PHYSICAL REVIEW A **99**, 022703 (2019)

Low-energy elastic scattering of positrons by O_2

Wagner Tenfen[*]
Physics Department, Universidade Federal da Fronteira Sul, 85770-000 Realeza, Paraná, Brazil

Marcos V. Barp and Felipe Arretche
Physics Department, Universidade Federal de Santa Catarina, 88040-900 Florianópolis, Santa Catarina, Brazil

(Received 21 November 2018; published 13 February 2019)

We employed the method of continued fractions in conjunction with the positron correlation polarization potential model with different levels of polarization to calculate the elastic integral and differential cross sections for positron scattering by O_2 molecules. We show how the addition of higher-order terms in the polarization interaction is necessary in order to achieve convergence of the scattering potential. Also, we present the effect that such terms have over the integral cross sections, comparing with results of previous studies. When convergence of the scattering potential is attained, the resulting cross sections fairly agree with the most recent total cross section measurements up to the positronium formation threshold and moreover exhibit good agreement with the available experimental quasielastic differential cross sections.

DOI: 10.1103/PhysRevA.99.022703

I. INTRODUCTION AND MOTIVATION

The study of positron collisions with atoms and molecules constitutes a major step towards the construction of a solid understanding of how matter and antimatter species interact in the energy range associated to chemical reactions [1].

Nowadays, there is a set of total cross sections (TCS) reported for several atomic and molecular targets. There is reasonable agreement that the TCS for noble gases are well established, mainly in the low-energy regime [2]. The situation is rather different regarding the scattering by molecules, even the simplest ones like the diatomic, mainly for energies below the positronium formation threshold. This point, as we wish to argue in the following, is particularly critical for molecular oxygen.

The first TCS data for positron scattering by O_2 was reported by Coleman *et al.* [3] in the 1970s. Later, in the beginning of the 1980s, Charlton *et al.* [4,5] presented two sets of TCS covering high to low energies. Before the end of the decade, two more sets of TCS had been measured by Katayama *et al.* [6] and Dababneh *et al.* [7]. Except for Charlton *et al.* [4] and Katayama *et al.* [6], all other authors presented TCS for energies below the positronium formation threshold (5.4 eV [8]). The first theoretical calculation, for energies below 10 eV, was performed by Mukherjee and Ghosh [9] using the positron correlation polarization potential (PCOP) [10,11]. In 1999, Przybyla *et al.* [12] reported quasielastic differential cross sections (DCS). After that, a set of TCS was measured by Marler [13], resolving the positronium formation and direct ionization cross sections of O_2 by positron impact. The most recent study on positron-O_2 is the one presented by Chiari *et al.* [14], where the authors presented TCS data measured with the Trento apparatus compared to theoretical calculations performed with the independent atom model combined with the screening corrected additivity rule, the IAM-SCAR method.

From Fig. 2 of the paper of Chiari *et al.* [14], we can see that, for energies below 10 eV, the measurements of Charton *et al.* [5] and Dababneh *et al.* [7] are well converged among each other and the data of Coleman *et al.* [3] and Marler [13] have similar magnitude but are a little bit higher than those of Charlton *et al.* [5] and Dababneh *et al.* [7]. The measurements of Chiari *et al.* [14] are significantly higher in magnitude towards lower energies than all other previous data and seem to be qualitatively different from all other experimental results, with exception when compared to the TCS of Marler [13] and Coleman *et al.* [3]. The theoretical calculations of Mukherjee and Ghosh [9] support the data of Charlton *et al.* [5] and Dababneh *et al.* [7] up to the positronium formation threshold. On the other hand, the results obtained by the IAM-SCAR method do not uphold the Trento TCS, particularly below 10 eV.

Above the opening of the inelastic channels, the absorption potential calculations present relatively good agreement with the available total cross section measurements [15–18]. Such agreement is significant above 100 eV, which leaves for the theoretical approaches some work in refining the calculated cross sections between 10 and 100 eV. It is desirable to explicitly determine the inelastic cross sections experimentally and theoretically, but in the absence of such calculations the absorption potential formulation seems to be doing notable work in the representation of the TCS in this energy range. Some adjustments may be necessary in order to represent the TCS more accurately and more studies of this nature shall bring clarity to the problem. Though the energy range above the opening of the inelastic channels is well covered theoretically and experimentally, it is important to note that the elastic interaction is almost unexplored, particularly from a theoretical point of view.

---

[*] wtenfen@uffs.edu.br

2469-9926/2019/99(2)/022703(12)

Given this scenario, it seems reasonable to develop more theoretical investigations on low-energy positron-O_2 cross sections. Motivated by the works of Buckingham and Orr [19,20], Gianturco *et al.* [21], Reid *et al.* [22], and Franz *et al.* [23,24], we examine how the inclusion of higher-order correction terms in the polarization component of the PCOP formulation affects the scattering potential and the integral and differential elastic cross sections for this target.

This paper is organized as follows. In Sec. II we provide a brief revision of the method of continued fractions (MCF), the details about the construction of the interaction potential, the numerical details of the calculations, and a brief discussion about the O_2 polarizabilities; in Sec. III we show and discuss the results obtained. Finally, in Sec. IV we state our conclusions and final comments. We also review the polarization interaction terms in the Appendix A.

II. THEORY

A. Method of continued fractions for scattering calculations

In the static plus correlation-polarization interaction level, the scattering potential is defined as

$$V(\vec{r}) = V_{\rm st}(\vec{r}) + V_{\rm cp}(\vec{r}), \tag{1}$$

where $V_{\rm st}(\vec{r})$ and $V_{\rm cp}(\vec{r})$ are, respectively, the static and correlation-polarization potentials, to be defined later in the text. Given the potential in Eq. (1) the Lippmann-Schwinger equation (we drop the $\vec{r}$ explicit dependence for simplicity)

$$|\psi\rangle = |\phi\rangle + G_0 V\, |\psi\rangle \tag{2}$$

can be numerically solved. In order to perform such a task, we employed the method of continued fractions (MCF) as proposed by Horáček and Sasakawa [25], and implemented by Lee *et al.* [26,27] and Ribeiro *et al.* [28]. This is a method in which the potential is weakened iteratively, until it becomes negligible in the scattering equation.

Considering that the K matrix in the first Born approximation is not equal to zero, we define the weakened potential as

$$V^{(1)} = V - \frac{V\,|\phi\rangle\,\langle\phi|\,V}{\langle\phi|\,V\,|\phi\rangle}, \tag{3}$$

and then rearrange the Eq. (2) as a function of $V^{(1)}$. Therefore, the solution of Eq. (2) can be written as

$$|\psi\rangle = |\phi\rangle + (1 - G_0V^{(1)})^{-1} G_0 V\,|\phi\rangle\,\frac{\langle\phi|\,V\,|\psi\rangle}{\langle\phi|\,V\,|\phi\rangle}. \tag{4}$$

From Eq. (4) we identify that the two new functions,

$$|\phi_1\rangle = G_0 V\,|\phi\rangle \tag{5}$$

and

$$|\psi_1\rangle = (1 - G_0V^{(1)})^{-1}\,|\phi_1\rangle\,, \tag{6}$$

lead to

$$|\psi\rangle = |\phi\rangle + |\psi_1\rangle\,\frac{\langle\phi|\,V\,|\psi\rangle}{\langle\phi|\,V\,|\phi\rangle}. \tag{7}$$

It is easy to verify (operate $\langle\phi|\,V$ and rearrange) that the K matrix is given by

$$K = \frac{\langle\phi|\,V\,|\phi\rangle^2}{\langle\phi|\,V\,|\phi\rangle - \langle\phi|\,V\,|\psi_1\rangle}, \tag{8}$$

and thus we only need to solve Eq. (6) to obtain the elements of the K matrix. The reader may observe that if $|\psi_1\rangle \approx |\phi_1\rangle$ (i.e., $V^{(1)} \approx 0$), the K matrix is completely determined. If these functions are considerably different, then one should proceed to obtain $|\psi_1\rangle$. We notice that Eq. (6) is actually the Lippmann-Schwinger equation for the potential $V^{(1)}$ and solution $|\psi_1\rangle$

$$|\psi_1\rangle = |\phi_1\rangle + G_0V^{(1)}\,|\psi_1\rangle\,. \tag{9}$$

Thus we follow the very same steps as before to solve it. Such procedure brings us the second-order weakened potential

$$V^{(2)} = V^{(1)} - \frac{V^{(1)}\,|\phi_1\rangle\,\langle\phi_1|\,V^{(1)}}{\langle\phi_1|\,V^{(1)}\,|\phi_1\rangle}, \tag{10}$$

and the functions

$$|\phi_2\rangle = G_0V^{(1)}\,|\phi_1\rangle, \tag{11}$$

$$|\psi_2\rangle = (1 - G_0V^{(2)})^{-1}\,|\phi_2\rangle. \tag{12}$$

The K matrix now reads

$$K = \frac{\langle\phi|\,V\,|\phi\rangle^2}{\langle\phi|\,V\,|\phi\rangle - \frac{\langle\phi_1|V^{(1)}|\phi_1\rangle^2}{\langle\phi_1|V^{(1)}|\phi_1\rangle - \langle\phi_1|V^{(1)}|\psi_2\rangle}}. \tag{13}$$

Again, if $|\psi_2\rangle \approx |\phi_2\rangle$, then the K matrix is fully determined. If not, then $|\psi_2\rangle$ should be determined from Eq. (12).

