Low-energy elastic positron cross sections for H_2 and N_2 using an *ab initio* target polarization

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Using an *ab initio* model to account the polarization effects of molecules in the presence of slow positrons, we have obtained low-energy positron cross sections for H_2 and N_2 molecules. The polarization model proposed here is calculated with the expected values of the positron-electron interaction operator in the polarized target wave function for each fixed distance of the positron. Together with the electrostatic potential, this polarization describes the interaction potential in a static-polarization approximation. Within this interaction level, we have obtained differential and integral cross sections that are in good agreement with recent measurements of the Trento group and other theoretical approaches.

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I. INTRODUCTION

The positron interaction with molecular targets is a very interesting problem. To consider the interactions correctly in the elastic regime, one must be able to represent the direct and polarization interactions. Temkin and Vasavada [1] showed that the scattering of electrons from molecular species is strongly dependent on polarization effects, which suggests that in the scattering of positrons these effects should be important. In this paper, we report a model potential with an *ab initio* technique to take into account the polarization effects. Many methodologies have been proposed to treat it and the results obtained so far are still matter of discussion [2–4].

Using the polarization correlation potential (PCOP) model [3], we were able to successfully obtain reliable differential and integral cross sections for positron scattering with CO, N_2O, and H_2O molecules [5–7]. All of them are polar molecules, therefore the dipole term presents a very strong contribution and dominates the characteristics of the scattering dynamics. In our most recent work [8], vibrational resolved cross sections for positron collisions with N_2 molecules were reported, and an interesting feature became noticeable: the integral cross section for this molecule using the PCOP model presented a minimum structure, which does not appear in any measurements [9–11] or in any theoretical results obtained using different methodologies for the polarization effects [2,12–18]. Among these methodologies we quote the *ab initio R* matrix [12,19], Kohn variational [13,20–22], Schwinger multichannel method (SMC) [14,23], and the models PCOP [3], distributed positron model [24], and semiclassical formulations [25].

Actually, this minimum is not a particularity of positron N_2 scattering, since a similar phenomenon was observed in the case of positron H_2 scattering [26] and in CH_4 and SiH_4 [27].

To date, this minimum has not been attributed to well-known effects such as the Ramsauer minimum, for example.

Recognizing the fact that the PCOP can generate unphysical structures in the cross sections of nonpolar molecules, we propose a potential model that is able to take into account both short- and long-range interactions properly, so the minimum presented in the theoretical scattering cross sections disappear in agreement with the experimental data. Our objective is to go beyond the PCOP and other polarization models. In order to perform such a task, we must identify the physical characteristics of the polarization model which could be the cause of the structures in the cross sections. First, we notice that the choice of the cutoff radius in the PCOP model is absolutely arbitrary. In that model, the first coordinate at which the polarization curve crosses the correlation curve defines the cutoff radius. The idea is that beyond that point the polarization term would be more relevant to describe dynamic effects of the target particles in the presence of the positron, even if the cutoff radius is located inside the molecular electronic cloud. Second, the correlation potential curve represents the polarization of a free electron gas in the presence of a positron [28], so using this potential curve is equivalent to considering the molecular orbitals as a free electron gas. The third aspect is that the polarization term (V_{pol}) of the PCOP curve should contribute only for very large distances from the molecule. Therefore, for coordinates located between the minimum of the interaction potential and the region where V_{pol} is valid, the behavior of the interaction should be slightly different.

Considering these aspects, we can propose an interaction model which is more realistic in the description of the polarization potential. Once the interaction is determined, we will be able to use the method of continued fractions (MCF) [29] to solve the scattering equations in order to obtain differential and integral cross sections. A comparison between our results and other recent theoretical and experimental data can be elucidative in the sense of understanding important physics in the polarization potential.

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II. THEORY

We write the interaction potential in the static-polarization approximation

$$V_{\text{int}}(\vec{r}_i,\vec{r}_p,\vec{R}) = V_{\text{stat}}(\vec{r}_i,\vec{r}_p,\vec{R}) + V_{\text{pol}}(\vec{r}_p,\vec{R}), \qquad (1)$$

where the static term is the Coulomb potential

$$V_{\text{stat}}(\vec{r}_i,\vec{r}_p,\vec{R}) = -\sum_i \frac{1}{|\vec{r}_i - \vec{r}_p|} + \sum_j \frac{Z_j}{|\vec{R}_j - \vec{r}_p|}. \qquad (2)$$

In order to fully describe the interaction we must determine the polarization term V_{pol} in such a way that, for large distances,

$$V_{\text{pol}}(\vec{r}_p \to \infty) = -\frac{1}{2}\left(\frac{\alpha_0}{r^4} + \frac{\alpha_2}{r^4} P_2\left[\cos(\theta)\right]\right), \qquad (3)$$

and, in the short-range region, $V_{\text{pol}}(\vec{r}_p,\vec{R})$ must be associated with the response effects of the target particles in the presence of a positron, a feature better known as the positron correlation potential. Some approximations have been made to consider these effects [2,3,24,25,30]; however, the obtained results were not satisfactory when compared to experimental data [8,26, 27].

