089-4
19. R. Carbó-Dorca, J. Math. Chem. **36**, 41 (2004)
20. R. Carbó-Dorca, J. Math. Chem. **38**, 89 (2005)
21. R. Carbó-Dorca, J. Math. Chem. **39**, 267 (2006)
22. R. Carbó-Dorca, J. Math. Chem. **41**, 209 (2007)
23. I.M. Vinogradov (ed.), *Encyclopaedia of Mathematics*, vol. 4 (Kluwer, Dordrecht, 1989)
24. A. Messiah, *Mècanique Quantique* (Tome I, Dunod, Paris, 1959), pp. 90, 400–401
25. P. Kaijsser, V.H. Smith Jr., Adv. Quantum. Chem. **10**, 37 (1977)
26. A. Thakkar, Adv. Chem. Phys. **128**, 303 (2004)