This procedure can be repeated as many times as necessary. Indeed, after n iterations we obtain

$$|\psi_n\rangle \approx |\phi_n\rangle\,, \tag{14}$$

and then we can construct the scattering wave function and the K matrix recursively. This method solves the scattering equation with the caution to observe that the obtained solution is approximate as it is the scattering potential.

B. Interaction potential

As stated above, the scattering potential is composed by the static potential $V_{\rm st}(\vec{r})$ and the correlation-polarization potential $V_{\rm cp}(\vec{r})$. In our scattering codes, the static potential is defined in the usual way, which is

$$V_{\rm st}(\vec{r}) = -\sum_i \int \frac{\phi_i^*(\vec{r}_i)\phi_i(\vec{r}_i)}{|\vec{r}_i - \vec{r}|}\,d\vec{r}_i + \sum_j \frac{Z_j}{|\vec{R}_j - \vec{r}|}, \tag{15}$$

where $\vec{r}_i$ and $\vec{R}_j$ represent the electronic and nuclear coordinates, respectively. So, a good representation of the molecular ground-state orbitals $\phi_i(\vec{r}_i)$ is fundamental for the determination of the electronic term of the static potential, which can be verified through the electrostatic moments of the molecule, for instance.

The correlation-polarization term is obtained with the PCOP model, as described by Jain [10,11], however, with a small modification in the spherical term of the polarization

TABLE I. Oxygen Gaussian basis set used to construct the O_2 HF wave function. This set is a slight modification of the SVP+Rydberg basis of Dunning and Hay [29].

Type	Exponent	Coefficient
S	7817.0	0.0011760
	1176.0	0.0089680
	273.20	0.0428680
	81.170	0.1439300
	27.180	0.3556300
	9.5320	0.4612480
	3.4140	0.1402060
S	9.5320	−0.1541530
	0.9398	1.0569140
S	0.2846	1.0000000
S	0.0320	1.0000000
S	0.0150	1.0000000
S	0.0070	1.0000000
P	35.180	0.0195800
	7.9040	0.1242000
	2.3050	0.3947140
	0.7171	0.6273760
P	0.2137	1.0000000
P	0.0280	1.0000000
P	0.0100	1.0000000
D	0.8500	1.0000000

part. Following Franz *et al.* [23,24], we consider the polarization potential given by

$$V_{\mathrm{pol}}(\vec{r}) = -\frac{\alpha_0}{2r^4} - \frac{\alpha_2}{2r^4}P_2(\cos\theta) - \frac{\alpha_Q}{2r^6} + \frac{B}{2r^7} - \frac{\gamma}{24r^8}, \quad (16)$$

containing the usual α_0 and α_2 contributions, but also the quadrupole polarization α_Q and the first (B) and second (γ) hyperpolarizabilities, described in the Appendix A. These polarizabilities and hyperpolarizabilities enter our scattering calculations as external parameters, so we can employ empirical or theoretical data freely.

C. Numerical details

For the representation of the ground state of the O_2 molecule, we employed a Hartree-Fock (HF) wave function constructed with the basis set given in Table I. This basis set is a slight modification of the SVP+Rydberg basis of Dunning and Hay [29], which can be obtained from the Basis Set Exchange database [30,31]. The equilibrium internuclear distance is $\mathrm{O}-\mathrm{O}(r_e) = 2.282a_0$, as determined by microwave spectroscopy [32].

The electronic orbitals generated by the HF calculation are expanded in the spherical harmonics basis with $l_{\max} = 40$. With these orbitals the electrostatic potential given in Eq. (15) is calculated. The accuracy of this potential is verified through the determination of the electrostatic moments. Nonetheless, the quadrupole, hexadecapole, and higher moments for l even are presented, and can be compared with reference values. In Table II, we compare the obtained electrostatic moments for O_2 with the values reported by Bartolomei *et al.* [33]. All calculations, including the scattering ones, were performed on a radial grid with 800 points, up to $125.35a_0$.

TABLE II. Electrostatic moments of O_2, compared with the theoretical values of Bartolomei *et al.* [33] and experimental data of Cohen and Birnbaum [34] and Buckingham *et al.* [35]; all values given in atomic units.

Multipole moments	This work	Calc. [33]	Expt. [34][a] [35][b]
Q_2	−0.3338	−0.2251	−0.25[a];−0.3 ± 0.1[b]
Q_4	4.7269	4.4821	
Q_6	20.5468	20.287	
Q_8	59.2943	50.138	

The comparison of the obtained electrostatic moments shows the adequacy of the employed wave function in the description of the ground state of the O_2 molecule. As stated above, this is particularly important for the correct calculation of the PCOP function and consequently for the determination of the matching radius. We then proceeded to the determination of the correlation-polarization potential, employing the PCOP function for the correlation part and Eq. (16) for the polarization. The values of the dipole polarizabilities employed in the present work are the frequency corrected values attributed to Hettema by Spelsberg and Meyer [36]. These values, $\alpha_0 = 10.60$ a.u. and $\alpha_2 = 4.77$ a.u., are fairly close to those calculated by Medved' *et al.* [37] on standard coupled cluster CCSD and CCSD(T) levels. For the quadrupole polarizability and first hyperpolarizability we have taken the values $\alpha_Q = 60.452$ a.u. and $B = -118.26$ a.u., both derived from the CASPT2/d-aug-cc-pVTZ calculations by North [38]. This calculation level was chosen because it reproduces more closely the values of α_0 and α_2 adopted here. It must be noticed that this quadrupole polarizability agrees with the values recommended by Bartolomei *et al.* [33] and Hettema *et al.* [39]. Finally, we considered $\gamma = 962.0$ a.u. for the second hyperpolarizability, as recommended by the experiment of Shelton [40] and by the calculation of Calamicini *et al.* [41].

Reviewing the literature on positron scattering by atoms and molecules, it appears that only Gianturco *et al.* [21], Reid *et al.* [22], and Franz *et al.* [23,24] considered the effects of the quadrupole polarizability and the first and second hyperpolarizabilities on the scattering cross sections. Gianturco *et al.* [21] calculated the integral and differential cross sections for positrons colliding with noble gas atoms, considering the DFTCP model as correlation-polarization interaction, and added the $\alpha_0 = \alpha_D$, α_Q, and α_O terms in the polarization component. Reid *et al.* [22] did the same for molecular hydrogen, but considering a different correlation scheme. Franz *et al.* [24] included the first and second hyperpolarizabilities to the polarization interaction and constructed a correlation-polarization potential with four different correlation models. From our point of view, the four correlation-polarization models lead to similar cross sections with subtle quantitative differences. Notwithstanding, these investigations did not clarify the effect of successive polarization enhancements over the convergence of the scattering potential.

In the present work, we study the effects of improving the polarization potential with higher orders of polarizability and

TABLE III. Nomenclature adopted in this work for the polarization potential corrections and the respective matching radius r_c, given in atomic units.