To overcome this difficulty, we propose a potential model to treat the polarization effects in the molecular target in the presence of a positron. We can represent the positron wave function based on the methodology of Assafrão *et al.* [31] and calculate the target molecular ground-state wave function in the presence of the positron ϕ_0^{pol}, for each distance between the positron and the molecule. With this target wave function we can obtain the energy differences in the electronic cloud as we fix the positron in different positions, obtaining a function V_{pol} which is parametrically constructed as

$$V_{\text{pol}}(\vec{r}_p,\vec{R}) = \left\langle \phi_0^{\text{pol}} \middle| h_1 \middle| \phi_0^{\text{pol}} \right\rangle - \langle \phi_0 | h | \phi_0 \rangle, \qquad (4)$$

where ϕ_0^{pol} is the positron-molecule bound-state wave function computed as in Ref. [31] as stated above, the operator h_1 is

$$h_1 = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_i \sum_j \frac{Z_j}{|r_i - r_j|} - \sum_i \frac{1}{|r_i - r_p|}, \qquad (5)$$

which represents the positron-molecule Hamiltonian without electron-electron interactions, and h is the same operator as h_1 for large positron molecule distances

$$h_1(r_p \to \infty) = h. \qquad (6)$$

Since the target wave function is explicitly dependent on the electron coordinates $[\phi_0^{\text{pol}} = \phi_0^{\text{pol}}(r_i; r_p, R)]$, the integration in Eq. (4) is carried out in those coordinates, implying that the polarization function depends parametrically on the positron distance from the molecule and on the internuclear distances which are maintained fixed during the calculations. This integral represents the expected value of the interaction energy between the positron and electrons related to the positron-molecule composite wave function. In order to construct V_{pol}, the energy of the composite disregarding electron-electron interactions is subtracted from the first term, within the hypothesis that only the positron-electron interactions gives rise to polarization effects.

Considering that Eq. (4) describes the polarization interaction in a good approximation, the problem now lies in the determination of the positron continuum wave function ψ by the scattering equation

$$|\psi\rangle = |s\rangle + G_0 V_{\text{int}} |\psi\rangle. \qquad (7)$$

In order to solve it, we employ the method of continued fractions [29]. Only a brief description of the referred method is explicitly shown here. The reader is directed to the original article of Horáček and Sasakawa for technical details. It was applied to treat positron-molecule scattering for the first time by Arretche *et al.* [5]. In this method, the interaction potential is weakened in each iteration, so it can be considered as negligible when it does not interfere anymore in the scattering wave function. Considering that the K matrix in the first Born approximation is not zero, let us write this weakened interaction potential (for simplicity $V_{\text{int}} = V$) as

$$V^{(1)} = V - \frac{V|s\rangle\langle s|V}{\langle s|V|s\rangle}, \qquad (8)$$

where s is the same plane wave of Eq. (7). Inserting Eq. (8) into Eq. (7), we obtain that

$$|\psi\rangle = |s\rangle + (1 - G_0 V^{(1)})^{-1} G_0 V|s\rangle \frac{\langle s|V|\psi\rangle}{\langle s|V|s\rangle}, \qquad (9)$$

using the orthogonality between Eq. (8) and $|s\rangle$. In order to rewrite Eq. (9) in the same form as Eq. (7), we define the functions

$$|s_1\rangle = G_0 V|s\rangle \qquad (10)$$

and

$$|\psi_1\rangle = (1 - G_0 V^{(1)})^{-1}|s\rangle, \qquad (11)$$

so it follows that

$$|\psi_1\rangle = |s_1\rangle + G_0 V^{(1)}|\psi_1\rangle. \qquad (12)$$

To solve Eq. (12), we write the potential $V^{(1)}$ as a new weakened potential

$$V^{(2)} = V^{(1)} - \frac{V^{(1)}|s_1\rangle\langle s_1|V^{(1)}}{\langle s_1|V^{(1)}|s_1\rangle}, \qquad (13)$$

and follow the same procedure as above, finding a new equation in the same form as Eq. (7):

$$|\psi_2\rangle = |s_2\rangle + G_0 V^{(2)}|\psi_2\rangle. \qquad (14)$$

We can repeat this until the potential $V^{(n)}$ is sufficiently weak, so that the scattering equation simply becomes

$$|\psi_n\rangle \approx |s_n\rangle, \qquad (15)$$

and then we can recursively construct the scattering wave function ψ, solving Eq. (7). However, it is easier to obtain the scattering amplitude than the scattering wave function itself. If we define the reactance matrix K_n as

$$K_n = \langle s_{n-1}|V^{(n-1)}|\psi_n\rangle, \qquad (16)$$

we can obtain it iteratively by using

$$K_n = \langle s_{n-1}|V^{(n-1)}|s_n\rangle + \frac{\langle s_n|V^{(n)}|s_n\rangle^2}{\langle s_n|V^{(n)}|s_n\rangle - K_{n+1}}. \qquad (17)$$

Once the reactance matrix K is obtained, we can calculate the transition matrix T through the expression

$$T = -\frac{2iK}{(1-iK)}. \tag{18}$$

The scattering amplitude is related to the transition matrix through the relation

$$f = -2\pi T, \tag{19}$$

and then the differential cross section for elastic positron molecule scattering averaged over the orientations of the molecule is calculated with

$$\frac{d\sigma}{d\Omega} = \frac{1}{8\pi^2} \int |f|^2 d\alpha \sin\beta \, d\beta \, d\gamma, \tag{20}$$

where (α, β, γ) are the Euler angles associated with the principal axes of the molecule.

III. NUMERICAL DETAILS

The parameters used in the calculations are presented in Table I. The internuclear distances were kept constant along the calculations. For the description of the ground state of the H_2 and N_2 molecules, we employed the Gaussian-type basis set from Dunning [32,33], with augmented functions as described in Table I.

All calculations were carried out in a 600-point radial grid, where the maximum value for the radial coordinate used was $r_{max} = 26a_0$. It was chosen this way to provide the normalization of the valence orbital both in H_2 and N_2. The highest partial wave considered in the K-matrix expansion was $l = 6$ and a maximum number of 10 iteration were needed to obtain convergence.

