

# Electron and Positron Scattering by Non-Central Potentials: Matrix Elements and Symmetry Properties in the First Born Approximation

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## Abstract

The Fourier transform of Cartesian Gaussian functions product is presented in the light of positron scattering. The calculation of this class of integrals is crucial in order to obtain the scattering amplitude in the first Born approximation framework for an *ab initio* method recently proposed. A general solution to the scattering amplitude is given to a molecular target with no restriction due to symmetry. Moreover, symmetry relations are presented with the purpose of identifying terms that do not contribute to the calculation for the molecules in the  $D_{\infty h}$  point group optimizing the computational effort.

**Keywords** — Positron and electron scattering, Fourier transform of the Gaussian product theorem, McMurchie-Davidson procedure, Obara-Saika procedure, linear molecules .

## Introduction and Motivation

The modeling of many physical and astrophysical environments demand the knowledge of positron (or electron) scattering cross sections by atoms and molecules. Electron cross sections are essential to model the energy deposition in planetary (Gan & Cravens, 1992; Fox et al., 2008) and stellar atmospheres (Jeffrey et al., 2019) for example. On the other hand, positrons show a crucial role in supernovae (missing citation) and in the central region of the Milky Way (Johnson III et al., n.d.). Moreover, one of the main problems is the electron and positron dynamics with biomolecules (Sanche, 2005) and biological environments (Champion, n.d.; (missing citation) with emphasis on DNA basis (missing citation); Mokrani et al., 2020). Even the positron thermalization dynamics with  $N_2$  gas is still an open problem (missing citation).

When a set o high energy positron (or electron) molecule cross sections are needed for some specific application, the most basic way to attack the problem is through the Independent Atom Model (IAM) (Massey et al., 1969). The IAM approach ignores multiple scattering and the chemical bond effects. Nonetheless, it is an easy-to-implement method that allows one to learn the basics with no great computational effort.

If one wishes to go beyond the simplistic IAM approximation, an elastic scattering calculation in first Born approximation (FBA) considering a genuine molecular wavefunction may be an adequate line of action. In the elastic scattering process, there is only momentum transfer between target and projectile, with no change in the quantum states. The FBA predicts reliable results at high energies where the target polarization is expected to be negligible. In this context, electron and positron cross sections are expected to be the same (Kauppila & Stein, 1989). The high energy region is also suitable for computational debugging since *ab initio*, model potential and IAM calculations must provide the same results. In this context, once a model for the molecular wavefunction is defined, the main issue is the non-central nature of the scattering potential.

Electron-molecule calculations performed in the FBA are definitely not new in literature. One can find the rovibrational calculation of Carson (Carson, 1954) performed with a model potential, the elastic and vibrational scattering calculation of Ford and Browne (Ford & Browne, 1973) where a Taylor expansion for the momentum transfer is adopted in order to simplify the evaluation of the matrix elements, followed by the works of Liu (Liu & Smith, 1973; Liu, 1985) using more sophisticated representations for the molecular target. The closest work to the one presented here is the calculations of Rescigno *et al.* (Rescigno *et al.*, 1975) except for the fact that these authors treat the Born calculation as a correction scheme to the T-matrix approach. This article is devoted to clarify, as the title propose, the matrix elements and symmetry considerations involved in electron and positron scattering calculations by non-central potentials in the FBA employing Cartesian Gaussian Functions (CGF's). The main challenge in the calculation of the matrix elements involves the incident particle and the spatial orbital of the molecular system integration, the last one deserves spacial attention due to its mathematical representation.

In the quantum chemistry research, the mathematical description of atomic orbitals have been studied mainly with the use of Slater (Slater, 1930; Bouferguene *et al.*, 1996) and Gaussian functions (Gill, 1994; Fernndez Rico *et al.*, 2001; Magalhes, 2014). The Slater function has the correct cusp at the origin and the physical exponential decay at long range (Kato, 1957; Liu, 2006), expected by the orbital representation, nevertheless, when a many-electron system is taken into account, the matrix elements become very hard to calculate in the coordinate space (Fernndez Rico *et al.*, 2001). On the other hand, in the Gaussian representation, the well known Gaussian product theorem allows one to reduce two Gaussian functions of different centers to a single one with well defined new center. Moreover, the integrals involving this type of function have analytic solution (Gill *et al.*, 1989; Gill & Pople, 1991). Furthermore, the same accuracy in the representation of the orbital can be expected when Gaussian functions are considered, however one might need to use a larger number of them (Shaw, 2020).

There are several applications that involve the integration of molecular integrals with Gaussian basis functions, for example, the calculation of magnetic field density (Cassam-Chena, 2001), structure factors in quantum crystallography (Genoni, 2020), positron and electron scattering (Čársky *et al.*, 1996; Tachikawa, 2001; rsky, 2007), molecular magnetic properties (Kiribayashi *et al.*, 1999), density functional theory (Mazur *et al.*, 2016), relativistic quantum electrodynamics (Grant & Quiney, 2000) and electronic dynamics (Kuchitsu *et al.*, 2009).

The computation of the Fourier transform of the Gaussian product has been investigated and several techniques have been introduced throughout the years, nonetheless two main approaches became widely used in literature. In the one based in the McMurchie-Davidson procedure (McMurchie & Davidson, 1978), the integrand of the Fourier transform is written in terms of Hermite Gaussian functions. Then, the Fourier transform is evaluated and the result can be expressed by a recurrence relation that involves the binomial product and the Hermite polynomials (Johnson *et al.*, 1991; Doll *et al.*, 2001). Another important procedure is the Obara-Saika approach (Obara & Saika, 1986; Obara & Saika, 1988) where the Fourier transform is evaluated and a recurrence formula is elaborated with the intention of writing the integral as a function of other ones of lower angular momenta (Bracken & Bartlett, 1997; Grabowsky *et al.*, 2020).