Nomenclature	Polarization potential	r_c
PCOP	$-\frac{\alpha_0}{2r^4} - \frac{\alpha_2}{2r^4}P_2(\cos\theta)$	2.54
PQ	$-\frac{\alpha_0}{2r^4} - \frac{\alpha_2}{2r^4}P_2(\cos\theta) - \frac{\alpha_Q}{2r^6}$	3.02
PB	$-\frac{\alpha_0}{2r^4} - \frac{\alpha_2}{2r^4}P_2(\cos\theta) - \frac{\alpha_Q}{2r^6} + \frac{B}{2r^7}$	3.20
PG	$-\frac{\alpha_0}{2r^4} - \frac{\alpha_2}{2r^4}P_2(\cos\theta) - \frac{\alpha_Q}{2r^6} + \frac{B}{2r^7} - \frac{\gamma}{24r^8}$	3.23

hyperpolarizability for positron scattering with O_2 molecules. In this sense, we denominate four different levels of polarization interaction, as stated in Table III. It seems reasonable to assume that the successive inclusion of correction terms in the polarization component enlarges the values of the matching radius since $B < 0$. The value of r_c must be consistent with the apparent size of the molecule, as observed by Franz *et al.* [23]. Since the transversal van der Waals radius of the O_2 molecule is $3.55a_0$ [42] and the PG polarization leads to $r_c = 3.23a_0$, we can conclude that the correlation potential acts only inside the electronic cloud region. This means that the inclusion of such terms in the polarization potential does not imply a nonphysical size of the O_2 molecule. In Fig. 1 we present the spherical term of the scattering potential, where the effects of each polarization level can be visually evaluated together with the electrostatic potential.

D. Comments about the polarizability

We consider important to discuss, even briefly, the values of the dipole polarizability of the O_2 molecule found in scientific articles and presented in previous works on positron scattering by this molecule.

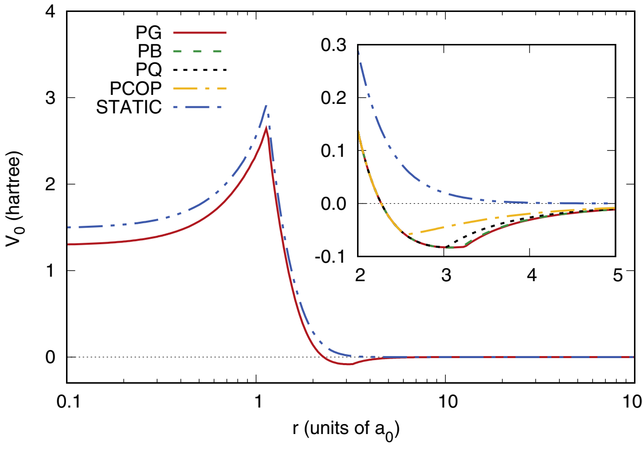

FIG. 1. Spherical components of the scattering potential; see Eq. (1). Legends are as follows: dashed-double-dotted line, static; dashed-dotted line, PCOP; dotted line, PQ; dashed line, PB; solid line, PG. The inset shows how different polarization potential affects the matching radius (r_c). Note that the solid and dashed lines are practically merged.

First, Chiari *et al.* [14] states that the dipole polarizability of the O_2 molecule is $\alpha_0 = 15.73$ a.u., which is reiterated by Brunger *et al.* [43]. Many values are available in literature for such polarizability [33,36–38,44–46]; however, none of them are close to the one used by Chiari *et al.* [14] and Brunger *et al.* [43]. Actually, the experimental value derived from the accurate refraction index measured by Newel and Baird [47] is $\alpha_0 = 10.67$ a.u., while the value obtained by Bridge and Buckingham [46] is $\alpha_0 = 10.78$ a.u. We note also that the value referenced by Chiari *et al.* [14] was not employed in the scattering calculations within the IAM-SCAR formalism, as the polarization interaction for positrons colliding with O_2 molecules was considered for isolated oxygen atoms, consistent with the central idea of the independent atom model.

Verifying the values available in the literature for the polarizability of the O_2 molecule, it seems that Chiari *et al.* [14] and Brunger *et al.* [43] took the α_{zz} component of the dipole polarizability tensor as the spherical symmetric dipole polarizability, namely α_D or α_0. Of course, since α_{zz} is a component of the dipole polarizability tensor, it can be formally regarded as a dipole polarizability. Nonetheless, it is customary to denote $\alpha_D = \alpha_0 = \overline{\alpha}$, and since atoms and molecules respond in all directions when subjected to the presence of an external electric field α_2 must be considered as well.

It is also noteworthy that the calculations of Mukherjee and Ghosh [9] employed the spherical polarizability $\alpha_0 = 10.9$ a.u. to the O_2 molecule, which is very close to the experimental value of Bridge and Buckingham [46], fairly close to the experimental value of Newel and Baird [47], and just a little higher than the value applied in the present work. At that time the TCS available for positron scattering with O_2 molecules were those of Coleman *et al.* [3], Katayama *et al.* [6], Dababneh *et al.* [7], and Charlton *et al.* [5]. The correlation polarization adopted by Mukherjee and Ghosh [9] reproduced the TCS of Dababneh *et al.* [7] and Charlton *et al.* [5] reasonably well. We do not consider the slight difference between the polarizability employed by Mukherjee and Ghosh [9] and by us as a hurdle to compare the results; however, the use of $\alpha_0 = 15.73$ a.u., as suggested by Chiari *et al.* [14] and Brunger *et al.* [43], would lead to elastic integral cross sections too large and improper in order to compare with other calculations and experimental data.

III. RESULTS AND DISCUSSION

In this section we present and discuss our results. We start with the elastic integral cross section for energies below 5 eV, since the positronium formation threshold is between 5 and 6 eV, and we report elastic cross sections only. For the sake of completeness we provide the elastic integral cross section up to 10 eV in Table IV. These results are shown and compared with theoretical and experimental data in Fig. 2.

When we consider the PCOP level of polarization with typical values for α_0 (10.9 a.u. in Mukherjee and Ghosh [9] and 10.6 a.u. in our calculation), the obtained integral cross sections clearly describe the experimental data of Dababneh *et al.* [7] until 3 eV. There is qualitative and some quantitative agreement with Charlton *et al.* [5] up to 2.5 eV. The present

TABLE IV. Calculated elastic integral cross sections from 0.1 to 10.0 eV.

Energy (eV)	ICS (10^{-16} cm^2)	Energy (eV)	ICS (10^{-16} cm^2)	Energy (eV)	ICS (10^{-16} cm^2)
0.1	39.4833	1.0	5.60022	3.0	3.74951
0.2	24.8098	1.1	5.23194	4.0	3.59581
0.3	17.5770	1.2	4.95684	5.0	3.47944
0.4	13.6484	1.3	4.74589	6.0	3.41210
0.5	10.6920	1.4	4.57782	6.75	3.37907
0.6	8.87582	1.5	4.44137	7.0	3.37109
0.7	7.70888	1.7	4.24748	8.0	3.34368
0.8	6.73342	2.0	4.06204	9.0	3.32511
0.9	6.06203	2.5	3.84749	10.0	3.31180

results and the results of Mukherjee and Ghosh [9] agree fairly well in this level of polarization, as it should be. Although we considered different wave functions, polarizabilities, and theoretical scattering methodology, we can observe the distinct minimum in the cross section around 0.8 eV as observed Mukherjee and Ghosh [9], which can be attributed to overcorrelation or, as we argue next, to underpolarization. Also, as we considered different polarizabilities and a different wave function from Mukherjee and Ghosh [9] it is expected that our results do not match precisely, even considering that we employed the same correlation-polarization model. The wave functions are somewhat different, as it can be observed in the quadrupole moments; see Table II. This significantly alters the electronic density, that is an important parameter for the calculation of the PCOP function. Still, the agreement between our calculation and theirs is satisfactory and illustrates the difficulty of the PCOP formulation in describing the intermediate range polarization. This question was briefly discussed by Gianturco *et al.* [21], and it is a relevant issue in the scattering of positrons with molecules that do not present permanent electric dipole, since the dipole interaction dominates at the intermediate and long range, overshadowing the underpolarization problem. This was anticipated in previous works where the PCOP model was employed to calculate the cross sections for positron collisions with polar molecules [48]. Nevertheless, even for such molecules the polarization potential must be considered in full form, or at least until convergence of the integral and differential cross sections is obtained.