IV. RESULTS AND DISCUSSION

The construction of the present model allows the determination of the polarization potential for all distances between the positron and the molecule. Using the numerical parameters given in Table I, we evaluate Eq. (4) for each position in the radial grid for H_2 and N_2 molecules. In the following sections, we present the results obtained for those molecules and compare them with other available data.

A. H_2

H_2 is the simplest neutral diatomic molecule, working as a model problem in the positron-molecule research field.

TABLE I. Numerical parameters used in the calculations.

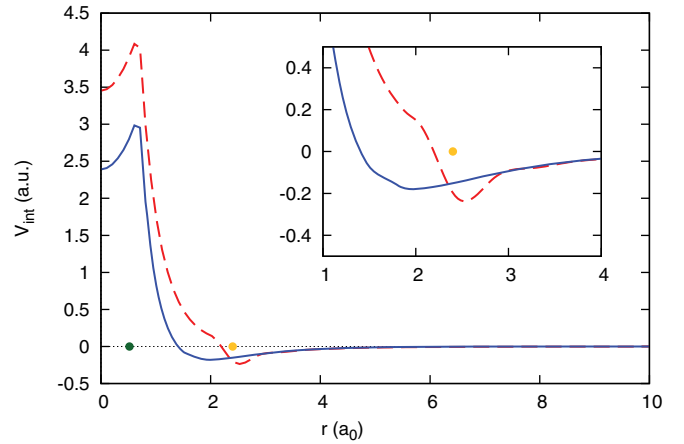|	H_2	N_2
Internuclear distance	$1.041a_0$ [49]	$2.0744a_0$ [49]
Dipole polarizability	$5.4142a_0^3$ [50]	$11.7442a_0^3$ [51]
Basis set	[33]	[32]
Augmented s functions		0.0653, 0.0213
Augmented p functions		0.0449, 0.0123
Augmented d functions		0.3730

FIG. 1. (Color online) Spherical component of the positron H_2 interaction potential. The solid blue line represents the result obtained in the present work. The dashed red line represents the interaction potential obtained within the PCOP approximation. The green and golden points are, respectively, the position of the hydrogen atoms and the cutoff radius. Inset shows the magnification of the curves from $1a_0$ to $4a_0$ showing the cutoff region ($r = 2.4a_0$). The points in this figure are connected by a cubic spline.

Because of that, the literature is rich with studies of positron-H_2 collisions. Many theoretical approaches have been made [12,23,25,26,34–40] and four experimental sets in the 1 to 10 eV energy range are available [9,41–43].

Considering the experimental studies, only the most recent measurement of Zecca *et al.* [41] provides data for the energy range from 0.1 to 1.0 eV. This is what we classify as the very-low-energy regime. For our potential this is the most striking test, since that in this energy range the polarization effects are the dominant ones.

In Fig. 1 we show our potential (solid blue line) computed according to Eq. (1) by using the static and the polarization potentials as respectively described in Eqs. (2) and (4), compared to the PCOP [3] curve (dashed red line) generated in the same radial grid. As we can see, these potentials have similar behaviors for distances greater than $\sim 3a_0$ from the molecular center, but they exhibit different dependencies as we approach the molecular target. The green and golden dot points given in the figure represent the position of the hydrogen atoms and the PCOP cutoff radius ($\sim 2.4a_0$), respectively. From the inset in Fig. 1, we can see that the present model potential is more attractive in the region closer to the molecular border and has a larger range. The PCOP curve has a "knee" structure followed by a minimum. This inflexion point comes from the functional form of the correlation potential used in the construction of the PCOP. For more details about this theme, we recommend the references given in Ref. [3]. The minimum present in the PCOP model comes from the matching of the correlation with the polarization potential at the cutoff radius ($\sim 2.4a_0$). On the other hand, our potential is constructed with no "matching schemes." It has no "cutoff" radius and no adjustable parameters such as the molecular polarizability, for example. As the positron coordinates are parametrically generated, the potential is calculated for each positron position. It follows that the minimum present in
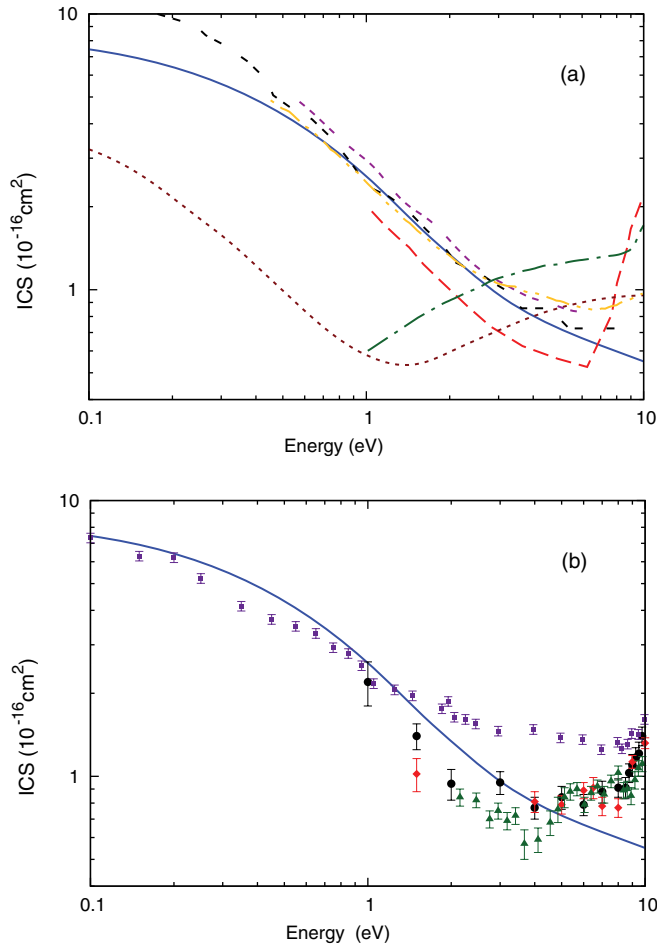
FIG. 2. (Color online) Integral elastic cross sections for positrons colliding with H_2. (a) Present work compared with other theoretical approaches. The solid blue line represents the present obtained results. The dotted maroon line is the result obtained using the PCOP. Other theoretical approaches are those of Reid *et al.* [25] (dashed red line), Zhang *et al.* [12] (dash-double-dotted golden line), Arretche *et al.* [23] (double-dash-space black line), Biswas *et al.* [36] (dash-dotted green line), and Mukherjee and Sarkar [34] (four-dashed-space purple line). (b) Present work compared with the available experimental sets: Zecca *et al.* [41] (purple squares), Zhou *et al.* [42] (red diamonds), Hoffmann *et al.* [9] (black dots), and Charlton *et al.* [43] (green triangles).