Recently, we have developed an *ab initio* model to evaluate the elastic cross sections of diatomic homonuclear molecules by positron and electron impact in the FBA framework. In this model, the molecular wavefunction is obtained by the unrestricted Hartree-Fock (UHF) procedure, where the molecular spatial orbitals are represented by a linear combination of CGF's. At the moment, the interaction of the incident particle and the molecular target is described by the electrostatic potential.

Due to the *ab initio* nature of the proposed model, combined with the non-central Coulomb potential, the calculation of the scattering amplitude demands the evaluation of several matrix elements involving the Fourier transform of product of Gaussian functions. A known fact is that with the increase of angular quantum number of the Gaussian functions used, the number of terms from the Fourier transform (Reine *et al.*, 2012; Tian *et al.*, 2021) rapidly grow. In the present work, we display the integration procedure involving the calculation of the scattering amplitude using an approach close to the McMurchie-Davidson

one. The integral results are exhibited in an explicit manner in order to visualize useful symmetry properties regarding the scattering amplitude. These are due to the product of the expansion coefficients of the molecular wavefunction obtained in the UHF formulation with the Fourier transform output.

This paper is organized as follows: The scattering model is summarized in section to set the background of the calculation; In section the CGF notation is given; The electronic scattering amplitude is discussed in section for an arbitrary symmetry system; In section the symmetry properties for the diatomic homonuclear molecules are presented and discussed; In section we acknowledge our final comments and conclusions. Atomic units (a.u.) are used in this paper unless stated otherwise.

## Basic Mathematical Definitions of the Scattering Model

Since the focus of this paper is the evaluation of the matrix elements involving CGF, the scattering model will be briefly described in order to exclusively bring the necessary information to understand the scope of this work. The physical background of the proposed model and results are addressed in a dedicated paper.

From the quantum scattering theory, the scattering amplitude in the FBA is given by

$$\mathcal{F}(\vec{k}_f, \vec{k}_i) = -\frac{1}{2\pi} S_{\vec{k}_f} \hat{V} S_{\vec{k}_i}, \quad (1)$$

where the homogeneous solution in the Born-Oppenheimer approximation,  $S_{\vec{k}} = \Phi_0^{nuc}(\vec{R}_A) \otimes \phi_0(\vec{s}_N) \otimes \vec{k}$ , includes the nuclear ( $\Phi_0^{nuc}(\vec{R}_A)$ ), electronic ( $\phi_0(\vec{s}_N)$ ) and incident particle ( $\vec{k}$ ) wavefunctions. The interacting potential is the electrostatic one, which is given in atomic units by  $V = q \sum_{A=1}^M \frac{Z_A}{|\vec{x}-\vec{R}_A|} - q \sum_{e=1}^N \frac{1}{|\vec{x}-\vec{r}_e|} = V_{nuc} + V_{elec}$ . With these considerations, it is possible to evaluate the nuclear and electronic scattering amplitudes separately. The scattering amplitude regarding the electronic part is the focus of this work, since the Gaussian functions do not appear in the nuclear counterpart. That being considered, it is possible to write the electronic amplitude for positron scattering as:

$$\mathcal{F}_{elec} = \frac{1}{2\pi} \int d^3\vec{x} e^{-i(\vec{k}_f - \vec{k}_i) \cdot \vec{x}} \sum_u \int d^3\vec{r} \psi_u^*(\vec{r}) \frac{1}{|\vec{x} - \vec{r}|} \psi_u(\vec{r}), \quad (2)$$

where the position vectors  $\vec{x}$  and  $\vec{r}$  are related to the positron and the molecular electrons, respectively. The incident wave vector is represented by  $\vec{k}_i$  and the scattered one by  $\vec{k}_f$ . The molecular wavefunction, obtained by the UHF calculation, is expressed by the molecular orbitals  $\psi_u$ , where the  $u$  label stands for the occupied orbital.

It is important to notice that the  $\vec{r}$  space integral in the amplitude (2) resembles a trivial electron repulsion integral (ERI) commonly found in molecular structure. However, the Coulomb potential involves the incident particle coordinate  $\vec{x}$ . Therefore, common techniques for the evaluation of ERI do not apply.

The Coulomb potential can be rewritten using the following (Taketa et al., 1966) relation:

$$\frac{1}{|\vec{x} - \vec{r}|} = \frac{1}{2\pi^2} \int \frac{d^3\vec{p}}{p^2} e^{i\vec{p} \cdot \vec{x}} e^{-i\vec{p} \cdot \vec{r}}.$$

(3)

The expression (3) enables one to split the dependence in  $\vec{r}$  and  $\vec{x}$  of the interacting potential. On the other hand, a new integration arises related to the auxiliary vector  $\vec{p}$ . This vector has no physical meaning and it is only a mathematical tool to support the calculation of the integral.

When the equality (3) is applied in the scattering amplitude (2), the definition of the Dirac delta function appears in the integration of the positron coordinates  $\vec{x}$ :

$$\int d^3\vec{x} e^{i[\vec{p}-(\vec{k}_f-\vec{k}_i)]\cdot\vec{x}} = (2\pi)^3\delta^3[\vec{p}-(\vec{k}_f-\vec{k}_i)].$$

(4)

Rearranging the terms of the amplitude, the sifting property of the delta can be applied considering the integration in the auxiliary vector. Therefore, the resulting amplitude takes the form:

$$\mathcal{F}_{elec} = \frac{2}{(\vec{k}_f - \vec{k}_i)^2} \sum_u \int d^3\vec{r} e^{-i(\vec{k}_f - \vec{k}_i)\cdot\vec{r}} \psi_u^*(\vec{r}) \psi_u(\vec{r}).$$

(5)

In order to obtain a solution to the amplitude, the integration over the spatial orbitals must be evaluated. Thus, a suitable mathematical representation to these molecular orbitals is desired. An interesting fact about this expression is that the entire term in the sum of  $u$  can be related to the well known form factors (Hubbell et al., 1975; Frishberg, 1986) found in literature.