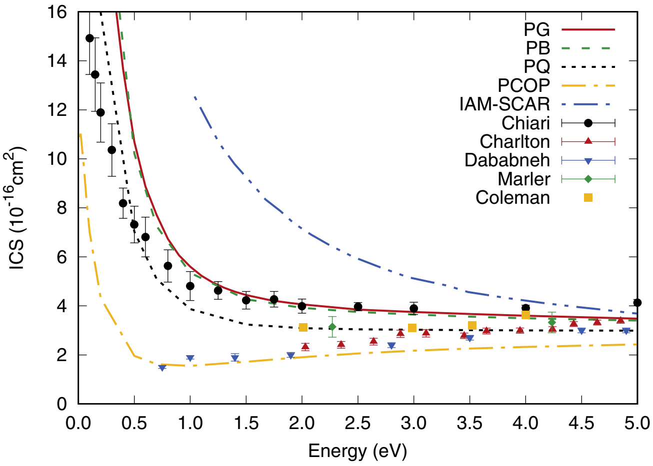

FIG. 2. Elastic integral cross section showing the contribution of each correction term present in the polarization potential [see Eq. (16)]. Theoretical approaches: solid line, PG; dashed line, PB; dotted line, PQ; dashed-dotted line, PCOP; dashed-double-dotted line, IAM-SCAR of Chiari *et al.* [14]. Experimental data: solid circles, Chiari *et al.* [14]; triangles, Charlton *et al.* [5]; inverted triangles, Dababneh *et al.* [7]; diamonds: Marler [13]; squares, Coleman *et al.* [3].

From Fig. 2, we see that the correction associated to the quadrupole polarizability (PQ) introduces significant improvement in the magnitude of the ICS. The experimental data of Dababneh *et al.* [7] could possibly suggest the existence of a minimum below 1 eV, corroborated by the present and previous PCOP results, but the inclusion of the quadrupole polarizability correction eliminates this effect. Hence one can state that the appearance of such minimum is partly due to the lack of polarization of the molecule. In this energy range, the PQ model presents reasonable agreement with the data of Coleman *et al.* [3] and of Marler [13]. Also, the PQ presents qualitative agreement with the data of Chiari *et al.* [14]; however, the magnitude of the cross sections concur only marginally. We expect that an angular correction for this TCS set [14] would make this comparison even worse for energies greater than 0.5 eV, since some enhancement in the TCS is expected making the comparison even more divergent.

The inclusion of the first hyperpolarizability correction (PB) raises the magnitude of the cross section leading to the agreement with the data of Chiari *et al.* [14] for energies above 1 eV. The second hyperpolarizability correction (PG), on the other side, becomes practically indistinguishable from the PB result. This suggests that convergence has been achieved in the polarization corrections, and higher-order corrections to the polarization interaction of positrons with O_2 molecules are unnecessary. The same feature can be observed in Fig. 1, which demonstrates that the PB and PG approaches are well converged with each other.

It is noteworthy that we compare our PG with the uncorrected TCS of Chiari *et al.* [14]. Some corrections for those data were obtained from the IAM-SCAR calculated DCS, indicating a 6% enhancement on the TCS for 1 eV positrons. We expect that this correction becomes more significant for lower incident energy positrons, which can potentially improve the agreement between our results and the data of Chiari *et al.* [14].

The observed enhancement of the cross sections calculated with the PG relative to those obtained with PCOP is not exclusively due to the increase of r_c, as the inclusion of the higher-order polarization terms implies in a different description of the intermediate range, i.e., the region right after the molecular border and before the asymptotic region. The correct description of interaction potential in this region is of fundamental importance for determining the cross sections at lower energies. This observation can be drawn when we compare the matching radius obtained by Mukherjee and Ghosh [9] with the matching radius obtained in the present work for each polarization level. Even their matching radius being larger the reported cross section is still lower than our PCOP in the 0 to 2 eV energy range, and then becomes a little bit larger. Therefore, the effect of the increase of r_c alone is not responsible for the correct description of the magnitude of the integral cross sections. There is a compromise between the effective size of the molecule, which is indicated by r_c, and the intermediate range polarization, which depends mainly on the adoption of the r^{-4}, r^{-6}, and r^{-7} polarization terms. For the purpose of obtaining physically meaningful scattering cross sections with the approximations made in this and similar works, consistent values for α_Q, B, and γ must be known.

Besides that, the correlation part of the interaction is very important and should be studied carefully. In order to evaluate how much the correlation affects the cross sections we set it as zero for $r < r_c$, with r_c still being defined with the aid of the PCOP model. We observed that the cross sections became very different from those that we report here. Particularly, the integral cross sections present a very distinct minimum and the magnitudes are not even close to any experimental data set or theoretical calculations. The differential cross sections for 4 eV positron collisions became very divergent qualitatively from the results that we present below, with a sensible drop at lower angles and a displacement of the minimum of the DCS by approximately 30° to lower angles. This is an interesting result, since it gives us some intuition about the behavior of the cross sections as a function of the correlation part of the total interaction, and we will discuss it further in the presentation of the differential cross sections.

A. Quasielastic differential cross sections

Our experience on the field of positron collisions with molecules taught us that the ultimate test for polarization-correlation models is the comparison between theoretical and experimental differential cross sections, since it is possible to obtain very similar integral cross sections with somewhat distinct differential cross sections. Also, we noticed that the correlation and polarization effects directly alter the qualitative and quantitative aspects of the cross sections for low and intermediate angles.

In order to visualize how the quadrupole polarizability and hyperpolarizability terms influence the angular dispersion of the scattered positrons, we present the elastic differential cross sections for some selected energies. These energies have been chosen in order to match the experimental relative differential cross section data measured by Przybyla *et al.* [12]. It is interesting to note that, as far as we know, no theoretical study has been reported concerning the elastic differential cross sections of positron scattering by O_2 molecules.

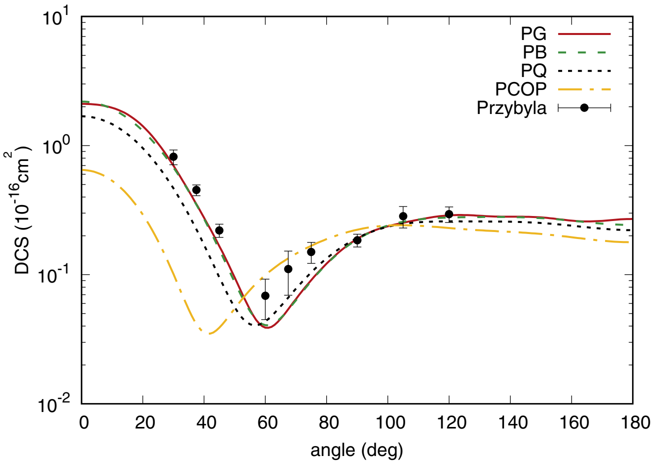

FIG. 3. Differential cross section for 4.0 eV. Legends are as follows: solid line, PG; dashed line, PB; dotted line, PQ; dashed-dotted line, PCOP. Experimental data from Przybyla *et al.* [12].

Figures 3 to 8 present the obtained elastic differential cross sections for PG and PCOP polarization levels compared to the available experimental data. For comparison between the calculated and the relative DCS measurements, the experimental data have been normalized at 120°. The reason for such a choice lies in the fact that the DCS at large angles is dominated by the static potential (see Fig. 7a of [49] for example). Choosing such a normalization scheme, we have a fair way to compare the effects in the angular distribution of the scattered positrons in both PCOP and PG formulations.

Likewise, we can clearly see that the differential cross sections are convergent with one another as the positron energy rises. This is expected, since the positron will become less and less sensible to polarization and correlation effects as its energy becomes greater. All these theoretical cross sections are well converged in partial wave expansion up to $l_{\max} = 14$ for high energies; however, for low energies, convergence was achieved with $l_{\max} = 8$. Also, the obtained K matrix converged within six iterations with $\Delta\delta_l = 10^{-5}$ rad, which is considered sufficient in order to obtain consistent cross sections with the desired numerical precision.

