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Implementation of a model potential in the Schwinger multichannel method to describe polarization in positron-atom and -molecule scattering: Studies for the noble-gas atoms, H_2, and N_2

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In this study, we evaluated a polarization scheme within the framework of the Schwinger multichannel method, using a model potential to describe positron-molecule polarization and correlation. Our aim was to calculate integral and differential cross sections for elastic scattering of positrons by noble gas atoms, hydrogen molecules, and nitrogen molecules. We compared our results with previous theoretical and experimental data, as well as with new results from a parallelized version of our computer codes, which allowed us to push the limits of our current *ab initio* methodology for small molecules. Our findings show that the model potential can recreate the s-wave integral cross sections from our best *ab initio* calculations, and also helps better understand the scattering process.

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I. INTRODUCTION

Understanding positron interactions with matter is of fundamental significance to many applications. For instance, positron annihilation is a core concept in the positron emission tomography (PET) scan for diagnostics in medicine [1,2], in positron annihilation spectroscopy for identification of defects in solids (especially in semiconductors) [3–6], and for the study of some astrophysical phenomena [7,8]. To correctly describe these processes, accurate experimental and theoretical data related to positron scattering, positronium formation, positron annihilation, and bound states [9,10] are required. Modeling these processes is a challenging task that usually requires cross-section (CS) data for positron scattering by different atoms and molecules. See, for instance, Refs. [11,12]. However, reliable experimental and theoretical CS data are not easy to determine since most of these data do not agree among themselves.

As of recently, for example, theoretical and experimental groups have encountered difficultiesin fully describing low-energy (below 10 eV) positron scattering even by simple nonpolar molecules such as methane [13]. In experiments, limitations in the angular resolution of different experimental apparatus seems to be responsible for the discrepancy among the results. On the other hand, in theoretical studies, the difficulties arise from accurately accounting for positron-molecule correlation-polarization interactions, especially in *ab initio* methods that rely on virtual single excitations to do it. These challenges likely explain the lack of agreement between theoretical predictions and experimental data, as well as the limited consistency among different theoretical approaches.

Usually, what is observed in the comparison of the calculated elastic scattering data with experiments is that the latter significantly underestimate the experimental results even when the positronium (Ps) formation channel is closed [13,14]. Particularly, it is expected for the measured total cross section (TCS) to be equal to the elastic cross section in positron-atom scattering in this energy region. In the case of a molecular target, even below the Ps formation threshold energy, other inelastic processes may occur (rotation and vibrational excitations). However, we expect their contribution to the TCS to be small when compared to the elastic process. Some hypotheses raised on why this happens are as folows: (i) lower than expected intensity of the calculated differential cross sections in smaller angles ($\theta < 30^\circ$) [14,15] and (ii) poor description of positron-molecule bound states, sometimes even identified as virtual states [16].

In theoretical *ab initio* methods such as the R-matrix and the Schwinger multichannel method (used in this work), the distortion of the electronic cloud due to the incoming positron (polarization) is described by virtual single excitations of the electrons of the target, an approximation known as static plus polarization (SP). According to Graves and Gorfinkiel [14,17], the current polarization schemes may be insufficient to describe the interaction between the incident positron and the electrons of the molecular target. Several strategies have been tested to improve this description such as use of extra chargeless centers and diffuse functions. The major problem with theses strategies is that it rapidly increased the cost of the calculation, limiting the targets we could scatter, and, even then, the results were not fully satisfactory [16–23]. Recently, we parallelized our computations' codes to take this approach even further pushing to the limits of what the *ab initio* strategy can obtain.

On the other hand, Tenfen *et al.* [24] suggested that these problems were related to the incapability of the calculations in the SP approximation to include higher polarizability terms other than the dipolar interaction in the polarization potential. The authors compared SMC results for the F_2 molecule with data obtained from the method of continued fractions (MCF) using the correlation-polarization potential proposed by Jain and Gianturco [25]. The difference in their work is that the polarization potential employed by Tenfen *et al.*

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includes terms all the way up to pure dipole hyperpolarizability, instead of only dipole polarizability as in Ref. [25]. The authors then compared their MCF and SMC results, showing that they agree only when the dipole polarizability term is included in the polarization potential, hence stating that the SMC method was unable to describe all the other higher-order terms. However, it is also important to notice that their correlation-polarization potential in the MCF calculation is single centered, which is not the case in the SMC method.

In light of these issues, different propositions on how to describe the correlation-polarization potential between the incident positron and the target molecules were made [24–27]. One such proposition, suggested by Swann and Gribakin [27], used an adapted form of the model potential of Mitroy and Ivanov [28] to describe the positron-molecule correlation-polarization potential. In their works, Swann and Gribakin [27,29–31] were able to calculate bound-state energies and annihilation parameters (Z_{eff}) with an excellent agreement with the measured experimental data. It is noteworthy that, since this is a semiempirical potential, they used one molecule as a way to obtain the value of the free parameter, by fitting of the experimental data, and then used the same parameter for similar systems. The results obtained for the other molecules were in good agreement with the experiment, showing that this potential could be used not only for understanding the positron-electron interactions but also to make predictions. They were also able to obtain scattering *s*-wave eigenphases with a good agreement with calculated theoretical data for many molecules. But it is worth mentioning that there are integral cross sections (ICS) and differential cross sections (DCS) using this model potential only for positron scattering by noble gas atoms [28].

As a way to further test this model potential and assess how well it can describe the ICS's and DCS's for the positron scattering from nonpolar molecules, we opted to include the model potential proposed by Swann and Gribakin [27,29–31] in the SMC method for positrons. Any successful new implementation should be able to reproduce previous benchmark data and provide improvements for new calculations. Thus, to test this implementation, in this work we calculated positron elastic scattering cross sections for noble gas atoms whose cross sections are benchmarked in the literature, and for the diatomic and nonpolar H_2 and N_2 molecules. These molecules have been chosen not only due to the availability of previous theoretical and experimental results, but also because (i) our codes allowed us to quickly perform the best calculations ever done with the SMC method for both molecules; (ii) Swann and Gribakin reported *s*-wave eigenphases for these systems, thus providing good test cases for our implementation; and (iii) simple enough to help us understand the physics behind the potential. This is also an important way to assess future possibilities of this model potential for bigger molecules since, as the size of the molecule increases, the computational cost becomes prohibitive.

This article will be organized as follows. In Sec. II we will briefly describe the SMC method, the correlation-polarization model potential and the polarization scheme used to achieve the results of this article. In Sec. III we present the calculated results for the integral cross section, differential cross sections, and s-wave eigenphases for positron elastic scattering from the systems of interest. Finally, Sec. IV we give some concluding remarks about the results.

II. THEORY

A. Schwinger multichannel method

The Schwinger multichannel method [32–36] has already been described in detail in other works in such a way that we will only review the most important aspects of the method. The resulting scattering amplitude from the Schwinger multichannel method for positron scattering from molecules or atoms has the following form:

$$f_{\text{SMC}}(\vec{k}_f,\vec{k}_i) = -\frac{1}{2\pi}\sum_{\mu,\nu}\langle S_{\vec{k}_f}|V|\chi_\mu\rangle(d^{-1})_{\mu\nu}\langle\chi_\nu|V|S_{\vec{k}_i}\rangle, \quad (1)$$

where

$$d_{\mu\nu} = \langle\chi_\mu|Q\hat{H}Q + PVP - VG_p^{(+)}V|\chi_\nu\rangle. \quad (2)$$

In the above expressions, P is the projection operator onto energetically open electronic states of the target; Q is the projection operator onto energetically closed electronic states of the target; $\hat{H}$ is the collision energy minus the full scattering Hamiltonian; $G_P^{(+)}$ is the free-particle Green's function projected on the P space; $|S_{\vec{k}_{i(f)}}\rangle$ is a solution of the unperturbed Hamiltonian H_0 and is given by the product of a target state and a plane wave with momentum $\vec{k}_{i(f)}$; V is the interaction potential between the incident positron and the electrons and nuclei of the target. Finally, $|\chi_\mu\rangle$ is an $(N+1)$ particles (N electrons and one positron) variational trial basis. Within the Schwinger multichannel method, the positron-molecule interactions can be treated in the static (S) and static plus polarization (SP) approximations.