## Cartesian Gaussian Functions as Spatial Orbitals and notation

With the purpose of representing the molecular wavefunction, the linear combination of atomic orbitals (LCAO's) is employed (Mintmire, 1979). In a molecule, the  $T$ -th atomic center has space coordinate  $\vec{R}_T$ . Since we use Gaussian functions to represent each atomic orbital, these will also be centered at  $\vec{R}_T$ . Within the LCAO's framework, the molecular orbital  $\psi_u$  can be represented by

In this expansion the  $\mu$  label represents any general type of Gaussian function. In addition, each S, P, D and F type CGF is related to the Greek letters  $\sigma$ ,  $\Pi$ ,  $\Delta$  and  $\phi$ , respectively.

The molecular wavefunction used in this model is obtained by the UHF method procedure, such that the expansion coefficients  $\{C_{u\mu}^T\}$  in the spatial orbital (??) are optimized values to represent the ground state

of the molecule. Such coefficients must not be confused with contraction ones, after all, at the moment, we are using uncontracted CGF's.

The normalized CGF are generally written (Taketa et al., 1966; Gill & Pople, 1991) as

$$\mathcal{G}(\vec{R}_T; \vec{r}) = \mathcal{N}(\epsilon, l, m, n) (x - X_T)^l (y - Y_T)^m (z - Z_T)^n e^{-\epsilon|\vec{r}-\vec{R}_T|^2}, \quad (6)$$

where  $\mathcal{G}(\vec{R}_T; \vec{r})$  is centered at  $\vec{R}_T = X_T\hat{x} + Y_T\hat{y} + Z_T\hat{z}$  and has angular quantum number  $\mathcal{L} = l + m + n$ . The normalization  $\mathcal{N}$  is a function of the Gaussian exponent  $\epsilon$  and the angular momentum quantum number components:

$$\mathcal{N}(\epsilon, l, m, n) = \left[ \frac{2^{2(l+m+n)+\frac{3}{2}} \epsilon^{l+m+n+\frac{3}{2}}}{(2l-1)!!(2m-1)!!(2n-1)!! \pi^{\frac{3}{2}}} \right]^{\frac{1}{2}}. \quad (7)$$

Since we are using CGF, the angular quantum number gives us information about the symmetry of the Gaussian-type orbital (GTO). For S type functions the angular quantum number is equal to zero ( $\mathcal{L} = 0$ ), and there is only one combination of  $l$ ,  $m$  and  $n$  that leads to this result. Therefore, each S type Gaussian function generates only one orbital, and such orbital has spherical symmetry. It could be said that a S-type function, due to the fact that  $\mathcal{L} = 0$ , has only one projection which is a S-GTO.

In the case of P type functions, where the angular quantum number is equal to one ( $\mathcal{L} = 1$ ), there are three different combinations of  $l$ ,  $m$  and  $n$ , *i.e.*, three projections. Hence, each P type Cartesian Gaussian function produces three distinct GTO with axial symmetry referred here as  $\Pi_x$ ,  $\Pi_y$  and  $\Pi_z$ . With that in mind, it makes more mathematical and computational sense to rewrite the labels related to the Gaussian type incorporating their projections explicitly:

$$\sum_{\Pi=1}^{\#P} C_{u \Pi}^T \mathcal{G}_{\Pi}(\vec{R}_T; \vec{r}) \xrightarrow{\Pi \rightarrow \Pi_i} \sum_{\Pi=1}^{\#P} \sum_{i=1}^3 C_{u \Pi_i}^T \mathcal{G}_{\Pi_i}(\vec{R}_T; \vec{r}). \quad (8)$$

The same procedure is applied to higher angular quantum numbers, as shown in table 1 with the respective  $\frac{(\mathcal{L}+2)!}{2(\mathcal{L})!}$  projections. Thus, using the summation to distinguish the projections related to the specific angular quantum number of each CGF the spatial orbital is represented by:

Table 1: Notation of the spatial orbitals with the projections of the Cartesian Gaussian function explicitly written, considering the summation in the index  $i, j$  and  $k$  related to the Cartesian components, *i.e.*,  $1 = x$ ,  $2 = y$  and  $3 = z$ .

Angular quantum number	Projection	Notation	Normalization relation
S type ( $\mathcal{L} = 0$ )	$\sigma$	$\sigma \rightarrow \sigma$	$N$
P type ( $\mathcal{L} = 1$ )	$\Pi_x, \Pi_y$ and $\Pi_z$	$\Pi \rightarrow \sum_{i=1}^3 \Pi_i$	$N_x = N_y = N_z$
D type ( $\mathcal{L} = 2$ )	$\Delta_{xx}, \Delta_{yy}, \Delta_{zz}, \Delta_{xy}, \Delta_{xz}$ and $\Delta_{yz}$	$\Delta \rightarrow \sum_{i=1}^3 \sum_{j \geq i}^3 \Delta_{ij}$	$N_{xx} = N_{yy} = N_{zz}$ $N_{xy} = N_{xz} = N_{yz}$
F type ( $\mathcal{L} = 3$ )	$\phi_{xxx}, \phi_{yyy}, \phi_{zzz}, \phi_{xxy}, \phi_{xxz}, \phi_{xyy}, \phi_{xzz}, \phi_{yyz}, \phi_{yzz}$ and $\phi_{xyz}$	$\phi \rightarrow \sum_{i=1}^3 \sum_{j \geq i}^3 \sum_{k \geq j}^3 \phi_{ijk}$	$N_{xyz}$ $N_{xxx} = N_{ijk} \delta_{ij} \delta_{ik}$ $N_{xxy} = N_{ijk} \delta_{jk}$