The agreement of the DCS reported here and the experimental data of Przybyla [12] for 4 eV is satisfactory. The cross sections clearly present a minimum, which is experimentally located somewhere between 45° and 60°. Except for PCOP, all of the polarization levels presented here were able to correctly represent the position of such minimum; however, fully quantitative agreement between the theoretical and experimental cross sections is not found at this energy. For the PCOP approach, it remains clear that lack of polarization prevents the cross sections from achieving the correct magnitude (evaluated through the integral cross sections; see Fig. 2). As for the PG approach, the correlation part may be stronger than it really is in the physical system; hence revisiting the correlation model can be necessary for obtaining cross sections at lower energies. Second, for higher and lower angles the agreement between the calculated differential cross

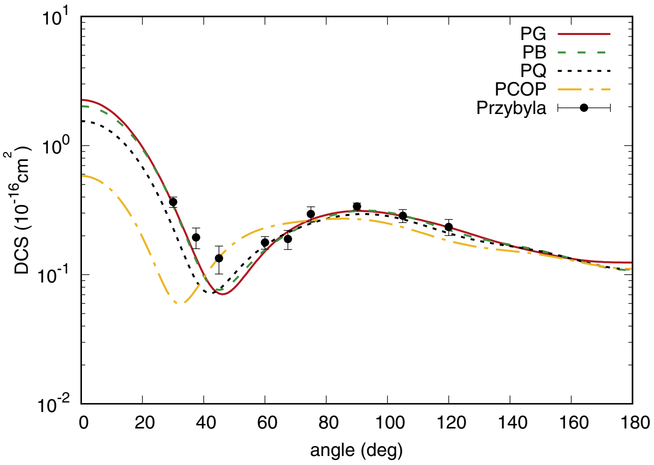

FIG. 4. Differential cross section for 6.75 eV. Legends are the same as Fig. 3.

sections is better with PG than with PCOP polarization level, independent of the adopted normalization criterium of the experimental data. So, it is sufficiently clear that the role of the polarization interaction part in the intermediate region is fundamental in order to achieve correspondence between calculated and measured cross sections. Of course, since the experimental data were recorded in arbitrary units, demanding normalization of the values for comparison, the quantitative agreement suggested by Fig. 3 may be artificial. However, we believe that the magnitude of the cross sections are correct since the integral cross section for this particular energy fairly agrees with the TCS data of Chiari *et al.* [14], and the available TCS data for this energy are not far from the most recent measurements.

Figure 4 presents the calculated differential cross sections for 6.75 eV positrons. Since the available experimental differential cross sections are quasielastic, our calculations can be compared directly with such data. We see that the agreement between our present results and the measurements of Przybyla *et al.* [12] is even better for this energy, as expected. It is so because the effects of the correlation part of the interaction become less significant as the projectile energy increases.

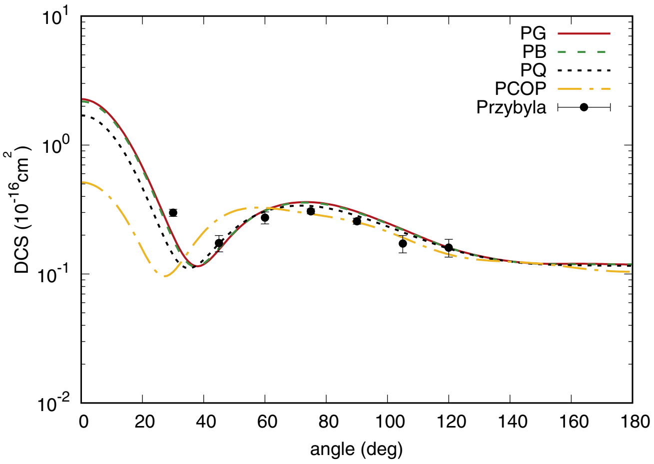

FIG. 5. Differential cross section for 10.0 eV. Legends are the same as Fig. 3.

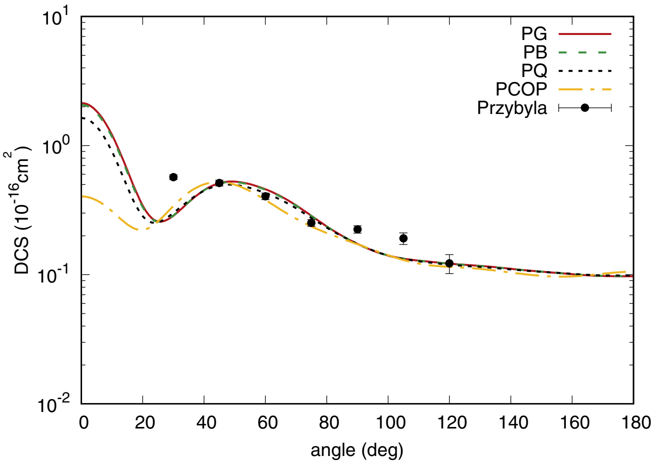

FIG. 6. Differential cross section for 20.0 eV. Legends are the same as Fig. 3.

Notwithstanding, the polarization part still has an important role in the determination of the qualitative and quantitative behavior of the differential cross sections, as we can see when comparing the results obtained within the PCOP and PG levels of polarization. The analysis of the experimental curve could indicate some kind of structure in this differential cross section around 67.5°, which is in contradiction with all the results that we obtained. So, in this angular region, the differential cross section is essentially smooth as it is observed systematically for all calculated elastic differential cross sections presented in this work. The presented differential cross sections for energies lower than 10.0 eV indicates that a richer set of experimental differential cross sections is necessary in order to evaluate the correlation and polarization models for positron molecule scattering.

Paying attention to the differential cross sections for higher energies, we find a similar behavior among them. The qualitative and quantitative agreement between theory and experiment is still observed, with exception, perhaps, for the 20.0 eV cross sections. Also, the considered polarization level becomes less and less significant as the positron energy rises, turning to almost unimportant at 50.0 eV and higher

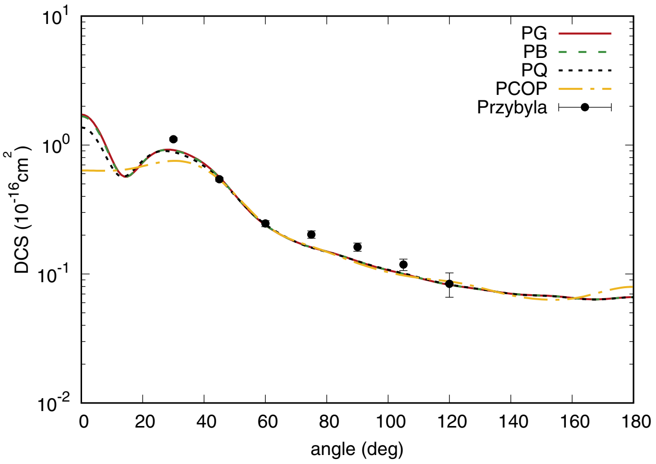

FIG. 7. Differential cross section for 50.0 eV. Legends are the same as Fig. 3.

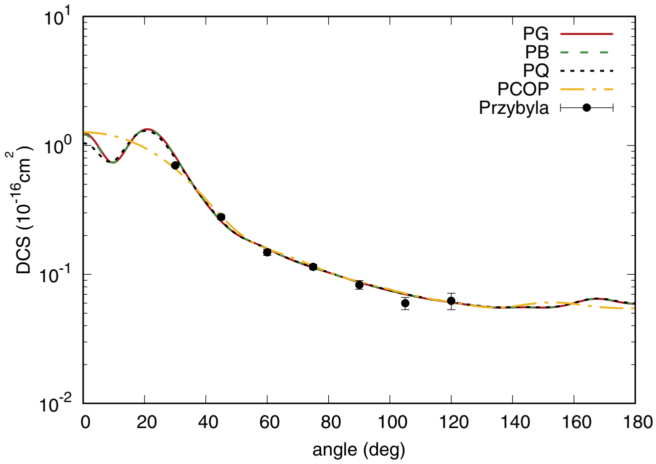

FIG. 8. Differential cross section for 100.0 eV. Legends are the same as Fig. 3.

energies. So, for positron collisions with O_2 molecules with energies lower than 50.0 eV we can state that the polarization part of the interaction potential must be considered carefully, warranting at least convergence of the polarization terms as we identified in Fig. 1.

IV. CONCLUSIONS

We presented theoretical integral and differential cross sections for positron collisions with O_2. Particularly, we report a study of how the polarization interaction levels in conjunction with the PCOP approach would affect these cross sections. Through this study, it seems that higher-order terms of the polarization interaction are necessary in order to calculate the cross sections for positron collisions with molecules, at least for molecular oxygen. This conclusion can be drawn from the analysis of the calculated integral and differential cross sections presented here.