In the S approximation, the target orbitals remain fixed in their calculated Hartree-Fock ground state. This means that correlation-polarization interactions are neglected in the scattering calculations conducted using this approximation. On the other hand, in the SP approximation, the electronic cloud of the target is allowed to distort due to the incoming particle through the use of virtual single excitations. To achieve this, the scattering wave function is expanded in a set of configuration states given by

$$|\Psi_{\vec{k}_i}^{(+)}\rangle = \sum_m c_{0m}^{(+)}(\vec{k}_i)|\chi_{0m}\rangle + \sum_r\sum_m c_{\text{rm}}^{(+)}(\vec{k}_i)|\chi_{\text{rm}}\rangle, \quad (3)$$

where $\{c_{\text{am}}^{(+)}(\vec{k}_i)\}$ are the variational coefficients. $|\chi_{0m}\rangle$ and $|\chi_{\text{rm}}\rangle$ are configuration state functions (CSF's) associated with the S and SP approximations, respectively, and are given by

$$|\chi_{0m}\rangle = |\Phi_0\rangle \otimes |\varphi_m\rangle, \quad (4)$$

and

$$|\chi_{\text{rm}}\rangle = |\Phi_r\rangle \otimes |\varphi_m\rangle, \quad (5)$$

where $|\Phi_0\rangle$ represents the ground state of the molecule obtained at the Hartree-Fock (HF) level, $|\varphi_m\rangle$ is a single-particle orbital used to represent the scattering orbital for the incident positron, and $|\Phi_r\rangle$ is obtained from a single virtual excitation of the target out of the HF reference state. In the present calculations, since only the elastic channel is open, $P = |\Phi_0\rangle\langle\Phi_0|$.

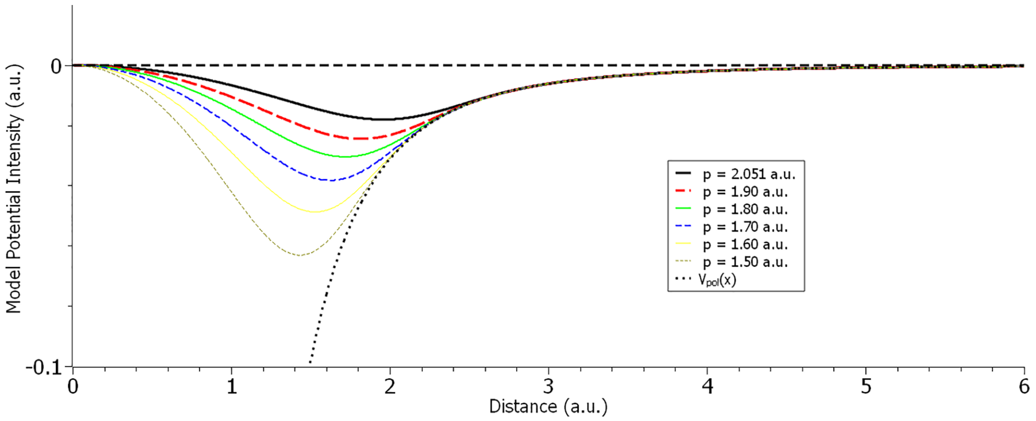

FIG. 1. Intensity of the model potential according to the distance from the origin for different values of ρ, considering $\alpha = 1$ a.u. $V_{\text{pol}}(x)$ corresponds to the expected asymptotic behavior of the correlation-polarization potential.

B. Model potential for correlation-polarization

The model potential proposed by Mitroy and Ivanov [28] to describe the correlation-polarization interactions between a positron and the electrons of an atom is the following:

$$V_{\text{CP}}(r) = -\frac{\alpha}{2r^4}\left[1 - \exp\left(-\frac{r^6}{\rho^6}\right)\right], \tag{6}$$

where α is the atomic polarizability of the target atom and ρ is the empirical parameter of the model potential. The behavior of the model potential in Eq. (6) with respect to the distance r for different values of ρ is presented in Fig. 1. This figure shows that the model potential exhibits the correct asymptotic behavior as r approaches infinity, namely, $V_{\text{CP}}(r) \xrightarrow[r\to\infty]{} -\alpha/(2r^4)$. Additionally, the exponential part of the model potential can account for short-range interactions (which may be associated with the correlation potential) other than the dipolar interaction. The choice of ρ regulates the strength of this short-range interaction.

Mitroy and Ivanov used positron s-wave eigenphases and bound-state energies to determine the optimal values of ρ in Eq. (6) for many atoms of interest. They compared their results with theoretical *ab initio* data available at the time and showed that a model potential that accurately reproduces scattering theoretical results could also reproduce the energy dependence of the annihilation parameter.

Encouraged by the success of the model potential in Eq. (6) for atoms, Swann and Gribakin decided to extend its application to positron scattering from molecules. To do so, they adapted the model potential, which now has the following form:

$$\begin{aligned} V_{\text{CP}}(\vec{r}) &= \sum_A V_{\text{CP}}^{(A)}(\vec{r}) \\ &= -\sum_A \frac{\alpha_A}{2|\vec{r}-\vec{r}_A|^4}\left[1 - \exp\left(-\frac{|\vec{r}-\vec{r}_A|^6}{{\rho_A}^6}\right)\right], \end{aligned} \tag{7}$$

where A is the index representing the atoms of the molecule, $V_{\text{CP}}^{(A)}$ is the model potential specific to atom A, α_A are the hybrid polarizabilities of atom A as according to the work of Miller [37], and ρ_A is the empirical parameters of the model potential for atom A. By using the hybrid polarizabilities for each atom A in the molecule, the model potential in Eq. (7) exhibits the correct asymptotic behavior as $r \to \infty$, corresponding to the expected asymptotic behavior of a molecule with a dipole polarizability $\alpha = \sum_A \alpha_A$.

In their calculations, Swann and Gribakin used a Gaussian approximation for the model potential $V_{\text{CP}}^{(A)}$ to simplify the computations. To achieve this, a group of Gaussian functions were fitted to each $V_{\text{CP}}^{(A)}$ using a least-squares method to determine the best coefficients $D_k^{(A)}$. The exponents $c_k^{(A)}$ for these Gaussian functions are provided in Ref. [27]

$$V_{\text{CP}}^{(A)}(r) = \sum_k D_k^{(A)} e^{-c_k^{(A)} r^2}. \tag{8}$$

To determine the optimal values of ρ_A in Eq. (7), Swann and Gribakin adopted a two-pronged approach. First, they assumed that ρ_A is the same for all atoms in a molecule and then calculated positron s-wave eigenphases [30] and bound-state energies [31] using their model potential. They then compared their results with existing theoretical and experimental data for a variety of molecules showing good agreement. In some cases, they used the same ρ from the work of Mitroy and Ivanov [28] (specifically, $\rho = 2.051$ a.u. for the hydrogen atom), showing that this could also reproduce the s-wave eigenphase for simple molecules (containing H, N, and C atoms).

In Ref. [31], Swann and Gribakin optimized the value of ρ for a specific molecule and then used the same value of ρ to predict results for other molecules with similar atomic compositions, such as the alkanes. By employing the model potential in Eq. (7), they were able to accurately reproduce existing theoretical results for the s-wave eigenphases and match experimental data for the bound-state energies of many molecules.