The aforementioned observations are important in order to simplify the integral solutions and are helpful to a computational implementation. This procedure allows one to identify the coefficients that produce terms that do not contribute to the scattering amplitude. It is important to notice that, even these terms cancel each other, in the calculation, they are evaluated, and depending of the complexity of the systems, it might consume time and computational power.

It is important to observe that the normalization (7) is also separate in order to reflect the related projection of the functions. In a few cases the normalization of the projections have the same value, however for D and F type functions some differences arise, as shown in table 1.

## scattering amplitude in the first born approximation

With the purpose of solving the electronic amplitude (5), one must consider the spatial orbital (??) along with its complex conjugate. Consequently, several integrals will arise due to the product of these spatial orbitals,

$$(9) \quad \int d^3\vec{r} e^{-i\vec{\xi}\cdot\vec{r}} \mathcal{G}_\mu(\vec{R}_T; \vec{r}) \mathcal{G}_\nu(\vec{R}_Q; \vec{r}),$$

where  $\vec{\xi} = \vec{k}_f - \vec{k}_i$  is the momentum transfer vector, used here to simplify the notation, and  $\mu$  and  $\nu$  are employed to represent a generic type of CGF. One of the reasons to apply these functions (instead of slater ones) is the Gaussian product theorem (Shaw, 2020), as commented before. In the light of this theorem, two non-concentric CGF can be written as a new CGF centered at a point between the two original functions.

To set up a general line of reasoning, let us consider a Gaussian function  $\mathcal{G}_\mu(\vec{R}_T; \vec{r})$  as defined in (6). In the same manner, a second CGF  $\mathcal{G}_\nu(\vec{R}_Q; \vec{r})$  localized at  $\vec{R}_Q = X_Q\hat{x} + Y_Q\hat{y} + Z_Q\hat{z}$  and with all other properties denoted by the  $\nu$  index. The product of these CGF's yields a new one centered at

$$\vec{P} = \frac{\epsilon_\mu \vec{R}_T + \epsilon_\nu \vec{R}_Q}{\epsilon_\mu + \epsilon_\nu},$$

(10)

and the product has the form:

The polynomial product  $(x - X_T)^{l_\mu}(x - X_Q)^{l_\nu}$  can be expressed considering the binomial theorem. It allows one to rewrite such product as a function of  $(x - P_x)$  being suitable to the evaluation of the integral. In order to do so, the position vector  $\vec{P}$  of the new CGF must be embedded in the polynomial product. It can be done simply expressing the terms as:  $(x - X_T)^l = ((x - P_x) + (P_x - X_T))^l = ((x - P_x) + (\overline{PT})_x)^l$ . This will result in one term that does not depend on the integration coordinate  $\vec{r}$  and other one, called  $\mathcal{B}$ , that is a function of known quantities. This is,

$$\begin{aligned}
 (x - X_T)^{l_\mu}(x - X_Q)^{l_\nu} &= \sum_{b_x=0}^{l_\mu} \sum_{b'_x=0}^{l_\nu} \binom{l_\mu}{b_x} \binom{l_\nu}{b'_x} (P_x - X_T)^{l_\mu - b_x} (P_x - X_Q)^{l_\nu - b'_x} (x - P_x)^{b_x + b'_x} \\
 &= \sum_{b_x=0}^{l_\mu} \sum_{b'_x=0}^{l_\nu} \mathcal{B}_{b_x + b'_x} (l_\mu, (\overline{PT})_x; l_\nu, (\overline{PQ})_x) (x - P_x)^{b_x + b'_x} \\
 &= \sum_{L=0}^{l_\mu + l_\nu} \mathcal{B}_L (l_\mu, (\overline{PT})_x; l_\nu, (\overline{PQ})_x) (x - P_x)^L .
 \end{aligned}$$

(11)

Considering the polynomial product (11), the Cartesian Gaussian product (??) can be expressed in a general way for any angular quantum numbers. Besides, this approach leads to well known analytic integrals. It is straightforward to see that one can take advantage of using CGF's and separate the three dimensional integral (9), considering the Gaussian product theorem, into the product of three integrals of Cartesian coordinates that are completely analogous. Such expression has the form:

The integration in the expression (??) can be written as a trivial Fourier transform of a Gaussian function and is found in a few works in literature (Taketa et al., 1966; Čársky et al., 1996; Genoni, 2020). One can disregard the polynomial considering the derivative in the quantity  $\xi$ . In addition, an exponential arise due

to a change in coordinates needed to perform the calculation. The result of the integration is connected to the generating function of the physicist's Hermite polynomial  $H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$ . Therefore,

It is worth noting that this procedure swaps the dependency from Cartesian Gaussian functions to Hermite Gaussian functions (Genoni, 2020). With the result of (??) extended to all Cartesian coordinates, one can write the integral (??) in its full form,

The expression (??), which is the general solution for (9), can be applied to the electronic scattering amplitude (5) in order to obtain an expression that has no restriction regarding the number of atomic centers and the level of CGF. For this reason, the present solution is suitable for the calculation of the scattering amplitude, consequently enabling one to obtain the differential cross section in the FBA for any molecular system. Moreover, it is possible to verify its validity to the special case of atoms, where all the CGF's are trivially centered at the origin.