our potential comes exclusively from the positron-molecule interaction and does not depend, as stated above, from the choice of any arbitrary cutoff point. Once the polarization effects dominate the scattering in the low-energy regime, a reasonable description of the interaction potential in the valence region of the molecule is very important to determine the cross sections.

In Fig. 2 we show the integral cross sections obtained for positron H_2 compared with different [Fig. 2(a)] calculations and [Fig. 2(b)] experimental data. The first feature we wish to highlight is that our cross section (solid blue line) does not show the minimum structure present in the PCOP model (dotted maroon line). In fact, our results have good agreement with the calculations reported by Zhang *et al.* [12] (dash-double-dotted golden line) and Arretche *et al.* [23] (double-dash-space black line) using respectively the *R*-matrix

and Schwinger multichannel methods. Both are *ab initio* methodologies that deal explicitly with the many-body aspect of the problem. Considering methods that treat the problem as the scattering of a single particle by a potential, we see that the calculation of Reid *et al.* [25] (dashed red line) has the same energy dependence as ours but in a smaller magnitude. We attribute it to the fact that the polarization potential was described in a semiclassical model, constructed to make $V_{pol} \rightarrow 0$ as $r \rightarrow 0$; that is, as the positron position coincides with the molecular center, the polarization potential vanishes in their approach. We also note that Reid *et al.* [25] includes the inelastic channels through an absorption potential. The first inelastic threshold in this case is the positronium formation channel. It becomes energetically open at ~8.2 eV. As a consequence, their cross section starts to grow above this energy. Mukherjee and Sarkar [34] (four-dash-space purple line) considered rovibrational excitations using the PCOP model to describe polarization. It is easy to see that the magnitude and the dependence of the reported cross section are similar to ours. The work of Lino and Christ [38] and Lino [39] employed an alternative form of polarization interaction with the Schwinger multichannel method and obtained reasonable results. Liu *et al.* [37] and Sun *et al.* [40] both employed optical potential approaches; however, their results together with those from Refs. [38,39] are not shown in Fig. 2(a). In Fig. 2(b) we compare our cross section to the experimental ones. In the lower scattering energies, below ~1.5 eV, the agreement between our results and the data of Zecca *et al.* [41] is remarkable. This strongly suggests that our methodology to treat the polarization effects is in the right direction. For energies above ~1.5 eV our results get lower in magnitude than the results obtained in Zecca *et al.* [41] but are very similar to the Hoffman *et al.* [9] data until ~5 eV. As we can visualize in Fig. 2(a), other theoretical methods follow the same trend. Synthesizing the scenario described above, our cross section agrees very well with the data of Zecca *et al.* below 1 eV and with the data of Hoffman *et al.* above 1 eV.

As stated above, the description of the polarization effects plays a fundamental role in the determination of the low-energy cross sections. However, the present work is so far limited to describe exclusively the elastic electronic channel, as the inelastic rotational and vibrational cross sections should not contribute significantly to the cross-section magnitude. This is apparent when we compare the rovibrational results of Mukherjee and Sarkar [34] with the present elastic calculation and with measurements of Zecca *et al.* [41]. This means that, even if the rovibrational excitations were considered in the present work, the results would not be as high as the measurements in the 2 to 10 eV range. Another consideration regarding the calculations of Mukherjee and Sarkar [34] is that they employed the PCOP model to account polarization effects and did not observe a minimum in the integral cross section. The previous work of Mukherjee *et al.* [26] showed that rotational resolved cross sections would not have such a minimum, so the rovibrational cross sections of Mukherjee and Sarkar [34] are expected to not have the minimum as well. Looking at the cross sections of Reid *et al.* [25], we see that those results are lower than the present ones in the whole elastic scattering range, as stated above. Since the behavior of the low-energy positron molecule cross sections is

strongly dependent on the polarization effects, we quote that this difference should be attributed to the polarization model.