C. Schwinger multichannel method implemented with the model potential

The central objective of this implementation is to provide a detailed description of the polarization potential using the SMC method and the model potential V_{CP} from Eq. (7), as opposed to relying on virtual excitations of the target atom or molecule. This is achieved by modifying the Schrödinger equation for the positron-molecule or atom scattering problem

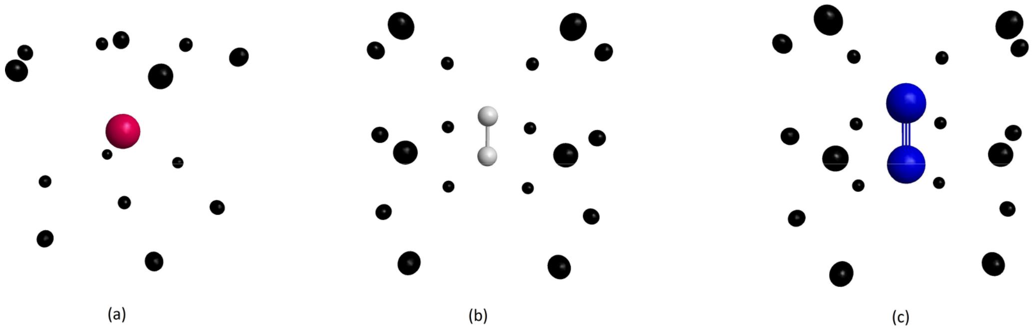

FIG. 2. Geometries and extra centers used in the calculations for the positron scattering from the systems of interest: (a) noble gas atoms, (b) hydrogen molecule, and (c) nitrogen molecule. Black spheres correspond to the extra centers, red sphere correspond to the noble gas atoms, white spheres correspond to hydrogen atoms, and blue spheres correspond to nitrogen atoms.

to explicitly incorporate the model potential V_{CP}. As a result, the equation that needs to be solved is now

$$(H_0 + V + V_{\mathrm{CP}})|\psi\rangle = E|\psi\rangle, \tag{9}$$

$$\langle\vec{r}|V_{\mathrm{CP}}|\vec{r}\,'\rangle = V_{\mathrm{CP}}(\vec{r})\delta(\vec{r} - \vec{r}\,'), \tag{10}$$

where $|\psi\rangle$ is the scattering wave function for the entire system, H_0 is theHamiltonian operator for the noninteracting system, V is the static potential between the incident positron and the target, and E is the total energy of the collision. The following expression for the scattering amplitude is obtained by proceeding in the same way as in the SMC method for the original Schrödinger equation for the problem of a positron scattering from a molecule or atom as follows:

$$f_{\mathrm{SMC-CP}}(\vec{k}_f, \vec{k}_i) = -\frac{1}{2\pi}\sum_{\mu,\nu}\langle S_{\vec{k}_f}|(V + V_{\mathrm{CP}})|\chi_\mu\rangle(d^{-1})_{\mu\nu} \times \langle\chi_\nu|(V + V_{\mathrm{CP}})|S_{\vec{k}_i}\rangle, \tag{11}$$

where

$$d_{\mu\nu} = \langle\chi_\mu|Q\hat{H}Q + P(V + V_{\mathrm{CP}})P - (V + V_{\mathrm{CP}})G_p^{(+)}(V + V_{\mathrm{CP}})|\chi_\nu\rangle. \tag{12}$$

Since polarization effects are taken into account through the model potential V_{CP}, we keep the molecular orbitals frozen throughout the calculations, just as in the S approximation. The fact that we describe the target as in the S approximation makes it possible to use all CSF's associated to the ground state of the molecule or atom besides being a much faster and simpler calculation. In this work, this procedure will be referred to as static plus model potential for correlation-polarization ($S + V_{\mathrm{CP}}$) approximation. The Gaussian fit in Eq. (8) is key in this implementation since SMC CSF's states are already expanded in a Gaussian-type basis set.

D. Computational details

We utilized a D_{2h} point group for all systems under investigation. We chose the basis functions from the aug-cc-pVDZ basis set for the noble gas atoms He, Ne, Ar, and Kr, as implemented in GAMESS [38]. To accurately capture the polarization potential, we incorporated extra functions centered in 14 chargeless centers around each atom, as shown in Fig. 2: two hexagons of side 2.0 Å, with centers 1.5 Å away from the atom center, and the two other centers positioned 1.75 Å from the atom center. We chose to incorporate two s-type Gaussian functions with exponents of 0.23 and 0.02, and two p-type Gaussian functions with exponents of 0.17 and 0.03 into each center. These extra centers were crucial as they helped to compensate for the limitations of Gaussian basis functions in describing atomic orbitals and enabled us to more accurately capture the polarization potential.

As previously mentioned, our primary motivation for calculating cross sections for positron-noble gas scattering was to demonstrate the consistency of our implementation. To this end, we used the same cutting distances in the SMC method with the $S + V_{\mathrm{CP}}$ approximation as Mitroy and Ivanov [28] did for the noble gases. Specifically, we used cutting distances of $\rho = 1.50$ a.u. for helium, $\rho = 1.51$ a.u. for neon, $\rho = 1.71$ a.u. for argon, and $\rho = 1.85$ a.u. for krypton, which were determined based on prior studies. By using these cutting distances, we aim to establish a direct comparison between our results and those reported by Mitroy and Ivanov and to demonstrate the reliability and accuracy of our implementation.

The interatomic distances $R_{\text{H-H}} = 1.39$ a.u. [30] and $R_{\text{N-N}} = 2.068$ a.u. [39] were used in the calculations done in the hydrogen and nitrogen molecules, respectively. To demonstrate that our implementation in the SMC method can reproduce the previous s-wave eigenphases reported by Swann and Gribakin [30], we perform calculations for the s-wave eigenphases using the $S + V_{\mathrm{CP}}$ approximation, the cutting distance $\rho = 2.051$ a.u., and the $12s8p8d$ Cartesian Gaussian basis set for both molecules, exactly as Swann and Gribakin did in their study.

To compute the integral cross sections for positron collisions with molecules, we employed the aug-cc-pVTZ basis set for the hydrogen molecule and the aug-cc-pVDZ basis set for the nitrogen molecule, both implemented in GAMESS [38]. Additionally, we use extra Cartesian Gaussian basis functions placed in 18 chargeless centers. These centers were positioned in hexagons vertices as shown in Fig. 2: one of these hexagons is placed at the midpoint between the atoms of both molecules and the other two at a distance of 1.5 Å from this midpoint.

Consistent with the approach of Swann and Gribakin [27,31], we applied the same cutting distance for all atoms in the molecules under consideration. For our initial calculations, we selected the cutting distance $\rho = 2.051$ a.u., which was previously used by Swann and Gribakin [27,29–31].