## the effect of symmetry in the scattering amplitude

For the purpose of observing the effect of symmetry in the calculation of the scattering amplitude, it makes sense to split the result of integral (??) in a few quantities to ease the visualization of the results. Thus, the quantity  $\Upsilon_{\mu T}^{\nu Q} = \Upsilon_{l_{\mu} m_{\mu} n_{\mu} T}^{l_{\nu} m_{\nu} n_{\nu} Q}(\vec{\xi}; \epsilon_{\mu}, \vec{R}_T; \epsilon_{\nu}, \vec{R}_Q)$  is introduced,

where it is important to notice that the dependence in the Gaussian centers is in the entity  $\mathcal{B}$ . In the special case where the Gaussian functions are in the same center, a commutation in the column index yields a symmetry to this expression,  $\Upsilon_{l_{\mu} m_{\mu} n_{\mu} T}^{l_{\nu} m_{\nu} n_{\nu} T} = \Upsilon_{l_{\nu} m_{\nu} n_{\nu} T}^{l_{\mu} m_{\mu} n_{\mu} T}$ , *i.e.*, the  $l_{\mu}$ ,  $m_{\mu}$  and  $n_{\mu}$  are interchangeable to  $l_{\nu}$ ,  $m_{\nu}$ , and  $n_{\nu}$  respectively. Looking back to the result of the Fourier transform (??), the exponential with explicit dependence in the Gaussian coordinate vector is represented by

$$E_T^Q(\epsilon_{\mu}, \vec{R}_T; \epsilon_{\nu}, \vec{R}_Q) = \exp \left[ -\frac{\epsilon_{\mu} \epsilon_{\nu}}{\epsilon_{\mu} + \epsilon_{\nu}} (\vec{R}_T - \vec{R}_Q)^2 \right]. \quad (12)$$

With these considerations, the integral (??) can be rewritten simply as:

$$I_{\mu}^{\nu}(\vec{R}_T; \vec{R}_Q) = e^{-i\vec{\xi} \cdot \vec{P}} E_T^Q(\epsilon_{\mu}, \vec{R}_T; \epsilon_{\nu}, \vec{R}_Q) \Upsilon_{l_{\mu} m_{\mu} n_{\mu} T}^{l_{\nu} m_{\nu} n_{\nu} Q}(\vec{\xi}; \epsilon_{\mu}, \vec{R}_T; \epsilon_{\nu}, \vec{R}_Q). \quad (13)$$

The representation (13) of the Fourier transform of the Gaussian product deserves some attention regarding symmetry. If both CGF's are in the same center, the exponential function  $E_T^Q(\epsilon_{\mu}, \vec{R}_T; \epsilon_{\nu}, \vec{R}_Q)$  will not contribute, no matter the symmetry of the system, since  $E_T^Q \delta_{T,Q} = 1$ .

From now on, diatomic homonuclear molecules will be considered, however, some comments may be highlighted regarding other symmetry groups. In this class of systems, the CGF's centers are symmetric and belong to the  $d_{\infty h}$  point group. As consequence, the Gaussian position vectors can be represented by  $\vec{R}_1$  and  $\vec{R}_2$  with the following properties:  $|\vec{R}_1| = |\vec{R}_2| = R$  and  $\vec{R}_2 = -\vec{R}_1$ . Because of that, the exponential function will always yield the result

$$E_1^2 = E_2^1 = \exp \left[ -\frac{\epsilon_{\mu} \epsilon_{\nu}}{\epsilon_{\mu} + \epsilon_{\nu}} R^2 \right] = \bar{E}. \quad (14)$$

In order to visualize the symmetry properties in a clear and concise manner, we will only demonstrate the calculation with S and P type CGF's. Nonetheless, comments on the high angular momentum calculations will be given in the text.

Let us consider the scattering amplitude (5) and the spatial orbital expansion (??) up to P type functions:

The first term in the amplitude (??), only dependent in the S type function  $T_{\sigma-\sigma}$ , can be expressed by the previous definition (13) simply as:

$$T_{\sigma-\sigma} = \sum_{T=1}^2 \sum_{Q=1}^2 \sum_{\sigma=1}^{\#S} \sum_{\sigma'=1}^{\#S} C_{u\sigma}^T C_{u\sigma'}^Q e^{-i\vec{\xi} \cdot \vec{P}} E_T^Q \Upsilon_{\sigma T}^{\sigma' Q}, \quad (15)$$

where the  $\Upsilon$  term can be expressed in both notations  $\Upsilon_{000T}^{000Q}$  or  $\Upsilon_{\sigma T}^{\sigma'Q}$ . One may use the first one to explicitly visualize the angular quantum number projections or use the second one for the sake of simplicity. In equation (15), apart from the Fourier transform, the expansion coefficients  $C$  also carry the Gaussian center information by the labels  $T$  and  $Q$ . Therefore, these quantities need crucial attention in the analysis of symmetry for the scattering amplitude. Likewise, the center information is encapsulated in the exponential term  $e^{-i\vec{\xi}\cdot\vec{P}}$ , more specifically in the  $\vec{P}$  vector.