A known problem on the calculation of positron cross sections with nonpolar molecules is the presence of a pronounced Ramsauer minimum in the integral cross sections when employing the PCOP model [48]. We observe here that this minimum comes from the underpolarization of the molecule in the presence of positrons when one considers only the dipole-dipole polarizability, i.e., terms proportional to r^{-4} in the polarization potential. With the addition of the quadrupole polarization potential term, related to the quadrupole-quadrupole polarizability, this effect already disappears for positrons interacting with the O_2 molecule; however, we also noticed that more terms are necessary in order to achieve convergence of the interaction potential, which is obtained considering the terms described in Table III.

Besides, with the inclusion of such corrections in the scattering potential, we observed satisfactory qualitative and quantitative agreement between our calculated cross sections and the experimental data available up to the positronium formation threshold. For whichever experimental data a different approach for the polarization level leads to agreement, nonetheless the converged interaction potential fairly agrees with the measurements of Chiari *et al.* [14], and the obtained differential cross sections for this level show good agreement with the quasielastic measurements of Przybyla *et al.* [12]. That being considered, we recommend the elastic cross sections obtained within the PG polarization level as reference for further experimental and theoretical works.

Finally, from this work, it is clear that more theoretical and experimental studies on positron collisions with O_2 are necessary, such as differential cross sections from lower energies up to the positronium formation threshold, in order to investigate the effects of the correlation models. Likewise, more theoretical studies are welcome in order to define criteria for the choice of the higher orders of polarizabilities and hyperpolarizabilities and also a correlation model that improves the description of the scattering phenomena at low and very low positron energies.

ACKNOWLEDGMENTS

W.T. would like to thank Universidade Federal da Fronteira Sul for supporting this research. M.V.B. and F.A. would like to thank the Programa de Pós-Graduação em Física of Universidade Federal de Santa Catarina for the support. M.V.B. would like to thank the Conselho Nacional de Desenvolvimento Científico e Tecnológico for the financial support.

APPENDIX: POLARIZABILITIES AND HYPERPOLARIZABILITIES

The potential described in this paper, in particular the asymptotic polarization potential (16), is constructed considering the long-range interaction. In the context of positron scattering, the presence of an external electric field produces a distortion in the molecule called polarizability; the induced moments are linearly proportional to the strength of the field applied. On the other hand, the description of the nonlinear responses to the external electric field are known as hyperpolarizabilities [50].

As discussed in a recent work [51], in Appendix A, the application of perturbation theory to the energy of diatomic homonuclear systems leads to an unperturbed energy being the ground-state energy of the molecule $E^{(0)}$ and a first correction $E^{(1)}$ related to the static potential.

When one considers the second correction $E^{(2)}$ and the multipole expansion of the many-body electrostatic potential it is possible to infer the nonzero terms that contribute to the energy correction. Then, comparing such second correction with the polarizability tensor [50,52]

$$\alpha_{lk,l'k'} = 2\sum_n \frac{\langle 0|\,\hat{Q}_{lk}\,|n\rangle\,\langle n|\,\hat{Q}_{l'k'}\,|0\rangle}{E_n - E_0}, \tag{A1}$$

it is easy to obtain the final expression for the polarization potential regarding the polarizability tensor $\alpha_{lk,l'k'}$. The multipole moments operator $\hat{Q}_{lk}$ is described in Cartesian components [50]; therefore, the expected value related to $\hat{Q}_{10}$ is the dipole, $\hat{Q}_{20}$ the quadrupole, and so forth. Applying this procedure, the following recursive formulas are attained for the polarization potential due to the second correction on the energy:

$$V_{\text{pol}} = -\sum_{l=1}^{\infty} \frac{\alpha_l}{2r^{2l+2}}. \tag{A2}$$

TABLE V. Polarizabilities and hyperpolarizabilities (nonlinear polarizabilities) nomenclatures used in literature compared with the tensor notation.

Polarizabilities and hyperpolarizabilities		
Multipole components	Commonly used [21,23,24,53,54]	Tensor notation [19,50]
Dipole-dipole	$\alpha_1, \alpha_{z,z} = \alpha_0 + \alpha_2 P_2(\cos\theta)$	$\alpha_{10,10}$
Dipole-quadrupole[a]	A	$\alpha_{10,20}$
Dipole-octupole	E	$\alpha_{10,30}$ [55]
Quadrupole-quadrupole	α_2, α_Q, C	$\alpha_{20,20}$
Octupole-octupole	α_3	$\alpha_{30,30}$
Dipole-dipole-dipole[a]	β	$\beta_{10,10,10}$
Dipole-dipole-quadrupole	B	$\beta_{10,10,20}$
Dipole-dipole-dipole-dipole	γ	$\gamma_{10,10,10,10}$

[a] Not applicable to diatomic homonuclear systems.

In this expression, r is the positron coordinate and α_l is the polarizability. From the summation raises the static dipole polarizability α_1, quadrupole polarizability α_2, and so on, it is important to note that the suppressed notation in Eq. (A2) is commonly used [21]. In order to avoid any misunderstanding regarding the notation, since the polarizability is described by a rank 2 tensor and Eq. (A2) uses only one index, following some previous works [19,21,24,50] such polarizabilities can be expressed as in Table V. Note that the index z is due to, without loss of generality, the choice of direction of the external electric field. Moreover, the α_0 and α_2 present in the dipole-dipole component are the spherical and nonspherical polarizabilities. These polarizabilities (Table V), as stated before, are the mathematical representation of the linear response of the molecule to the external electric field.

Looking back to perturbation theory, the third correction $E^{(3)}$ is given by

$$E^{(3)} = \sum_{p\neq 0}\sum_{n\neq 0} \frac{\langle 0|V|p\rangle\langle p|V|n\rangle\langle n|V|0\rangle}{(E_0-E_n)(E_0-E_p)} - \sum_{p\neq 0}\frac{\langle 0|V|p\rangle\langle p|V|0\rangle}{(E_0-E_p)^2}\langle 0|V|0\rangle . \tag{A3}$$

Considering the multipole expansion in the potential V,

$$V(\vec r, \vec r_i, \vec R_j) \overset{r\to\infty}{\longrightarrow} \sum_j\sum_\lambda Z_j \frac{R_j^\lambda}{r^{\lambda+1}} P_\lambda(\hat R_j\cdot\hat r) - \sum_i\sum_\eta \frac{r_i^\eta}{r^{\eta+1}} P_\eta(\hat r_i\cdot\hat r), \tag{A4}$$

as before $\vec r_i$ are the electron coordinates and $\vec R_j$ the nuclei coordinates, mathematically, any monopole contribution leads the third energy correction (A3) to zero due to the orthogonality of the states. In what concerns the dipole contribution, considering $|i\rangle$ the electronic molecular states, it is possible to write

$$\langle i|V|i\rangle = \sum_{l,m}\frac{4\pi}{2l+1}\left[\int d^3\vec r_i\, r_i^l \rho(\vec r_i) Y_l^{m*}(\hat r_i)\right] Y_l^m(\hat r). \tag{A5}$$

Considering $\rho(\vec r_i)$ as a simple representation of the charge density at normalized internuclear distance $\rho(x,y,z) = \delta(x)\delta(y)[\delta(z+1)+\delta(z-1)]$, from the integration only terms of even power on z will not vanish.

The first nonzero term is due to the expansions in two dipole terms and a third one in quadrupole, such that

$$E^{(3)} = \frac{1}{r^7}\left[\sum_{p\neq 0}\sum_{n\neq 0}\frac{\langle 0|\hat Q_{1,0}|p\rangle\langle p|\hat Q_{1,0}|n\rangle\langle n|\hat Q_{2,0}|0\rangle}{(E_0-E_n)(E_0-E_p)} - \sum_{p\neq 0}\frac{\langle 0|\hat Q_{1,0}|p\rangle\langle p|\hat Q_{1,0}|0\rangle}{(E_0-E_p)^2}\langle 0|\hat Q_{2,0}|0\rangle\right]. \tag{A6}$$

It is possible to relate Eq. (A6) to the first hyperpolarizability tensor [19,50], also known as dipole-dipole-quadrupole hyperpolarizability; see Table V. Aforesaid tensor is given by

$$\beta_{lk,l'k',l''k''} = \mathcal{S}\sum_{p\neq 0}\left[\sum_{n\neq 0}\frac{\langle 0|\hat Q_{l,k}|p\rangle\langle p|\hat Q_{l',k'}|n\rangle\langle n|\hat Q_{l'',k''}|0\rangle}{(E_0-E_n)(E_0-E_p)} - \frac{\langle 0|\hat Q_{l,k}|p\rangle\langle p|\hat Q_{l',k'}|0\rangle}{(E_0-E_p)^2}\langle 0|\hat Q_{l'',k''}|0\rangle\right], \tag{A7}$$

where $\mathcal{S}$ denotes a sum of all permutations, in this context $\mathcal{S} = 2!$. Comparing Eqs. (A6) and (A7) the third correction on the energy leads to the potential

$$V = \frac{\beta_{1,1,2}}{2r^7} = \frac{B}{2r^7}. \tag{A8}$$

It must be noted that this potential is attractive, since the element tensor $\beta_{1,1,2}$ is negative; see Sec. II C.