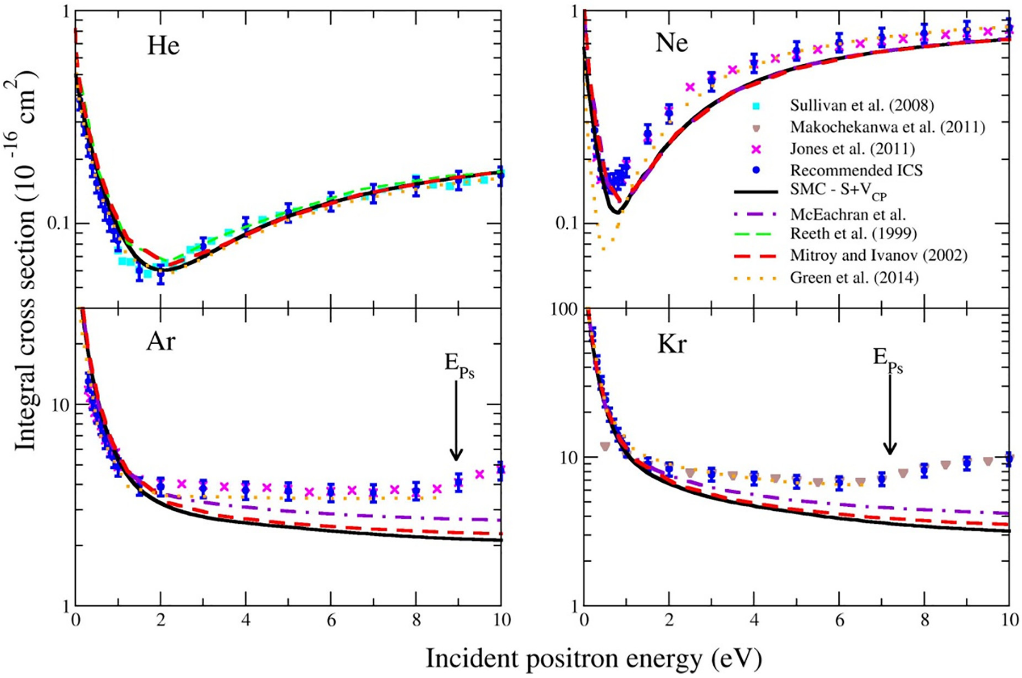

FIG. 3. ICS for positron scattering from the noble gas atoms: helium, neon, argon, and krypton. Our $S + V_{\mathrm{CP}}$ results (solid black line) are compared with previous calculations by Mitroy and Ivanov [28] (dashed red line), Reeth *et al.* for helium [43] (thin dashed green line); McEarhan *et al.* for neon [44], argon [45], and krypton [46] (dot dashed violet line); and of Green *et al.* [47] (dotted orange line) and with the previous experimental TCS data from Sullivan *et al.* for helium [48] (cyan squares), Makochekanwa *et al.* for krypton [49] (brown down triangles), Jones *et al.* for neon and argon [50] (violet crosses), and the recommended experimental TCS from Ratnavelu *et al.* [51] (blue circles) (uncorrected for the forward scattering). The vertical arrows correspond to the energy at which the positronium channel opens for argon ($E_{\mathrm{Ps}} = 8.95$ eV) [45] and krypton ($E_{\mathrm{Ps}} = 7.2$ eV) [46].

To fully understand how model potential calculations compares with *ab initio* methods, we performed the biggest calculations thus far in the *SP* approximation using the SMC method for both molecules. The calculations were performed using the same basis sets as in the $S + V_{\mathrm{CP}}$ approximation considering all possible single virtual excitations to generate the CSF's. This resulted in 36 100 CSF's and 174 040 CSF's for the hydrogen and nitrogen molecules, respectively. With these results, we were able to obtain, by a direct fit, the parameter ρ that best fit our *SP* data and compared with the one obtained by Swann and Gribakin [27].

To carry out these calculations in the *SP* approximation, we parallelized the serial codes of the SMC method for positron scattering. This improvement of the codes did not affect how the scattering process is described, but it allowed to greatly increase the number of CSF used in the expansion of the scattering wave function. Similar to the approach used in the SMCPP method for electron scattering [36], we utilized OPENMP directives [40] for the calculation of the numerator matrix elements $\langle S_{\vec{k}_f} | V | \chi_\mu \rangle$ in Eq. (1) and the denominator matrix elements $d_{\mu\nu}$ in Eq. (2). Additionally, we employed LAPACK routines [41] for LU factorization in the inversion of the denominator matrix $d_{\mu\nu}$ in Eq. (1).

III. RESULTS AND DISCUSSIONS

In this section, our main goal is to assess the consistency of our implementation by presenting ICS for noble gas atoms and comparing them with the results reported by Mitroy and Ivanov [28]. In addition, we computed the scattering *s*-wave eigenphases obtained from the SMC method in the $S + V_{\mathrm{CP}}$ approximation for H_2 and N_2 molecules, and compared our results with those reported by Swann and Gribakin [30]. A major advantage of our implementation is that it enables ICS and DCS's calculations for positron-molecule collision, which allows for direct comparison with experimental data. Furthermore, we analyzed the model potential and compared it to the asymptotic analytic form of the polarization potential, as described in Refs. [42] and [26], as a way to better understand the physics of this model potential.

A. Noble gas atoms (He, Ne, Ar, Kr)

In Fig. 3, we present the ICS for elastic scattering of positrons from noble gas atoms (He, Ne, Ar, and Kr) obtained through the SMC method in the $S + V_{\mathrm{CP}}$ approximation using the same ρ as in Ref. [28]. Our results are compared with the theoretical data of Mitroy and Ivanov [28] with the same model potential; Reeth *et al.* for helium [43] with the Kohn variational method; McEarhan *et al.* for neon [44], argon [45], and krypton [46] with polarized orbitals (PO); and of Green *et al.* [47] with many-body theory (MBT). On the experimental side, we include the TCS data from Sullivan *et al.* for helium [48], Makochekanwa *et al.* for krypton [49], Jones *et al.* for neon and argon [50], and the recommended experimental TCS from Ratnavelu *et al.* [51]. We also remark that the experimental data shown here are uncorrected for the

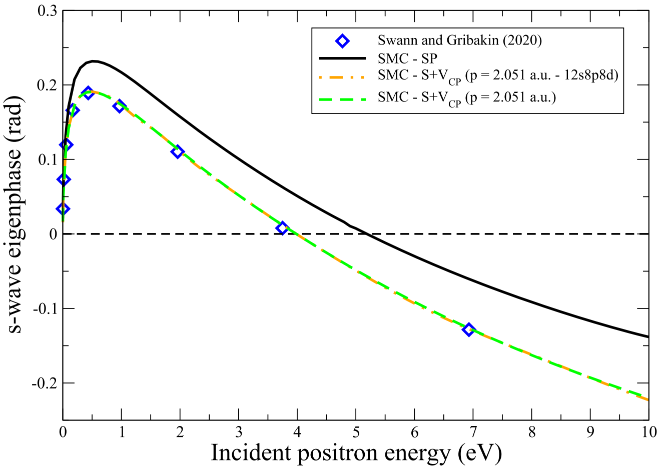

FIG. 4. *S*-wave eigenphases for the positron scattering from hydrogen molecule calculated with the SMC method on the $S + V_{\mathrm{CP}}$ approximation, calculated with the SMC method on the SP approximation and the one calculated by Swann and Gribakin [30].

forward scattering. Our results are consistent with the ones from Mitroy and Ivanov [28] and Reeth *et al.* [43] at all energy ranges.

It is worth noting that the values of ρ used by Mitroy and Ivanov, as well as in our current calculations, were derived to best fit the theoretical calculations of Reeth *et al.* for helium [43] and of McEachran *et al.* for neon [44], argon [45], and krypton [46]. Overall, we observe that the theoretical curves are in better agreement with the experimental data at very low energies (typically <2.0 eV), but are slightly below the data from Refs. [45] and [46] for Ar and Kr above ≈2 eV and, also at this energy range, consistently below the calculations from Green *et al.* [47]. This last piece of theoretical data seems to perfectly fit, at energies below positronium formation, the experimental data. While Gaussian basis sets, as used in the SMC method, are not ideal for atomic calculations, we perform such calculations to confirm the computational implementation of the model potential in our codes. However, our primary objective is to evaluate cross sections for positron-molecule scattering.

B. Hydrogen molecule (H_2)

To further evaluate the implementation of the model potential in our method, we reproduced the *s*-wave eigenphase calculations for positron scattering previously performed by Swann and Gribakin [30]. Figure 4 displays a comparison between our calculated *s*-wave eigenphase, obtained using the SMC method on the $S + V_{\mathrm{CP}}$ approximation with a $12s8p8d$ basis set and a cutting distance of $\rho = 2.051$ a.u. (dot-dashed orange curve), and the eigenphase calculated by Swann and Gribakin [30] (blue diamonds). Our results demonstrate excellent agreement with the earlier findings of Swann and Gribakin [30], as expected.