The position vector of the Gaussian product  $\vec{P}$  is defined as the weighted average (10) of the vectors  $\vec{R}_T$  and  $\vec{R}_Q$ . Recalling the properties  $|\vec{R}_1| = |\vec{R}_2| = R$  and  $\vec{R}_2 = -\vec{R}_1$ , due to the fact that there are 2 possible centers ( $\vec{R}_1$  and  $\vec{R}_2$ ), represented by the sum in  $T$  and  $Q$ , there are three possible scenarios here:

- both Gaussian functions in the same center ( $\vec{R}_1$  or  $\vec{R}_2$ )

$$\vec{P} = \frac{\epsilon_\sigma + \epsilon'_\sigma}{\epsilon_\sigma + \epsilon'_\sigma} \vec{R}_1 = \vec{R}_1 = \vec{R} \quad \text{or} \quad \vec{P} = \vec{R}_2 = -\vec{R}; \quad (16)$$

- Gaussian function defined by  $\epsilon_\sigma$  in  $\vec{R}_1$  and the one with exponent  $\epsilon'_\sigma$  in  $\vec{R}_2$

$$\vec{P} = \frac{\epsilon_\sigma \vec{R}_1 + \epsilon'_\sigma \vec{R}_2}{\epsilon_\sigma + \epsilon'_\sigma} = \frac{\epsilon_\sigma - \epsilon'_\sigma}{\epsilon_\sigma + \epsilon'_\sigma} \vec{R} = \epsilon_R^{\sigma\sigma'} \vec{R}, \quad (17)$$

where the term  $\epsilon_R^{\sigma\sigma'} = \frac{\epsilon_\sigma - \epsilon'_\sigma}{\epsilon_\sigma + \epsilon'_\sigma}$  has been introduced to simplify the notation ;

- Gaussian function with exponent  $\epsilon'_\sigma$  in  $\vec{R}_1$  and the one related to the exponent  $\epsilon_\sigma$  in  $\vec{R}_2$

$$\vec{P} = \frac{\epsilon_\sigma \vec{R}_2 + \epsilon'_\sigma \vec{R}_1}{\epsilon_\sigma + \epsilon'_\sigma} = \frac{-\epsilon_\sigma + \epsilon'_\sigma}{\epsilon_\sigma + \epsilon'_\sigma} \vec{R} = -\left(\frac{\epsilon_\sigma - \epsilon'_\sigma}{\epsilon_\sigma + \epsilon'_\sigma}\right) \vec{R} = -\epsilon_R^{\sigma\sigma'} \vec{R}. \quad (18)$$

Considering the exponential definition (14), for Gaussian exponents of S type functions it has the representation  $\bar{E}_{\sigma\sigma'} = \exp\left[-\frac{\epsilon_\sigma \epsilon'_\sigma}{\epsilon_\sigma + \epsilon'_\sigma} R^2\right]$ . In addition with the consideration (16), (17) and (18), the first term (15) of the scattering amplitude can be expressed as,

As stated before, the expansion coefficients from the UHF calculations play an important role in the analysis of symmetry, in fact their product allows one to simplify the equations. Observing the product of the coefficients for S type CGF we have:  $C_{u\sigma}^1 C_{u\sigma'}^1 = C_{u\sigma}^2 C_{u\sigma'}^2$  and  $C_{u\sigma}^1 C_{u\sigma'}^2 = C_{u\sigma}^2 C_{u\sigma'}^1$ . Moreover, for the special case of diatomic homonuclear molecules, if the Gaussian functions are in the same center,  $\Upsilon_{\mu 1}^{\nu 1} = \Upsilon_{\mu 2}^{\nu 2}$ . Thus, the exponential functions in (??) can be rewritten as cosine functions through the Euler's formula  $2 \cos(x) = e^{ix} + e^{-ix}$ , hence

$$T_{\sigma-\sigma} = 2 \sum_{\sigma=1}^{\#S} \sum_{\sigma'=1}^{\#S} \left[ C_{u\sigma}^1 C_{u\sigma'}^1 \Upsilon_{\sigma 1}^{\sigma' 1} \cos(\vec{\xi} \cdot \vec{R}) + C_{u\sigma}^1 C_{u\sigma'}^2 \bar{E}_{\sigma\sigma'} \Upsilon_{\sigma 1}^{\sigma' 2} \cos(\vec{\xi} \cdot \vec{R} \epsilon_R^{\sigma\sigma'}) \right]. \quad (19)$$

For the second term in the scattering amplitude (??), the previous comments regarding the vector  $\vec{P}$  are valid. nevertheless, one must pay attention to the projections that arise from the P type Gaussian functions, already commented in previous sections. These projections, mathematically embedded in the expression as a sum in the index  $i$ , *i.e.*, the sum  $\sum_{i=1}^3$ , will affect the expansion coefficients  $C$  and the term  $\Upsilon$  defined in (??). So,

$$\begin{aligned} T_{\sigma-\Pi} &= \sum_{T=1}^2 \sum_{Q=1}^2 \sum_{\sigma=1}^{\#S} \sum_{\Pi=1}^{\#P} \sum_{i=1}^3 \left[ C_{u\sigma}^T E_T^Q e^{-i\vec{\xi} \cdot \vec{P}} C_{u\Pi_i}^Q \Upsilon_{\sigma T}^{\Pi_i Q} \right] \\ &= \sum_{T=1}^2 \sum_{Q=1}^2 \sum_{\sigma=1}^{\#S} \sum_{\Pi=1}^{\#P} \left[ C_{u\sigma}^T E_T^Q e^{-i\vec{\xi} \cdot \vec{P}} \left( C_{u\Pi_x}^Q \Upsilon_{000T}^{100Q} + C_{u\Pi_y}^Q \Upsilon_{000T}^{010Q} + C_{u\Pi_z}^Q \Upsilon_{000T}^{001Q} \right) \right]. \end{aligned} \quad (20)$$

Using the compact notation above, due to simplicity, the term (20) can be treated considering the sum in the Gaussian centers. One can rewrite  $T_{\sigma-\Pi}$  as,

The product of the coefficients  $C$  for S and P type CGF have the following symmetry:  $C_{u\sigma}^1 C_{u\Pi_i}^1 = -C_{u\sigma}^2 C_{u\Pi_i}^2$  and  $C_{u\sigma}^1 C_{u\Pi_i}^2 = -C_{u\sigma}^2 C_{u\Pi_i}^1$ .