The fourth energy correction on the energy is described, from perturbation theory, by

$$\begin{aligned}E^{(4)} =& \sum_{q\neq 0}\sum_{p\neq 0}\sum_{n\neq 0}\frac{\langle 0|\,V\,|q\rangle\,\langle q|\,V\,|p\rangle\,\langle p|\,V\,|n\rangle\,\langle n|\,V\,|0\rangle}{(E_0-E_n)(E_0-E_p)(E_0-E_q)} - \sum_{q\neq 0}\sum_{n\neq 0}\frac{\langle 0|\,V\,|n\rangle\,\langle n|\,V\,|0\rangle}{(E_0-E_n)}\,\frac{\langle 0|\,V\,|q\rangle\,\langle q|\,V\,|0\rangle}{(E_0-E_q)^2}\\ &-\sum_{q\neq 0}\sum_{p\neq 0}\frac{\langle 0|\,V\,|q\rangle\,\langle q|\,V\,|p\rangle\,\langle p|\,V\,|0\rangle}{(E_0-E_p)^2(E_0-E_q)}\,\langle 0|\,V\,|0\rangle - \sum_{q\neq 0}\sum_{n\neq 0}\frac{\langle 0|\,V\,|q\rangle\,\langle q|\,V\,|n\rangle\,\langle n|\,V\,|0\rangle}{(E_0-E_q)^2(E_0-E_n)}\,\langle 0|\,V\,|0\rangle\\ &+\sum_{q\neq 0}\frac{\langle 0|\,V\,|q\rangle\,\langle q|\,V\,|0\rangle}{(E_0-E_q)^3}\,\langle 0|\,V\,|0\rangle\,\langle 0|\,V\,|0\rangle\,. \end{aligned}\tag{A9}$$

Considering the first term in the multipole expansion (A4), i.e., the dipole, and the given fourth energy correction (A9), the following energy is found for diatomic homonuclear systems:

$$E^{(4)} = \frac{1}{r^8}\left[\sum_{q\neq 0}\sum_{p\neq 0}\sum_{n\neq 0}\frac{\langle 0|\,\hat{Q}_{1,0}\,|q\rangle\,\langle q|\,\hat{Q}_{1,0}\,|p\rangle\,\langle p|\,\hat{Q}_{1,0}\,|n\rangle\,\langle n|\,\hat{Q}_{1,0}\,|0\rangle}{(E_0-E_n)(E_0-E_p)(E_0-E_q)} - \sum_{q\neq 0}\sum_{n\neq 0}\frac{\langle 0|\,\hat{Q}_{1,0}\,|n\rangle\,\langle n|\,\hat{Q}_{1,0}\,|0\rangle}{(E_0-E_n)}\,\frac{\langle 0|\,\hat{Q}_{1,0}\,|q\rangle\,\langle q|\,\hat{Q}_{1,0}\,|0\rangle}{(E_0-E_q)^2}\right].\tag{A10}$$

Note that all the terms ($\langle 0|\,V\,|0\rangle$) are equal to zero since this is the expected value of the dipole moment. In the same way as previously done, such correction (A10) can be related to the second hyperpolarizability tensor [20],

$$\begin{aligned}\gamma_{lk,l'k',l''k'',l'''k'''} =& \,\mathcal{S}\sum_{q\neq 0}\sum_{p\neq 0}\sum_{n\neq 0}\frac{\langle 0|\,\hat{Q}_{l,k}\,|q\rangle\,\langle q|\,\hat{Q}_{l',k'}\,|p\rangle\,\langle p|\,\hat{Q}_{l'',k''}\,|n\rangle\,\langle n|\,\hat{Q}_{l''',k'''}\,|0\rangle}{(E_n-E_0)(E_p-E_0)(E_q-E_0)}\\ &-\mathcal{S}\sum_{q\neq 0}\sum_{n\neq 0}\frac{\langle 0|\,\hat{Q}_{l,k}\,|n\rangle\,\langle n|\,\hat{Q}_{l',k'}\,|0\rangle}{(E_n-E_0)}\,\frac{\langle 0|\,\hat{Q}_{l'',k''}\,|q\rangle\,\langle q|\,\hat{Q}_{l''',k'''}\,|0\rangle}{(E_q-E_0)^2},\end{aligned}\tag{A11}$$

where $\mathcal{S}$ is, as commented before, the sum of all permutations (in this specific case $\mathcal{S} = 4!$), leading to a term for the potential in the form of

$$V = -\frac{\gamma_{10,10,10,10}}{24r^8} = -\frac{\gamma}{24r^8}.\tag{A12}$$

Such second hyperpolarizability $\gamma_{10,10,10,10}$ is also denoted by dipole-dipole-dipole-dipole hyperpolarizability, as shown in Table V. Both first and second hyperpolarizabilities represent the nonlinear response to the electric external field.

[1] G. F. Gribakin, J. A. Young, and C. M. Surko, Positron-molecule interactions: Resonant attachment, annihilation, and bound states, Rev. Mod. Phys. **82**, 2557 (2010).

[2] L. Chiari and A. Zecca, Recent positron-atom cross section measurements and calculations, Eur. Phys. J. D **68**, 297 (2014).

[3] P. Coleman, T. Griffith, G. Heyland, and T. Killeen, *Atomic Physics* (Plenum, New York, 1975).

[4] M. Charlton, T. C. Griffith, G. R. Heyland, and G. L. Wright, Total scattering cross sections for intermediate-energy positrons in the molecular gases H_2, O_2, N_2, CO_2 and CH_4, J. Phys. B **13**, L353 (1980).

[5] M. Charlton, T. C. Griffith, G. R. Heyland, and G. L. Wright, Total scattering cross sections for low-energy positrons in the molecular gases H_2, N_2, CO_2, O_2 and CH_4, J. Phys. B **16**, 323 (1983).

[6] Y. Katayama, O. Sueoka, and S. Mori, Inelastic cross section measurements for low-positron-O_2 collisions, J. Phys. B **20**, 1645 (1987).

[7] M. S. Dababneh, Y.-F. Hsieh, W. E. Kauppila, C. K. Kwan, S. J. Smith, T. S. Stein, and M. N. Uddin, Total-cross-section measurements for positron and electron scattering by O_2, CH_4, and SF_6, Phys. Rev. A **38**, 1207 (1988).

[8] J. P. Marler and C. M. Surko, Positron-impact ionization, positronium formation, and electronic excitation cross sections for diatomic molecules, Phys. Rev. A **72**, 062713 (2005).

[9] T. Mukherjee and A. S. Ghosh, Total and rotational cross sections in-scattering, J. Phys. B **29**, 2347 (1996).

[10] A. Jain, Low-energy positron-argon collisions by using parameter-free positron correlation polarization potentials, Phys. Rev. A **41**, 2437 (1990).

[11] A. Jain, A treatment of low-energy positron-CO collisions using a new parameter-free positron correlation polarization (PCOP) potential, J. Phys. B: At. Mol. Opt. Phys. **23**, 863 (1990).

[12] D. A. Przybyla, W. Addo-Asah, W. E. Kauppila, C. K. Kwan, and T. S. Stein, Measurements of differential cross sections for positrons scattered from N_2, CO, O_2, N_2O, and CO_2, Phys. Rev. A **60**, 359 (1999).

[13] J. P. Marler, *New Results for Positron Scattering from Noble Gas Atoms and Diatomic Molecules* (University of California, San Diego, 2005).

[14] L. Chiari, A. Zecca, S. Girardi, E. Trainotti, G. García, F. Blanco, R. P. McEachran, and M. J. Brunger, Positron scattering from O_2, J. Phys. B **45**, 215206 (2012).