In addition to our primary results, we also include eigenphase data obtained from other calculations. Specifically, we show the eigenphase data obtained from the *ab initio SP* calculation and the eigenphase data obtained using the $S + V_{\mathrm{CP}}$ approximation with the same ρ as before, but with the basis

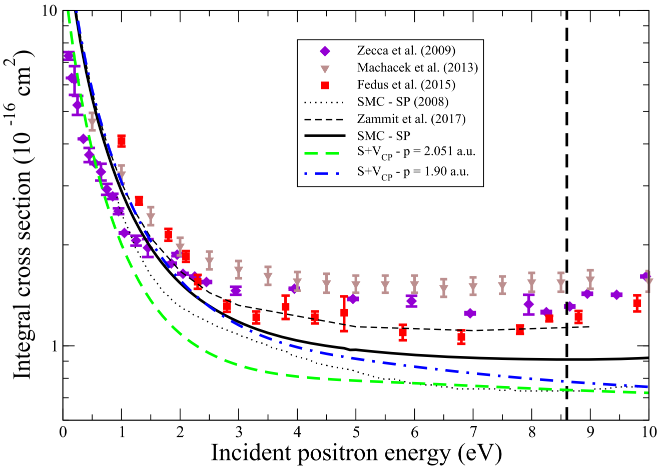

FIG. 5. ICS for positron scattering from hydrogen molecule. Our calculations in the *SP* approximation (solid black line) and $S + V_{\mathrm{CP}}$ approximation with the cutting distances $\rho = 2.051$ a.u. (dashed green line) and $\rho = 1.90$ a.u. (dot dashed blue line) are compared with previous calculations of Sanchez *et al.* [55] (dotted black line) and Zammit *et al.* [56] (thin dashed black line) and experimental data from Zecca *et al.* [52] (purple diamonds), Machacek *et al.* [53] (brown down triangels), and Fedus *et al.* [54] (red squares) (the experimental data shown here are uncorrected for the forward scattering). The vertical dashed line corresponds to the energy at which the positronium channel opens ($E_{\mathrm{Ps}} = 8.6$ eV) [52].

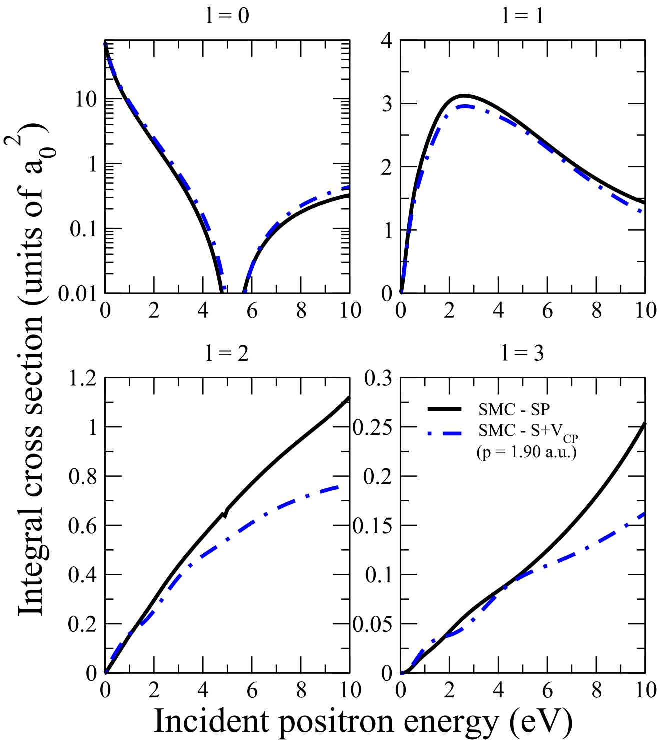

FIG. 6. Angular momentum decomposition of the ICS for positron scattering from hydrogen molecule (in units of a_0^2) from our calculations in the *SP* approximation (solid black line) and $S + V_{\mathrm{CP}}$ approximation with the cutting distance $\rho = 1.90$ a.u. (dot dashed blue line).

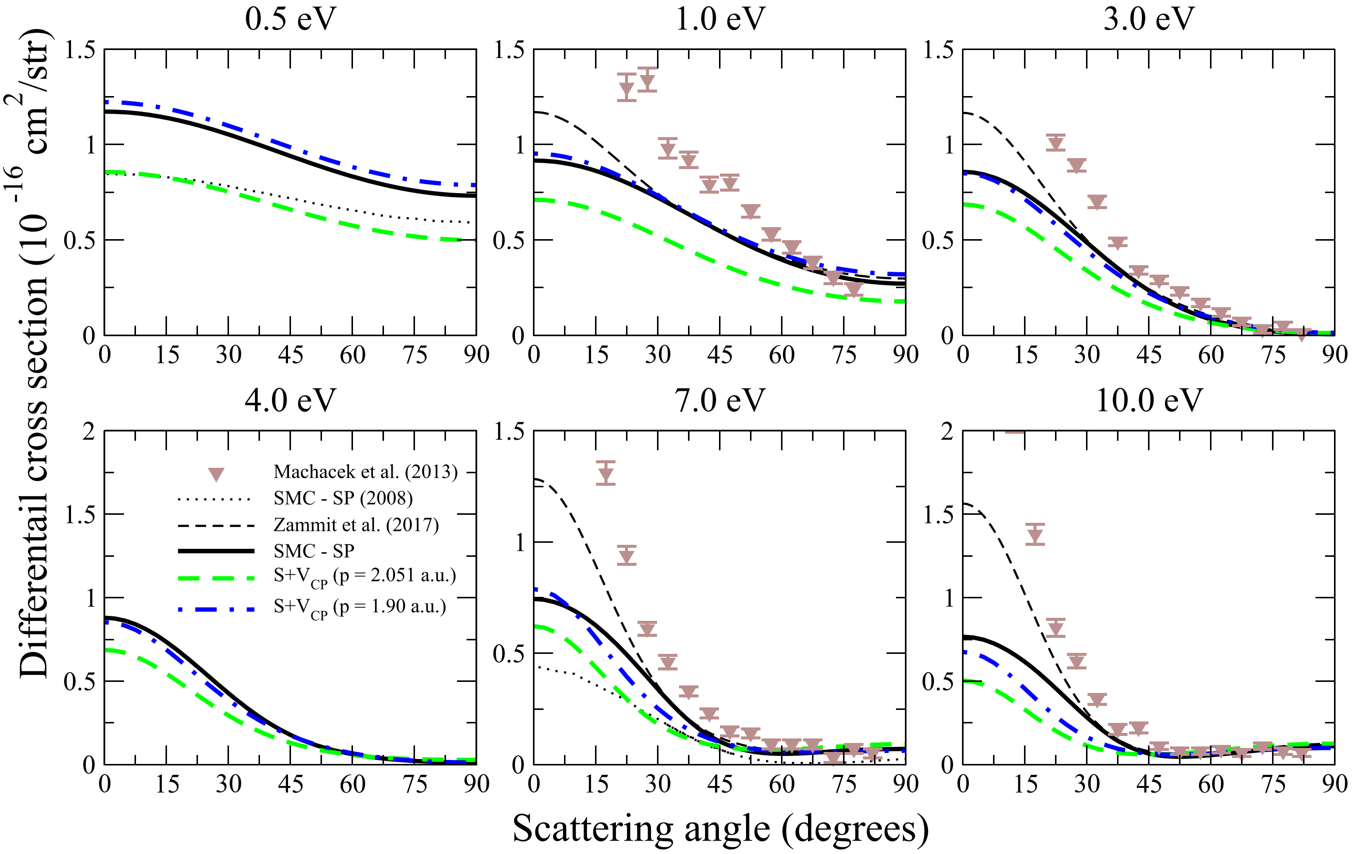

FIG. 7. Folded DCS's for positron scattering from hydrogen molecule. Our calculations in the SP approximation (solid black line) and $S + V_{\mathrm{CP}}$ approximation with the cutting distances $\rho = 2.051$ a.u. (dashed green line) and $\rho = 1.90$ a.u. (dot dashed blue line) are compared with previous calculations of Sanchez *et al.* [55] (dotted black line) and Zammit *et al.* [56] (thin dashed black line), and experimental data from Machacek *et al.* [53] (brown down triangles).

set employed in the *SP* approximation. We find that our calculations using the same value for ρ but different basis sets produce practically no difference. However, there is a significant difference between our results in the *SP* approximation and the findings of Swann and Gribakin [30].