Apart from the special case of S type Gaussian functions, the  $\Upsilon$  quantity has real and imaginary parts. Therefore, it is useful to define  $\Upsilon_{\mu T}^{\nu Q} = \text{Re}(\Upsilon_{\mu T}^{\nu Q}) + i \text{Im}(\Upsilon_{\mu T}^{\nu Q})$ . The terms related to angular quantum number sum of the Gaussian functions ( $L$ ,  $M$  and  $N$ ) are subjected to symmetry due to the binomial theorem (11) and the imaginary component of the Fourier transform (??). This is applicable observing their upper limits: if the upper limit is odd the real part is antisymmetric to change of center and the imaginary part is symmetric, *i.e.*,  $\text{Re}(\Upsilon_{\sigma 1}^{\Pi_i 2}) = -\text{Re}(\Upsilon_{\sigma 2}^{\Pi_i 1})$  and  $\text{Im}(\Upsilon_{\sigma 1}^{\Pi_i 2}) = \text{Im}(\Upsilon_{\sigma 2}^{\Pi_i 1})$ ; if the upper limit is even,

regarding the change of center, the real part is symmetric and the imaginary one is antisymmetric, *i.e.* ,  $\text{Re}\left(\Upsilon_{\sigma_1}^{\Pi_i 2}\right) = \text{Re}\left(\Upsilon_{\sigma_2}^{\Pi_i 1}\right)$  and  $\text{Im}\left(\Upsilon_{\sigma_1}^{\Pi_i 2}\right) = -\text{Im}\left(\Upsilon_{\sigma_2}^{\Pi_i 1}\right)$ .

In addition, in the scenario where both Gaussian functions are in the same center, the analysis is straightforward from the Fourier transform (??). So, for angular quantum number sum ( $L$ ,  $M$  and  $N$ ) odd the  $\Upsilon$  term is purely imaginary  $\Upsilon_{\nu_1}^{\mu 1} = i \text{Im}\left(\Upsilon_{\nu_1}^{\mu 1}\right)$ . On the other hand, with the upper limits even, it is purely real  $\Upsilon_{\nu_1}^{\mu 1} = \text{Re}\left(\Upsilon_{\nu_1}^{\mu 1}\right)$ .

From these observations, in the term considering S and P type Gaussian functions it is possible to observe that

$$\text{Re}\left(\Upsilon_{\sigma_1}^{\Pi_i 2}\right) = -\text{Re}\left(\Upsilon_{\sigma_2}^{\Pi_i 1}\right) \quad \text{and} \quad \text{Im}\left(\Upsilon_{\sigma_1}^{\Pi_i 2}\right) = \text{Im}\left(\Upsilon_{\sigma_2}^{\Pi_i 1}\right) . \tag{21}$$

Thus, one can rewrite the term related to S and P Gaussian functions  $T_{\sigma-\Pi}$  taking the exponential functions in evidence:

Considering the Euler's formula  $2 \cos(x) = e^{ix} + e^{-ix}$  and  $2i \sin(x) = e^{ix} - e^{-ix}$ , this expression can be displayed with dependence to the trigonometric functions:

The third term in the scattering amplitude (??) involves only P type functions. This kind of Gaussian function has three projection ( $\Pi_x$ ,  $\Pi_y$  and  $\Pi_z$ ) and as consequence there would be nine distinct term from these projections. Further, due to the permutation in the centers  $T$  and  $Q$ , and the fact that these terms have real and imaginary components, the total of sixty four terms could arise from each P function pair. In a compact notation it is written as:

Observing the expansion coefficients  $C$  for the  $D_{\infty h}$ , since it is a linear group:  $C_{u \Pi_i}^T C_{u \Pi'_j}^Q \equiv \delta_{ij}$ . Likewise, the product of these coefficients allow one to observe that they are symmetric by change of center:  $C_{u \Pi_i}^1 C_{u \Pi'_j}^1 = C_{u \Pi_i}^2 C_{u \Pi'_j}^2$  and  $C_{u \Pi_i}^1 C_{u \Pi'_j}^2 = C_{u \Pi_i}^2 C_{u \Pi'_j}^1$ .

Regarding the function  $\Upsilon$ , since the angular quantum number sum is even, in the scenario when the Gaussian functions are in the same center, it is a pure real quantity, *i.e.*,  $\Upsilon_{\Pi_i 1}^{\Pi'_i 1} = \text{Re} \left( \Upsilon_{\Pi_i 1}^{\Pi'_i 1} \right)$ . Also, as commented before, in the case of even upper limit, by the change of center the real part is symmetric and the imaginary one is antisymmetric.

Rearranging the terms and considering the Euler's formula, it is possible to express  $T_{\Pi-\Pi}$  in terms of trigonometric functions:

Therefore, with the application of the symmetries of the functions, specially the product of the expansion coefficients  $C$ , it is possible to reduce from the original sixty four terms of  $T_{\Pi-\Pi}$  to nine (considering the sum in the index  $i$ ).

With the use of the presented properties, one can evaluate the electronic scattering amplitude taking into account the symmetry of the system with a compact expression that disregard a few terms. Along with its nuclear counterpart, the scattering amplitude for the proposed system can be readily obtained.