[15] K. L. Baluja and A. Jain, Total (elastic and inelastic) scattering cross sections for several positron-molecule systems at 10–5000 eV: H_2, H_2O, NH_3, CH_4, N_2, CO, C_2 H_2, O_2, SiH_4, CO_2, N_2O, and CF_4, Phys. Rev. A **45**, 7838 (1992).

[16] D. Raj, Total cross sections for positron scattering by molecules, Phys. Lett. A **174**, 304 (1993).

[17] D. D. Reid and J. Wadehra, Scattering of intermediate-energy positrons by C, N, O atoms and the corresponding diatomic molecules: elastic and total cross-sections, Chem. Phys. Lett. **311**, 385 (1999).

[18] S. De-Heng, L. Yu-Fang, S. Jin-Feng, Z. Zun-Lue, and Y. Xiang-Dong, Positron total cross sections for collisions with O_2, H_2O, and CH_4 in energy range from 30 to 3000 eV, Chin. Phys. **14**, 964 (2005).

[19] A. D. Buckingham, Theory of long-range dispersion forces, Discuss. Faraday Soc. **40**, 232 (1965).

[20] A. D. Buckingham and B. J. Orr, Molecular hyperpolarisabilities, Q. Rev. Chem. Soc. **21**, 195 (1967).

[21] F. A. Gianturco, A. Jain, and J. A. Rodriguez-Ruiz, Test of local model potentials for positron scattering from rare gases, Phys. Rev. A **48**, 4321 (1993).

[22] D. D. Reid, W. B. Klann, and J. M. Wadehra, Scattering of low- to intermediate-energy positrons from molecular hydrogen, Phys. Rev. A **70**, 062714 (2004).

[23] J. Franz, K. Fedus, and G. P. Karwasz, Do positrons measure atomic and molecular diameters?, Eur. Phys. J. D **70**, 155 (2016).

[24] J. Franz, Positron-electron correlation-polarization potentials for the calculation of positron collisions with atoms and molecules, Eur. Phys. J. D **71**, 44 (2017).

[25] J. Horáček and T. Sasakawa, Method of continued fractions with application to atomic physics, Phys. Rev. A **28**, 2151 (1983).

[26] M.-T. Lee, I. Iga, M. Fujimoto, and O. Lara, The method of continued fractions for electron (positron)-atom scattering, J. Phys. B **28**, L299 (1995).

[27] M.-T. Lee, M. Fujimoto, and I. Iga, Application of the method of continued fractions to low-energy electron scattering by the hydrogen molecule, J. Mol. Struct.: THEOCHEM **394**, 117 (1997).

[28] E. M. S. Ribeiro, L. E. Machado, M.-T. Lee, and L. M. Brescansin, Application of the method of continued fractions to electron scattering by polyatomic molecules, Comput. Phys. Commun. **136**, 117 (2001).

[29] T. H. Dunning and P. J. Hay, Gaussian basis sets for molecular calculations, in *Methods of Electronic Structure Theory* (Springer, New York, 1977), pp. 1–27.

[30] D. Feller, The role of databases in support of computational chemistry calculations, J. Comput. Chem. **17**, 1571 (1996).

[31] K. L. Schuchardt, B. T. Didier, T. Elsethagen, L. Sun, V. Gurumoorthi, J. Chase, J. Li, and T. L. Windus, Basis set exchange: a community database for computational sciences, J. Chem. Inf. Model. **47**, 1045 (2007).

[32] D. R. Lide *et al.*, *CRC Handbook of Chemistry and Physics* (CRC Press, Boca Raton, 2012).

[33] M. Bartolomei, E. Carmona-Novillo, M. I. Hernández, J. Campos-Martínez, and R. Hernández-Lamoneda, Long-range interaction for dimers of atmospheric interest: Dispersion, induction and electrostatic contributions for O_2-O_2, N_2-N_2 and O_2-N_2, J. Comput. Chem. **32**, 279 (2011).

[34] E. R. Cohen and G. Birnbaum, Influence of the potential function on the determination of multipole moments from pressure-induced far-infrared spectra, J. Chem. Phys. **66**, 2443 (1977).

[35] A. Buckingham, R.-L. Disch, and D. Dunmur, Quadrupole moments of some simple molecules, J. Am. Chem. Soc. **90**, 3104 (1968).

[36] D. Spelsberg and W. Meyer, Static dipole polarizabilities of N_2, O_2, F_2, and H_2O, J. Chem. Phys. **101**, 1282 (1994).

[37] M. Medved', M. Urban, V. Kellö, and G. H. Diercksen, Accuracy assessment of the ROHF–CCSD(T) calculations of static dipole polarizabilities of diatomic radicals: O_2, CN, and NO, J. Mol. Struct.: THEOCHEM **547**, 219 (2001).

[38] S. C. B. North, *Interactions Between Oxygen Molecules, for Atmospheric Applications* (Michigan State University, East Lansing, MI, 2016).

[39] H. Hettema, P. Wormer, P. Jo/rgensen, H. A. Jensen, and T. Helgaker, Frequency-dependent polarizabilities of O_2 and van der Waals coefficients of dimers containing O_2, J. Chem. Phys. **100**, 1297 (1994).

[40] D. P. Shelton, Nonlinear-optical susceptibilities of gases measured at 1064 and 1319 nm, Phys. Rev. A **42**, 2578 (1990).

[41] P. Calaminici, K. Jug, and A. M. Köster, Density functional calculations of molecular polarizabilities and hyperpolarizabilities, J. Chem. Phys. **109**, 7756 (1998).

[42] S. S. Batsanov, van der Waals radii of elements, Inorg. Mater. **37**, 871 (2001).

[43] M. J. Brunger, S. J. Buckman, and K. Ratnavelu, Positron scattering from molecules: An experimental cross section compilation for positron transport studies and benchmarking theory, J. Phys. Chem. Ref. Data **46**, 023102 (2017).

[44] Y. N. Kalugina and V. Cherepanov, Multipole electric moments and higher polarizabilities of molecules: Methodology and some results of ab initio calculations, Atmos. Oceanic Opt. **28**, 406 (2015).

[45] A. Kumar, W. J. Meath, P. Bündgen, and A. J. Thakkar, Reliable anisotropic dipole properties, and dispersion energy coefficients, for O_2 evaluated using constrained dipole oscillator strength techniques, J. Chem. Phys. **105**, 4927 (1996).

[46] N. J. Bridge and A. D. Buckingham, The polarization of laser light scattered by gases, Proc. R. Soc. London. Ser. A **295**, 334 (1966).

[47] A. Newell and R. Baird, Absolute determination of refractive indices of gases at 47.7 gigahertz, J. Appl. Phys. **36**, 3751 (1965).

[48] W. Tenfen, K. T. Mazon, S. E. Michelin, and F. Arretche, Low-energy elastic positron cross sections for H_2 and N_2 using an *ab initio* target polarization, Phys. Rev. A **86**, 042706 (2012).

[49] A. Jain and F. Gianturco, Low-energy positron collisions with CH_4 and SiH_4 molecules by using new positron polarization potentials, J. Phys. B **24**, 2387 (1991).

[50] A. J. Stone, *The Theory of Intermolecular Forces*, 2nd ed. (Oxford University Press, Oxford, 2013).

[51] M. V. Barp, E. P. Seidel, F. Arretche, and W. Tenfen, Rotational excitation of N_2 by positron impact in the adiabatic rotational approximation, J. Phys. B **51**, 205201 (2018).

[52] See Eq. (2.3.8) of Ref. [50].

[53] D. M. Bishop and J. Pipin, Dipole, quadrupole, octupole, and dipole-octupole polarizabilities at real and imaginary frequencies for H, He, and H_2 and the dispersion-energy coefficients for interactions between them, Int. J. Quantum Chem. **45**, 349 (1993).

[54] G. Maroulis and A. J. Thakkar, Multipole moments, polarizabilities, and hyperpolarizabilities for N_2 from fourth-order many-body perturbation theory calculations, J. Chem. Phys. **88**, 7623 (1988).

[55] E.-A. Reinsch and W. Meyer, Finite-perturbation calculation of static quadrupole and mixed dipole-octupole polarizabilities for the ground states of the first-row atoms, Phys. Rev. A **18**, 1793 (1978).