In contrast to Swann and Gribakin's [30] work, our implementation allowed for ICS and DCS calculations. We present our computed integral cross section for the positron-H$_2$ scattering in Fig. 5 in the *SP* approximation and in the $S + V_{\mathrm{CP}}$ approximation with $\rho = 2.051$ a.u. and $\rho = 1.90$ a.u. We compare our results with the experimental data from Zecca *et al.* [52], Machacek *et al.* [53], and Fedus *et al.* [54], as well as previous theoretical calculations from Sanchez *et al.* [55] using the SMC method and from Zammit *et al.* [56] using the convergent-close-coupling (CCC) method. It should be noted that the experimental data shown here are uncorrected for the forward scattering. To improve clarity, we only include the most recent data, but we acknowledge the earlier works by Hoffman *et al.* [57], Charlton *et al.* [58], Zhou *et al.* [59], and Sullivan *et al.* [60].

Parallelizing our codes significantly improves the ICS results across all energy ranges, as demonstrated by the comparison of our current SP calculation with the one by Sanchez *et al.* Our SP data show good agreement with the experimental data up to 3 eV, after which it consistently remains below the experiments and the calculation results from Zammit *et al.* [56]. Analysis of the different values of ρ used shows that our $S + V_{\mathrm{CP}}$ approximation with $\rho = 2.051$ a.u. accurately reproducing the data from Zecca *et al.* [52] for energies $\leqslant 1.5$ eV, but deviating rapidly thereafter. This could be due to the fact that the value of ρ used by Mitroy and Ivanov [28] is obtained by comparing the scattering length of the model with one from close-coupling calculations, hence prioritizing energies closer to zero. Conversely, the value of $\rho = 1.90$ a.u. appears to perfectly reproduce our current *SP* calculation for energies up to 3 eV, before deviating towards smaller values.

Mitroy and Ivanov mentioned in their work [28] that the level of agreement obtained in their *s*-wave cross sections does not extend for higher partial waves, which becomes crucial as energy increases. To further analyze it, we compute partial integral cross sections for $l = 0, 1, 2, 3$ as shown in Fig. 6 for our current *SP* and $S + V_{\mathrm{CP}}$ approximation with $\rho = 1.90$ a.u. The major differences between both data can be seen in this case for *d* and *f* waves precisely for energies above 3.0 eV. As mentioned in Ref. [28], this could be fixed by a different value of ρ for a different l and this shall be further investigated in the future.

The analysis of the folded DCS's presented in Fig. 7 supports the hypothesis that fully *ab initio* methods like SMC or *R*-matrix have difficulty in accurately describing low-

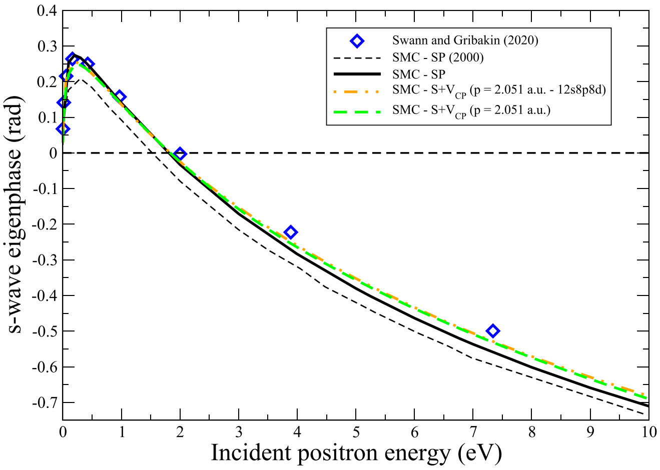

FIG. 8. Comparison between the *s*-wave eigenphase for the positron scattering from nitrogen molecule calculated with the SMC method on the $S + V_{\mathrm{CP}}$ approximation, with the SMC method on the *SP* approximation [39] and the one calculated by Swann and Gribakin [30].

scattering angles ($\leqslant 30^\circ$) due to a poor representation of the long-range polarization potential. However, this issue is not present in the work of Ref. [56], which successfully captures the forward angle peak as the impact energies increase. Additionally, our current calculation, which is performed using a parallelized version of our codes, significantly improves upon our previous work by Sanchez *et al.* [55]. Furthermore, calculations in the $S + V_{\mathrm{CP}}$ approximation with $\rho = 1.90$ a.u. adequately reproduce the available theoretical DCS's for energies up to 4.0 eV, once again deviating as the energy increases.

C. Nitrogen molecule (N_2)

We begin our N_2 results similarly to that of H_2, by comparing our calculated *s*-wave eigenphase obtained using the $S + V_{\mathrm{CP}}$ approximation and the SMC method, with the results calculated by Swann and Gribakin [30] using the same basis set and $\rho = 2.051$ a.u. The excellent agreement between both curves is shown in Fig. 8. Additionally, we present several other results for comparison, including a previous calculation performed with the SMC method by Carvalho *et al.* [39], a current calculation with the SMC method in the *SP* approximation using the aug-cc-pVDZ basis set, which is very close to the results of the authors of Ref. [30], and another in $S + V_{\mathrm{CP}}$ approximation, with the aug-cc-pVDZ basis set and $\rho = 2.051$ a.u. The last one provides the best fit to our most recent *SP* calculation but deviates slightly as the energy increases. Only the results from Ref. [39] differ in magnitude from the other calculations in all energy ranges.

In Fig. 9 we present the ICSs for positron scattering from the nitrogen molecule calculated in this work, as well as those from earlier experimental works by Karwasz *et al.* [61], Przybyla *et al.* [62], and Zecca *et al.* [63], and theoretical works by Carvalho *et al.* [39] with the SMC method in the *SP* approximation, Franz [26] with the quantum Monte Carlo (QMC) parametrization for the correlation potential, and Ellis-Gibbings *et al.* [64] with the independent atom model with screening-corrected additivity rule plus interference terms (IAM-SCAR+I) method. Similarly to H_2, the experimental data shown here are uncorrected for the forward scattering. To improve clarity, we only include the most recent

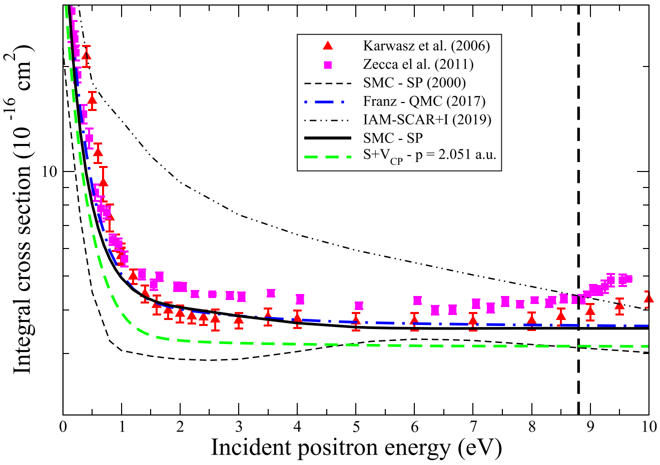

FIG. 9. ICS for positron scattering from nitrogen molecule. Our *SP* (solid black line) and $S + V_{\mathrm{CP}}$ (green dashed line) results are compared with previous calculations by Carvalho *et al.* [39] (black thin dashed line), Franz [26] (blue dot dashed line), and Ellis-Gibbings *et al.* [64] (black thin double dot dashed line), and experimental data from Karwasz *et al.* [61] (red up triangles) and Zecca *et al.* [63] (magenta squares) (the experimental data shown are not angle corrected). The vertical dashed line corresponds to the energy at which the positronium channel opens ($E_{\mathrm{Ps}} = 8.8$ eV) [63].