This procedure can be extended to higher angular quantum numbers as commented before. In that case, the part of the  $T_{\mu\nu}$  expression where the Gaussian functions are in the same center is quite trivial and will generate only one term *per*  $\mu - \nu$  pair. This component can always be written as a trigonometric function, as noted in the previous equations.

With the increase of the angular quantum numbers more terms will arise in the sector where the Gaussian functions are in separate centers, leading to real and imaginary terms. However, these can be expressed as a function of sine and cosine functions with real and imaginary components, always considering the symmetric relations commented in the text.

In order to summarize the symmetry relations regarding the expansion coefficients from the UHF calculation, the product of these quantities is given in table 2. The S, P, D and F type Gaussian functions are represented by  $\sigma$ ,  $\Pi$ ,  $\Delta$  and  $\phi$ , respectively. In each cell, the product symmetry of the coefficients  $C$  is given considering the  $\mu - \nu$  pairs. Below the product symmetry, in each cell of the table, a few conditions to identify the non-vanishing values are also pointed out in the form of Kronecker delta, *i.e.*, the index must be in accordance to the delta in order to obtain nonzero values, further, the ones with arrow indicates special conditions observed in this symmetry group. All this operations can be extended to the symmetry group  $D_{\infty h}$  paying attention to the index  $T$  and  $Q$ .

Table 2: Symmetry relations involving the expansion coefficients from the unrestricted Hartree-Fock calculation, more specifically, the symmetry of the product of the coefficient. Also, relations that enable one to verify the non-vanishing values is given with the Kronecker delta. These relations are applicable to diatomic homonuclear molecules, nonetheless they can be extended to all systems in the  $D_{\infty h}$  symmetry point group.

	$\sigma$	$\Pi$	$\Delta$	$\phi$
$\sigma$	$C_{u\sigma}^T C_{u\sigma'}^Q = C_{u\sigma}^Q C_{u\sigma'}^T$	$C_{u\sigma}^T C_{u\Pi_i}^Q = -C_{u\sigma}^Q C_{u\Pi_i}^T$	$C_{u\sigma}^T C_{u\Delta_{ij}}^Q = C_{u\sigma}^Q C_{u\Delta_{ij}}^T$	$C_{u\sigma}^T C_{u\phi_{ijk}}^Q = -C_{u\sigma}^Q C_{u\phi_{ijk}}^T$
$\Pi$		$C_{u\Pi_i}^T C_{u\Pi_j}^Q = C_{u\Pi_i}^Q C_{u\Pi_j}^T$ $\delta_{ij}$	$C_{u\Pi_i}^T C_{u\Delta_{jk}}^Q = -C_{u\Pi_i}^Q C_{u\Delta_{jk}}^T$ $\delta_{iz} \rightarrow \delta_{jk}$ $\delta_{ji}\delta_{kz}$	$C_{u\Pi_i}^T C_{u\phi_{jkl}}^Q = C_{u\Pi_i}^Q C_{u\phi_{jkl}}^T$ $\delta_{jk}\delta_{li}$
$\Delta$			$C_{u\Delta_{ij}}^T C_{u\Delta'_{kl}}^Q = C_{u\Delta_{ij}}^Q C_{u\Delta'_{kl}}^T$ $\delta_{ij} \rightarrow \delta_{kl}$ $\delta_{ik} \rightarrow \delta_{jl}$	$C_{u\Delta_{ij}}^T C_{u\phi_{klm}}^Q = -C_{u\Delta_{ij}}^Q C_{u\phi_{klm}}^T$ $\delta_{ij} \rightarrow \delta_{kl}\delta_{mz}$ $\delta_{jz} \rightarrow \delta_{kl}\delta_{mi}$
$\phi$				$C_{u\phi_{ijk}}^T C_{u\phi'_{lmn}}^Q = C_{u\phi_{ijk}}^Q C_{u\phi'_{lmn}}^T$ $\delta_{ij}\delta_{lm}\delta_{kn}$

## Conclusions

In this work, we have presented Fourier transform of Gaussian functions related to a recently proposed positron-molecule scattering model. More precisely, the model enables one to evaluate the scattering amplitude of diatomic homonuclear molecules considering the electrostatic potential in the FBA framework. The molecular wavefunction is described by a superposition of CGF and it is obtained by an UHF calculation.

The Fourier transform terms are directly connected to the Gaussian product, from the UHF procedure, and the exponential function that represents the scattered particle. The appearance of these classes of integrals are also caused by the non-central potential that describes the interaction of the particle with the molecular system. We have employed a similar procedure to the McMurchie-Davidson one (McMurchie & Davidson, 1978) in order to evaluate the integrals, however, in this manuscript, the integrals are exhibited in a more explicit manner with the intention to highlight the terms that are more relevant to the scattering process. With these results, the method of calculation of the scattering amplitude can be easily extended to molecules belonging to any symmetry group.

Apart from the general solution, we have studied the symmetry properties that arise from the product of the expansion coefficients (from the UHF calculation) with the integral results. Such analysis enables one to disregard terms that would be calculated but do not contribute to the scattering amplitude. With this approach it is possible to reduce considerably the number of terms that must be taken into account in the computational calculation. The symmetry properties are conceived for diatomic homonuclear molecules, but they can be readily extended, paying attention to the atomic centers, to any system belonging to the  $D_{\infty h}$  point group.

The relations that comes from the analysis can be used to ease the calculation of future *ab initio* scattering methods for this class of molecules. Moreover, these considerations combined with new computational techniques (Mazur et al., 2016) may be useful in the investigation of larger molecules with  $D_{\infty h}$  symmetry. The extension to the  $C_{\infty h}$  point group can be considered recalculating a few terms in the model.

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## Conflict of interest

The authors declare no conflict of interest.

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