The monotonic decrease in the present elastic cross section from the point it begins to diverge from the measurements until the positronium formation threshold, can be addressed to the monochannel nature of our calculations. Above ∼2 eV up to the positronium threshold 8.6 eV, the cross section of the most recent measurement is practically constant, with values of about 1.5×10^{-16} cm^2 [41]. We notice that the two-channel calculation of Biswas *et al.* [36] provides the best theoretical comparison with the measurements of Zecca *et al.* [41] in this range. Biswas *et al.* [36] did not consider polarization effects, and this affects their very-low-energy cross sections; however, their calculation showed that the coupling between elastic and positronium formation scattering channels impacts over the cross sections in the vicinity of the opening channel. By adding the present cross sections with those calculated by Biswas *et al.* [36], we obtain an interesting curve, which even overestimated, gives a reasonable approximation to the measurements of Zecca *et al.* [41]. This suggests that, in a multichannel formulation, our results would agree with the measurements in the whole low-energy range. Even being in a monochannel approach, the present work is a considerable advance in the study of polarization effects over scattering in the very-low-energy range, where the coupling between elastic and positronium formation channels should not interfere in the cross sections. This analysis can be extended for the case of positron scattering with N$_2$.

Of course, polarization will interfere with the differential cross-section shape; therefore, comparing such curves will give us better insight into understanding the polarization effects. Figures 3(a) and 3(b) show the obtained differential elastic cross sections (solid blue lines) compared to those of Reid *et al.* [25] (dashed red lines) and Lino *et al.* [35] (dash-dotted green lines) for an impact energy of 4.5 and 6.9 eV, respectively. Overall, the agreement is satisfactory, but some divergences should be noted. It is interesting to observe the difference in all those curves in the midangle region, showing how the description of the polarization effects modifies the cross sections, as the calculations of Lino *et al.* [35] are performed within the same methodology of Arretche *et al.* [23]. The position of the minimum in the differential cross sections is different for each result; however, in the present calculations, this minimum is shifted towards higher angles. In the absence of experimental differential cross sections, it is not possible to state the correct position of the minimum. Nevertheless, there are such data for positron collisions with N$_2$ [44]. Table II brings other DCS values for H$_2$ in other energies to be compared with the results of Refs. [24,25,35].

B. N$_2$

The N$_2$ is a very interesting diatomic nonpolar molecule to study, for the same reasons cited for H$_2$. There are several available theoretical works of positron elastic collisions with the nitrogen molecule with different methodologies [2,14,15, 17,45]. In the experimental frontier, we identify four works which reported total cross sections [9–11,46]. As in the H$_2$ case, Zecca *et al.* [46] is the main set of data in the "very-low-energy range" with good energy resolution and small error
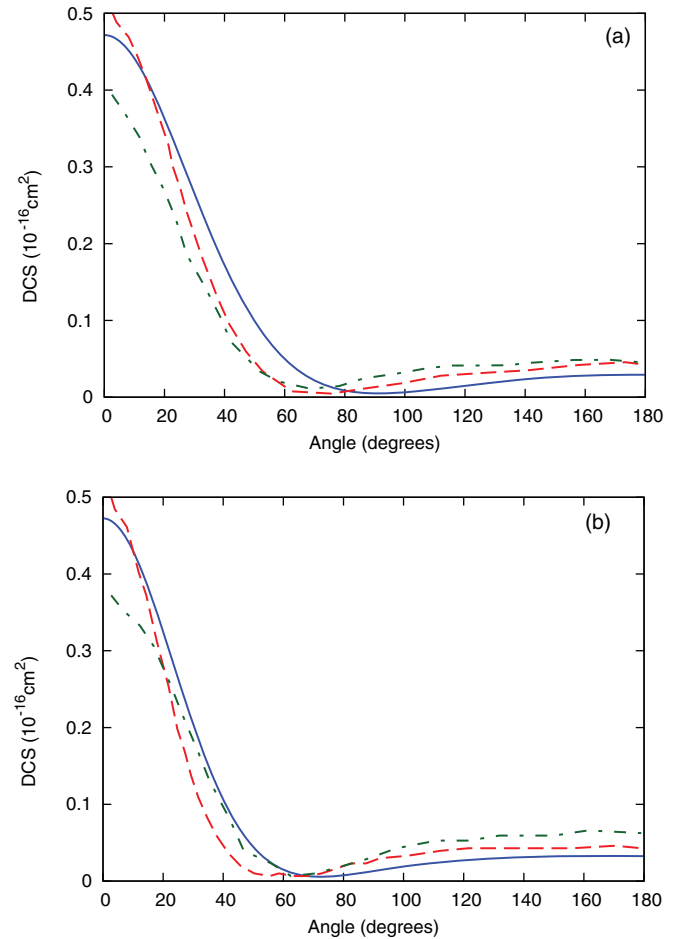

FIG. 3. (Color online) Differential elastic cross sections for positrons colliding with H$_2$. (a) Incident energy equal to 4.5 eV. (b) Incident energy equal to 6.9 eV. The solid blue lines represent the results of the present calculations. The dashed red lines are the results of Reid *et al.* [25]. The dash-dotted green lines are the results of Lino *et al.* [35].

bars. As far as we know, Przybyla *et al.* [44] reported the only set of experimental differential cross sections (DCSs) for positron N$_2$.

Comparing all the experimental cross sections, we clearly notice that no minimum structure is visible. This means that, if some minimum appears in the calculated cross sections, it should be attributed to difficulties in the determination of the interaction potential. There is a relatively good agreement between the measurements of Zecca [46] and Karwasz [11] as higher measurements. The data of Hoffman [9] and Sueoka [10] agree as well; however, their results seem to be underestimated when compared to the more recent one which can be attributed to lower angular resolution in the measurement apparatus. To date, there are no theoretical approaches which reproduce quantitatively the most recent measurements.