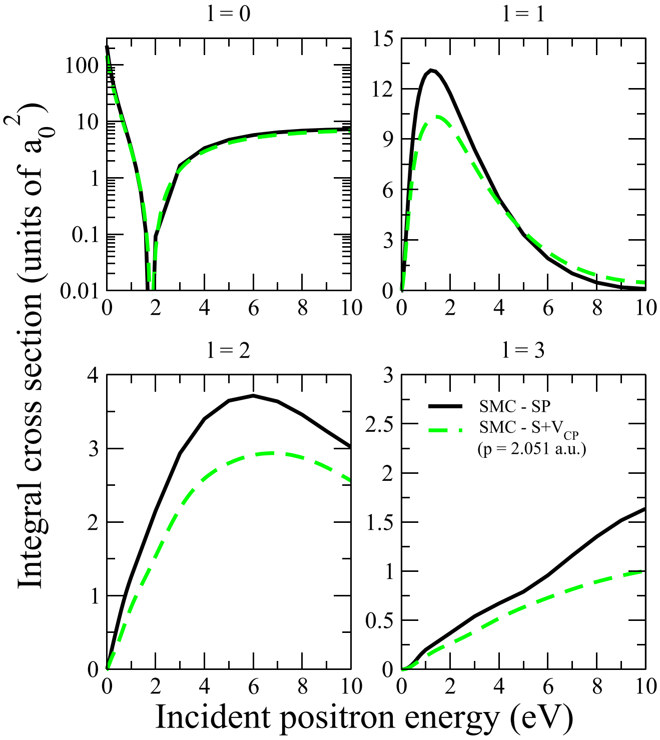

FIG. 10. Angular momentum decomposition of the ICS for positron scattering from nitrogen molecule (in units of a_0^2) from our calculations in the SP approximation (solid black line) and $S + V_{\mathrm{CP}}$ approximation (dashed green line).

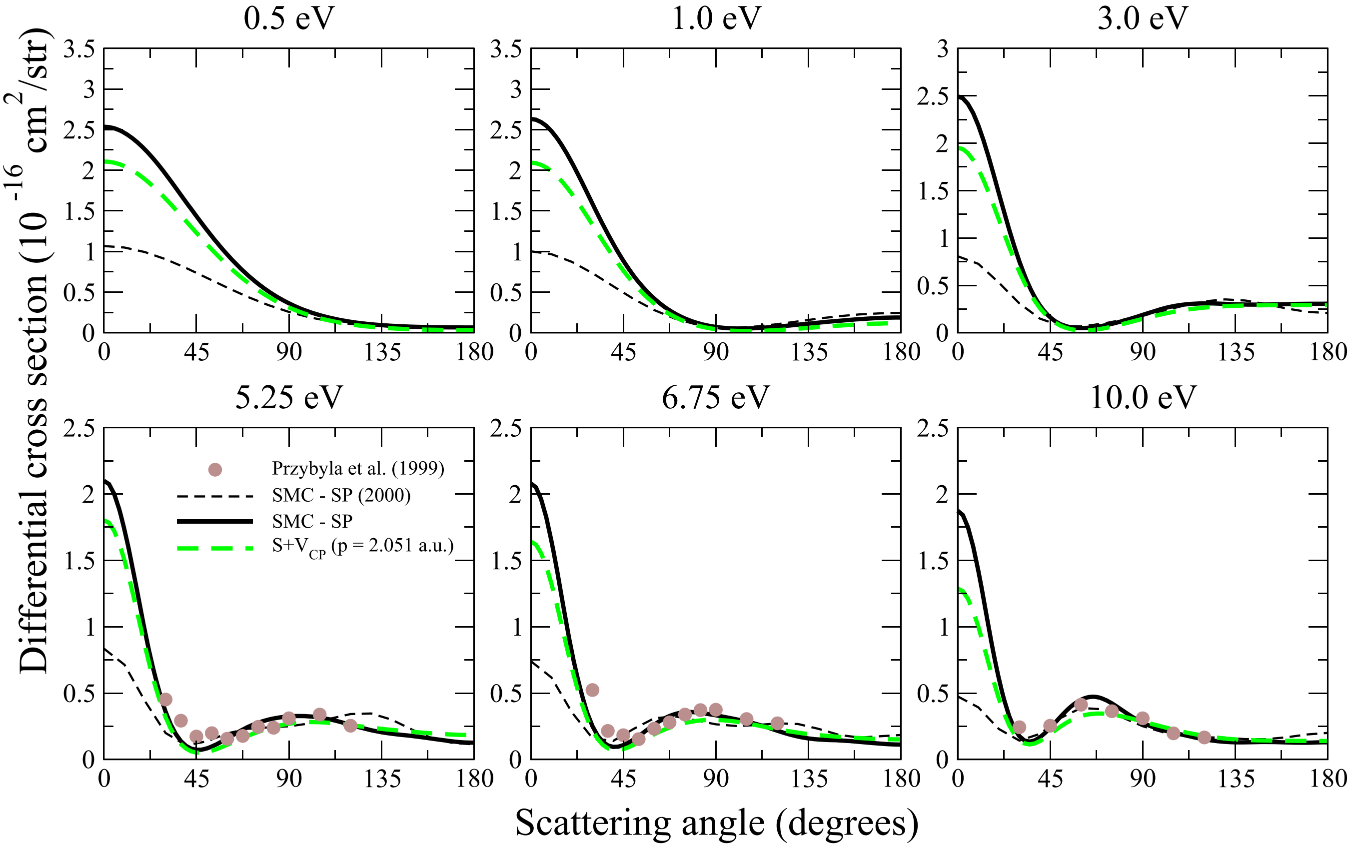

FIG. 11. Calculated DCS's for positron scattering from nitrogen molecule. Our *SP* (solid black line) and $S + V_{\rm CP}$ (green dashed line) results are compared with previous calculations by Carvalho *et al.* [39] (black thin dashed line) and experimental data from Przybyla *et al.* [62] (brown circles) for the relative DCS's as normalized in Ref. [39].

data, but we acknowledge the earlier works by Hoffman *et al.* [57] and Sueoka *et al.* [65].

Our current SP calculations of nitrogen (N_2) almost perfectly agree with the theoretical curve of Franz [26] in all the energy ranges shown. They also exhibit very good agreement with the experimental data up to the opening of the positronium channel. In contrast, the previous SMC method calculation by Carvalho *et al.* [39] greatly underestimated the results, while the IAM-SCAR+I method calculation by Ellis-Gibbings *et al.* [64] overestimated them. Unlike the H_2 calculation, we observe a larger discrepancy between our *SP* calculation and the one in the $S + V_{\rm CP}$ approximation with the cutting distance $\rho = 2.051$ a.u. They only agree at very low energies, which is expected since this value of ρ was chosen to obtain the best fit for the *s*-wave calculation. We tested different values of ρ and only a marginal improvement in the agreement with our *SP* calculation was observed, hence we opted to use $\rho = 2.051$ a.u. due to the better agreement with the *s*-wave partial cross section. The analysis of the decomposition of partial waves confirms this, as bigger differences than for H_2 are already visible for $l = 1, 2, 3$ for energies higher than 1.0 eV, as shown in Fig. 10.

The DCS's presented in Fig. 11 shows that our current calculated results in the *SP* approximation seems to accurately reproduce the experimental DCS's of Przybyla *et al.* [62]. Additionally, our current *SP* calculation significantly improves upon our previous work by Carvalho *et al.* [39], especially in the low angles region ($\leqslant 45^\circ$). Furthermore, calculations in the $S + V_{\rm CP}$ approximation with $\rho = 2.051$ a.u. adequately reproduce the available theoretical DCS's for angles higher than 30°, below which deviates slightly from the theoretical DCS's.