As for the H$_2$ system, we constructed the interaction curve as described in Eq. (4) and compared it with the PCOP model reported by Mazon *et al.* [8]. Curves representing both potentials are displayed in Fig. 4 for comparison. The captions are the same as those in Fig. 1. The minimum structure originated in the cutoff radius ($\sim 2.9a_0$) of the PCOP model is

TABLE II. Differential cross sections (units of 10^{-16} cm^2) for positron collisions with H$_2$. The energies are selected to be compared with those of Gibson [24], Reid *et al.* [25], and Lino *et al.* [35]. The notation $a(b)$ represents $a \times 10^b$.

Angle	2.72 eV	3.5 eV	4.08 eV	5.44 eV
0	0.4641	0.4682	0.4704	0.4729
10	0.4438	0.4434	0.4424	0.4377
20	0.3900	0.3784	0.3696	0.3482
30	0.3185	0.2940	0.2768	0.2396
40	0.2435	0.2092	0.1868	0.1428
50	0.1746	0.1364	0.1134	7.2826(−2)
60	0.1174	8.1110(−2)	6.1344(−2)	3.1111(−2)
70	7.3985(−2)	4.3696(−2)	2.9216(−2)	1.1300(−2)
80	4.3438(−2)	2.1095(−2)	1.2314(−2)	5.3604(−3)
90	2.3590(−2)	9.3549(−3)	5.6192(−3)	6.8076(−3)
100	1.1865(−2)	4.7901(−3)	4.9612(−3)	1.1276(−2)
110	5.9328(−3)	4.5928(−3)	7.4617(−3)	1.6354(−2)
120	3.9552(−3)	6.8948(−3)	1.1421(−2)	2.1085(−2)
130	4.4378(−3)	1.0387(−2)	1.5799(−2)	2.5174(−2)
140	6.1045(−3)	1.4060(−2)	1.9859(−2)	2.8476(−2)
150	7.8992(−3)	1.7114(−2)	2.3020(−2)	3.0795(−2)
160	9.1758(−3)	1.9105(−2)	2.4991(−2)	3.2052(−2)
170	9.8354(−3)	2.0108(−2)	2.5944(−2)	3.2534(−2)
180	1.0031(−2)	2.0402(−2)	2.6515(−2)	3.2641(−2)

visible for this molecule as well, and in the present calculated interaction potential the minimum originates exclusively from differences among the static and polarization potentials at the molecular border. The attractive part of the N$_2$ potential clearly has a larger range when compared to the similar one for H$_2$ (see the inset in Fig. 1), so we expect larger positron-N$_2$ cross sections when compared to the positron-H$_2$ cross sections.

In Fig. 5 we show the integral cross sections obtained for positron collisions with N$_2$ (solid blue line) compared with
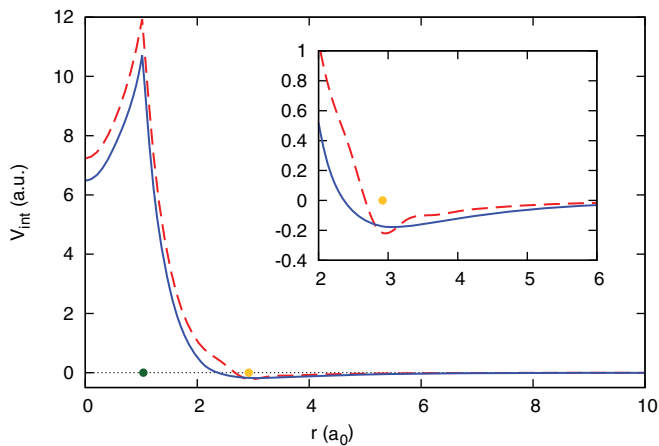

FIG. 4. (Color online) Spherical component of the positron N$_2$ interaction potential. The solid blue line represents the result obtained in the present work. The dashed red line represents the interaction potential obtained within the PCOP approximation. The green and golden points are, respectively, the position of the hydrogen atoms and the cutoff radius. Inset shows the magnification of the curves from $2a_0$ to $6a_0$ showing the cutoff region ($R = 2.9a_0$). The points in this figure are connected by a cubic spline.
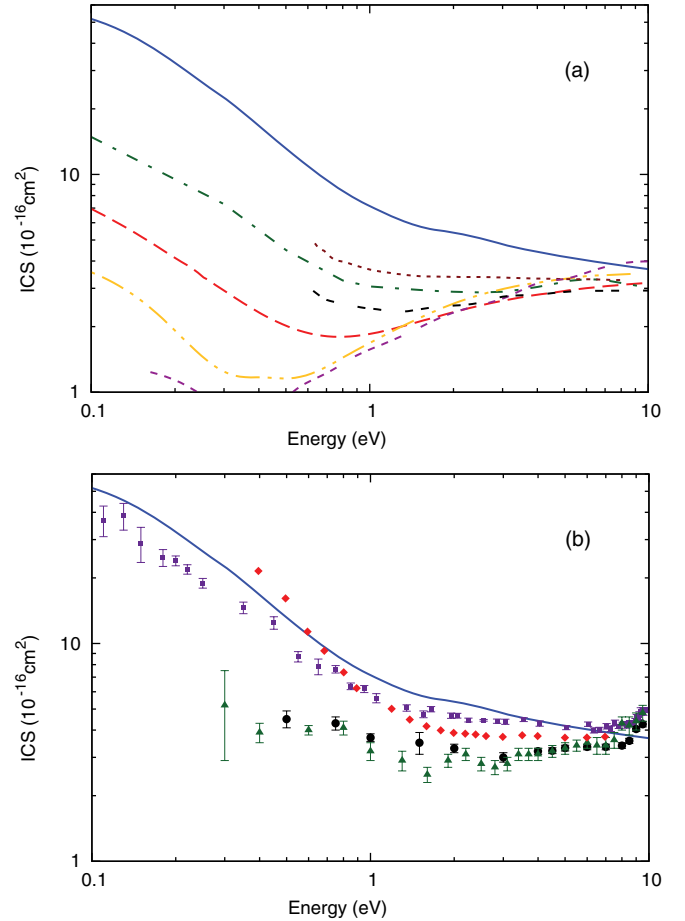