D. Model potential in molecules

To provide a better understanding of how the model potential $V_{\rm CP}$ is used in our calculations for positron scattering from molecules, we include a comparison between $V_{\rm CP}$ for the studied cutting distances and the asymptotic polarization potential $V_{\rm pol}$ up to the dipole polarizability and the second hyperpolarizability, along the radial coordinate [$\theta = 0^\circ$ in Eq. (13) below]. These comparisons are shown in Fig. 12 for the hydrogen molecule and Fig. 13 for the nitrogen molecule. We use the following form of $V_{\rm pol}$ for this comparison, as presented in previous studies [26,42]:

$$V_{\rm pol}(r) = -\frac{\alpha_{D,0}}{2r^4} - \frac{\alpha_{D,2}}{2r^4}P_2(\cos\theta) - \frac{\alpha_Q}{2r^6} + \frac{B}{2r^7} - \frac{\gamma}{24r^8}, \tag{13}$$

where $\alpha_{D,0}$ is the isotropic static dipole polarizability, $\alpha_{D,2}$ is the anisotropic static dipole polarizability, α_Q is the isotropic static quadrupole polarizability, B is the dipole-dipole-isotropic quadrupole hyperpolarizability, and γ is the the dipole-dipole-isotropic dipole-dipole hyperpolarizability.

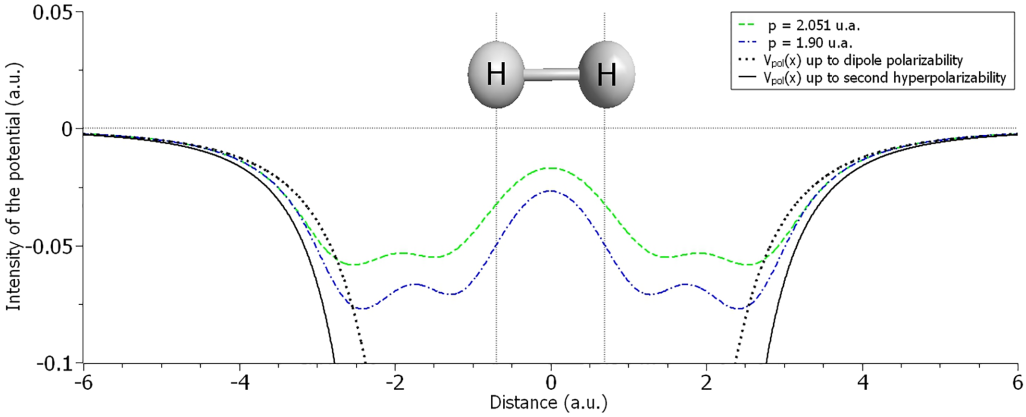

FIG. 12. Model potential V_{CP} for the hydrogen molecule along the radial coordinate. The vertical dotted lines correspond to the positions of the hydrogens in the hydrogen molecule.

For the hydrogen molecule, the values $\alpha_{D,0} = 5.180$ a.u., $\alpha_{D,2} = 1.210$ a.u., $\alpha_Q = 7.889$ a.u., $B = -74.8$ a.u., and $\gamma = 620.3$ a.u. were obtained through the results presented in the work of Miliordos and Hunt [66] with the basis set D6Z in the equilibrium interatomic distance ($r = r_e$). For the nitrogen molecule, the values $\alpha_{D,0} = 11.070$ a.u., $\alpha_{D,2} = 4.593$ a.u., $\alpha_Q = 83.26$ a.u., $B = -151.53$ a.u., and $\gamma = 927$ a.u. were used, which are the same values as those in the work of Franz [26] for the nitrogen molecule.

In Fig. 12, we can see that the model potential seems to be closer to the full potential of Eq. (13) than to only the dipole term for $r \gtrsim 2.75\ a_0$ for both values of ρ. This seems to indicate that the *SP* SMC calculation, which is reproduced with $\rho = 1.90$ a.u., is able to describe higher-order terms of the long-range potential than only the dipole one as mentioned by Tenfen *et al.* [24]. This may be explained by the fact that both *SP* SMC and the $S + V_{\mathrm{CP}}$ does not use single center expansion in their description of polarization effects, as done in the work of Franz [26] and Tenfen *et al.* [24]. However, what seems to be relevant to get the magnitude of the integral cross section right is to get a better description for $l > 0$, as can be seen in Fig. 6, which shows a considerable contribution for $l = 1$ even as energy as low as 1.5 eV.

This discussion is reinforced by Fig. 13 since also for $r \gtrsim 2.75\ a_0$ there seems to be a perfect agreement between the model potential and the full potential of Eq. (13). Furthermore, in the same way as done in the work of Franz [26], we calculated the crossing point r_c at which $V_{\mathrm{pol}} > V_{\mathrm{corr}}$ for the QMC parametrization of V_{corr} and along the radial coordinate in the nitrogen molecule to be $r_c \approx 3.6\, a_0$. This means that the model potential V_{CP} is able to capture the same polarization as captured in the potential presented in the work of Franz [26]. The difference in the ICS between the $S + V_{\mathrm{CP}}$ and the *SP* SMC calculation, as mentioned before, lies in a poorer description, in the case of N_2, for $l > 0$, not in the long-range potential.

IV. SUMMARY

In this work, we tackled the problem of positron scattering by molecules in two different ways: by parallelization of our previous computer codes and the inclusion of a model potential with a free parameter in our calculations. With the improved version of our computer codes, we were able to make our best calculations to date to both H_2 and N_2 molecules. However, to obtain such good results, we had to

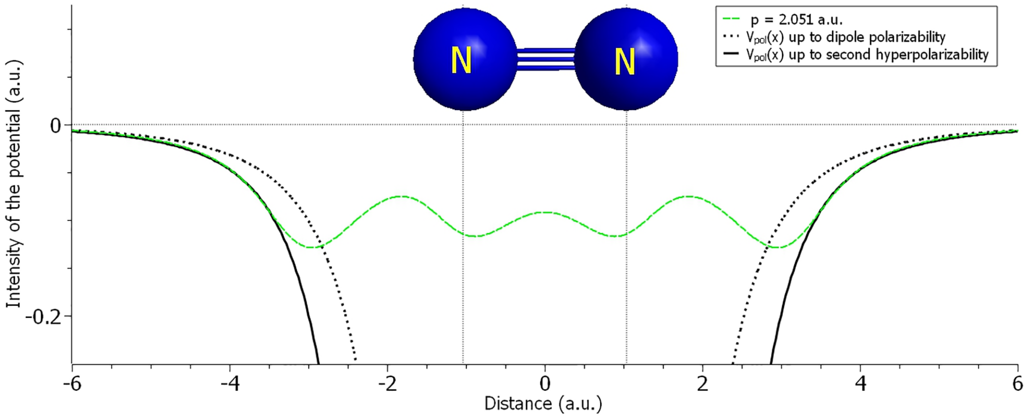

FIG. 13. Model potential V_{CP} for the nitrogen molecule along the radial coordinate. The vertical dotted lines correspond to the positions of the nitrogens in the nitrogen molecule.

resort to 36 100 CSF's and 174 040 CSF's for the hydrogen and nitrogen molecules, respectively, reaching the limit of *ab initio* calculations, which was only possible due to the diatomic nature of both molecules. However, performing similar calculations for bigger systems would be computationally prohibitive. Hence, the use of a model potential as proposed by Mitroy and Ivanov [28], later modified by Swann and Gribakin [30] for positron-molecule scattering was tested. Our calculations, in the $\mathrm{S} + \mathrm{V}_{\mathrm{CP}}$ approximation, were able to reproduce in part our current *SP* calculations, deviating at higher energies due to a poorer description of high angular momenta.

These first results with the model potential did not intend to make any predictions, but rather to (i) test the inclusion of the model potential by comparing with previous calculations, (ii) analyze the capability of the model potential to obtain good ICS and DCS's for positron-molecule scattering since it was previously tested only for s-wave eigenphases, and (iii) brings further understanding of the scattering process by comparison with the analytic form of the long-range potential. Since all these three were consistent, further investigation of what this model potential can bring to scattering calculations is now due. In this sense, one can inquiry if it can have the same success for ICS and DCS's as it had for positron binding energy as done in Ref. [29]. In their work, the value of the free parameter was optimized for a particular system and good results were obtained for similar molecules. These would then allow to obtain at least good estimates of scattering cross sections for bigger systems, which our current *ab initio* methodology does not allow.

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