FIG. 5. (Color online) Integral elastic cross sections for positron colliding with N$_2$. (a) Present work compared with other theoretical approaches. The solid blue line represents the present obtained results. The dashed red line is the result obtained using the PCOP [8]. Other theoretical approaches are those of Elza *et al.* [2] (dotted maroon line), Gianturco and Mukherjee (BFVCC) [45] (two-dash-space black line), De Carvalho *et al.* [14] (dash-dotted green line), Mukherjee *et al.* (rotationally unresolved) [26] (dash-double-dotted golden line), and Danby and Tennyson [17] (four-dashed-space purple line). (b) Present work compared with the available experimental sets: Zecca *et al.* [46] (purple squares), Karwasz *et al.* [11] (red diamonds), Hoffmann *et al.* [9] (black dots), and Sueoka and Hamada *et al.* [10] (green triangles).

different [Fig. 5(a)] calculations and [Fig. 5(b)] experimental data. We start by paying attention to Fig. 5(b), where we can compare the "state of the art" of the experimental measurements. Clearly, no minimum is present in any experimental dataset. Taking it as the genuine physical condition, we assume that, if some minimum structure appears in the calculated cross section, it must be attributed to difficulties in the construction of the interaction potential, as stated above.

Considering the results presented in Fig. 5(a), our result (solid blue line) does not have any minimum structure, in contradiction to the calculations of Mazon *et al.* (dashed red line), Mukherjee *et al.* [26] (dash double-dotted golden line), Gianturco *et al.* (double-dashed black line), and Danby and Tennyson [17] (four-dashed purple line). We identify the calculations like those of De Carvalho *et al.* [14] (dash-dotted

green line) and Elza *et al.* [2] (dotted maroon line) as mono-tonically increasing toward lower energies. All PCOP model [8,26,45] elastic calculations clearly exhibit the undesired minimum structure. It is also present in the *R*-matrix result of Danby and Tennyson [17]. In the case of *ab initio* methods like *R* matrix and SMC, the generation of the interaction potential must be carefully considered. Both, as said before, attack the problem in the many-body context. It happens that, under these circumstances, the many-body basis set used can present overcorrelation, undercorrelation, and also linear-dependence problems. The RMPS (*R*-matrix with pseudostates method) is designed to go beyond the static plus polarization approxima-tion and take into account the correlations effects. For further details, see Tennyson [47]. We are not aware of any recent results obtained with the *R*-matrix method for positron N_2 since the former reported by Danby and Tennyson [17]. On the other hand, a fair representation of the polarization effects in the context of SMC is still not clear. An illustration of how the lack of polarization of the scattering basis set can affect the calculated cross sections can be found in Sanchez *et al.* [48] and in references therein. Despite this, calculations of De Carvalho *et al.* [14] for positron N_2 present good agreement with older experimental data [9–11]. The model employed by Elza *et al.* [2] is not *ab initio* or even complicated and presents a higher magnitude compared with the results of De Carvalho *et al.* [14] or Danby and Tennyson [17]. Our results are higher than all other theoretical approaches. This suggests that the interaction potential used in our calculation has a larger range than those considered by other methods.

The comparison of the present results with experimental data is interesting, because we observe good agreement with the most recent measurements. Our results clearly favor the recent data of Karwasz *et al.* [11] and Zecca *et al.* [46]. For very low energies, the agreement between the present results and measurements of Zecca *et al.* [46], as obtained for the H_2 molecule, indicates that the polarization interaction is fairly described. For the entire range, the present results follow the measurements of Karwasz *et al.* [11] and Zecca *et al.* [46], which do not hold true for H_2 molecule comparison with data of Zecca *et al.* [41]. We attribute this to the electronic structure of the molecules, as the nitrogen is more polarizable than hydrogen. The outermost orbital of the N_2 molecule is more responsive to the presence of a positron, so Eq. (4) describes the polarization interaction in a more accurate way to this molecule than to H_2, hence the description of the peripheral region of the N_2 molecule is better than that for H_2.

The calculated differential cross sections for positrons colliding with N_2 are presented in Figs. 6(a) and 6(b) for the incident energies of 6.75 and 10.0 eV, respectively. For the selected energies, comparison is made with theoretical available data of Elza *et al.* [2] (dotted maroon line), Mazon *et al.* [8] (dashed red line), the SMC calculation of De Carvalho *et al.* [14] and the quasielastic relative measurements of Przybyla *et al.* [44] as presented in Ref. [8]. In both presented energies, the presented differential cross sections show interesting features in the low-angle region. First, we observe that the decrease from low angles to the position of the minimum agrees very well with the measured point. This is a very clear difference in the theoretical cross sections. The position of the minimum is in better agreement with the
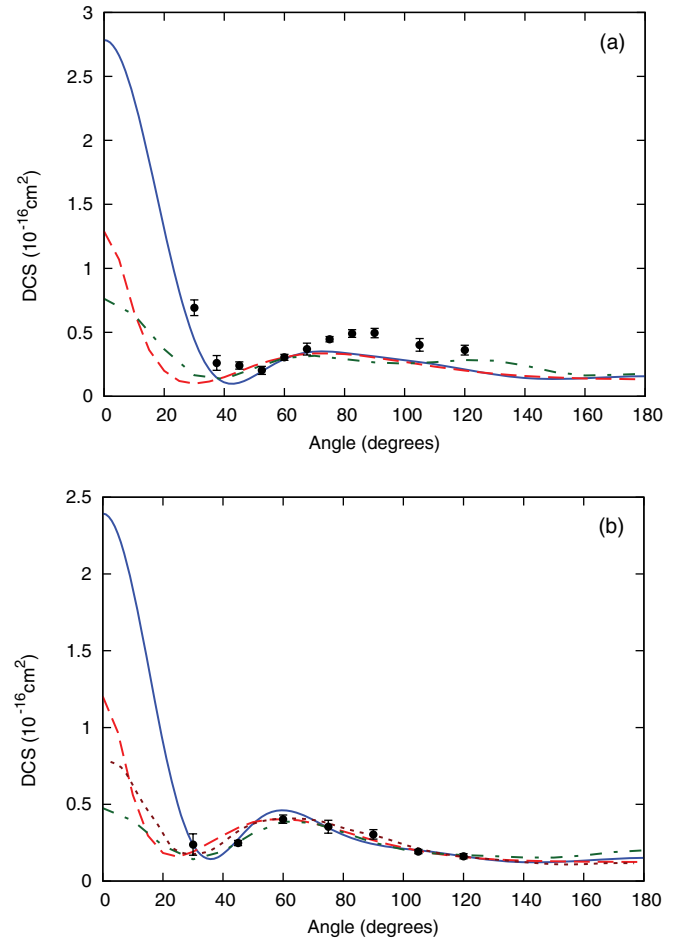

FIG. 6. (Color online) Differential elastic cross sections for positrons colliding with N_2. (a) Incident energy equal to 6.75 eV. (b) Incident energy equal to 10.0 eV. The solid blue lines represent the results of the present calculations. The dashed red lines represent the same calculation using the PCOP approximation to account for polarization effects [8]. The dash-dotted green lines are the results of de Carvalho *et al.* [14]. The dotted maroon line in panel (b) is the result of Elza *et al.* [2]. The black dots are the the relative measurements of Przybyla *et al.* [44] normalized as in Ref. [8].

measurements than other results, which once again will be attributed to the polarization model, as pointed out by Mazon *et al.* [8].

The description of the cross sections in mid and high angles seems to be independent of the polarization model and, partic-ularly for an incident energy of 6.75 eV, the available results still do not agree perfectly with the measured cross sections in this angular region. In the DCS for an incident energy of 10.0 eV this is not an issue, since the previous calculations already showed a good agreement with the measurements; however, we must point out that the present results reproduce the position of the minimum with better quality than previous calculations. Considering all these points, the present work shows a good progress in understanding the effects of polar-ization in a positron molecule scattering problem. Table III brings other DCS values for N_2 in other energies to be compared with the results of Refs. [2,8,14,44].

TABLE III. Differential cross sections (units of 10^{-16} cm^2) for positron collisions with N$_2$. The energies are selected to be compared with the calculations of Elza *et al*. [2], Mazon *et al*. [8], De Carvalho *et al*. [14], and Przybyla *et al*. [44]. The notation $a(b)$ represents $a \times 10^b$.

Angle	1.0 eV	4.0 eV	5.25 eV	6.0 eV
0	3.0496	3.0171	2.9302	2.8617
10	2.9443	2.6682	2.5177	2.4216
20	2.6513	1.8270	1.5663	1.4303
30	2.2288	0.9344	0.6582	0.5386
40	1.7473	0.3299	0.1694	0.1264
50	1.2705	8.1645(−2)	7.9237(−2)	0.1136
60	0.8470	6.7796(−2)	0.1663(−2)	0.2313
70	0.5072	0.1427	0.2519	0.3112
80	0.2624	0.2226	0.3074	0.3308
90	0.1086	0.2802	0.3212	0.3209
100	3.0413(−2)	0.3116	0.3150	0.3007
110	7.8320(−3)	0.3173	0.2923	0.2708
120	2.0328(−2)	0.3011	0.2551	0.2303
130	5.0271(−2)	0.2724	0.2134	0.1883
140	8.4624(−2)	0.2438	0.1804	0.1580
150	0.1153	0.2238	0.1632	0.1454
160	0.1384	0.2144	0.1602	0.1471
170	0.1524	0.2123	0.1641	0.1548
180	0.1571	0.2123	0.1667	0.1589

V. CONCLUSIONS

This work presents an *ab initio* model potential, designed to take into account the polarization effects in the low-energy elastic scattering of positrons by nonpolar molecules. As a first application, we considered the positron scattering by H$_2$ and N$_2$, since recent total cross section measurements are available for these targets. For H$_2$, we observe that our elastic cross sections agree with the Zecca *et al*. [41] data for energies below ∼1.5 eV and with the Hoffman *et al*. data [9] for higher energies. For N$_2$, our elastic cross sections clearly favor the more recent data of Karwasz *et al*. [11] and Zecca *et al*. [46] in the whole energy range. The computed differential cross sections have the midangle minimum shifted to higher angles. We attribute it to the polarization potential used, since in the previous work of Mazon *et al*. [8] exactly the same method was employed to solve the scattering equations, but with the PCOP model potential [3]. Further investigations will reveal if the model potential proposed is able to treat with success other nonpolar molecules.

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