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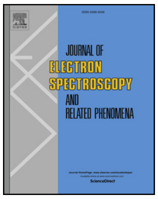

Elastic scattering and rotational excitation of Li_2 by positron impact

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ABSTRACT

We report an *ab initio* and model potential investigation of elastic and rotational excitation cross sections for positron impact with Li_2 molecule in the energy range from 0.1 to 10.0 eV. The *ab initio* cross sections were calculated with the Schwinger Multichannel Method, while the model potential calculations were performed with the Method of Continued Fractions, applying the correlation–polarization interaction known as PCOP. The converged elastic cross sections suggest a spherical polarizability for Li_2 between 150 and 160 a_0^3, a value considerably lower than the experimental one ($\approx 216\,a_0^3$). Rotational excitation cross sections obtained corroborate previous results available, with some discrepancy for the quadrupolar transition for energies below 3 eV. Our results indicate that such divergence comes from the consideration of a correlation-potential properly designed to treat positron-molecule scattering.

1. Introduction and motivation

Positrons have an interesting role in condensed matter physics [1]. For example, the development of slow positron beams is historically related to the study of moderators [2] as also to the annihilation dynamics in different condensed matter environments [3]. The comparison between the electron and positron processes, like energy deposition and penetration depth constitutes a theme of investigation [4,5] where interesting physics can be learned and tested. In the same fashion, the study of metallic clusters offers a very special environment to study strongly correlated systems. The bonding process, the geometry and the appearance of “magic numbers” are examples of interesting phenomena under intense investigation nowadays [6].

Among many atomic species, lithium sounds as an attractive system to be investigated theoretically because it is the lightest metallic element and it has a single s valence electron. Between the atomic and cluster structure, we find the Li_2 molecule, which usually is experimentally manipulated in the gas phase.

Li_2 is a system with several peculiar characteristics. For example, the internuclear distance in the equilibrium geometry is 5.05 a_0 [7], a value expressively larger than the one found for H_2 (1.400 a_0) and N_2 (2.068 a_0). Also, the static dipole polarizability of Li_2 (140–270 a_0^3) presents a considerable magnitude when compared to the corresponding ones for H_2 (5.4 a_0^3) and N_2 (11.4 a_0^3).

Beyond the particular molecular characteristics, Li_2 is a system that invites for a theoretical investigation in the context of positron scattering, mainly in the low energy region. For Li_2, the inelastic electronic thresholds are open at relatively small energies when compared to other similar systems. For example, the ionization potential of Li_2 is ≈ 4.94 eV. It means that positronium formation channel is present even when positrons reach the molecule with zero energy. The first threshold for electronic excitation, which corresponds to the channel ${}^1\Sigma_g \rightarrow {}^1\Sigma_u$, is of the order of 1.8 eV ([8], Table 3). To make things more interesting, the threshold for vibrational transition $v = 0 \rightarrow v = 1$ is about 0.04 eV. So we have a molecular system where the inelastic components, electronic and nuclear, are present for impact energies as small as ≈ 1 eV, such that, a rigorous investigation about the positron-Li_2 scattering should take into account all these collision channels and its couplings.

As far as we know, the only existing calculation for positron-Li_2 is the one performed by [9]. They have used the Lab-Frame Close-Coupling (LFCC) approximation with a model potential to calculate elastic and rotational cross sections. In that work, the positronium formation, the electronic and the vibrational excitations were fully disregarded.

It is a common practice in the field of electron and positron scattering by molecules to develop a systematic investigation of a given system, considering increasing levels of sophistication in order to understand how the inclusion of inelastic channels affect the dominant elastic cross section. Let us consider, for example, the study of positron scattering by Li atom, the atomic counterpart of Li_2 molecule.

The first set of works about positron-Li scattering was developed along the 70s and 80s [10–12]. These initial initiatives were focused in the calculation of the elastic cross sections, the main concern being to go beyond the static approximation, i.e., taking into account the target polarization effects. Only in the 90s, due to the improvement of the

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computational facilities, the first cross sections generated with close-coupling scattering models appeared in literature [13–15]. Those were the first set of calculations that included the positronium formation channel. Several models and different levels of approximations have been tested. In the present days, considerable progress exists in the determination of the positronium formation cross section in low energy positron-Li collisions [16] but its effect over the elastic channel is still a matter of discussion. We find interesting to observe that Watts and Humberston [17,18], working with the Kohn variational method and performing calculations for energies below the first electronic excitation threshold (1.84 eV) of the Li atom, have found an infinite positronium formation cross section at zero energy. The important result to us here is that, in this sophisticated model, the elastic cross section was practically unaffected by the coupling with the positronium channel.

In order to study the effect of the inelastic collisional channels over the elastic cross section, we should perform a complete calculation involving all states. However, it is necessary to first determine the elastic cross section in a reliable way.

In this work, we calculate the elastic positron-Li_2 cross section comparing two independent methodologies. The first one is the *ab initio* many-body Schwinger Multichannel Method (SMC) [19]. The second one is the single-body Positron Correlation-Polarization Potential (PCOP) of [20]. The model potential calculations were performed with the Method of Continued Fractions (MCF) [21]. In both cases only the elastic channel was considered in the computation of the respective T matrices. The elastic cross section was determined from the convergence between the results obtained with these two different methodologies. Such strategy to determine elastic cross sections has been successfully applied before by our group, as in the case of positron-N_2O [22] and positron-H_2O [23] investigations. In other words, in the lack of any experimental data, this is the elastic cross section we recommend for this molecule until the present moment.

This paper is organized as follows: in Section 2, we discuss the essential points about the methodologies used to compute the cross sections, with focus in the description of the criteria adopted to construct the trial scattering basis sets used in this work. In Section 3 we present our results and finally, in Section 4, we state our conclusions.

2. Methodology

2.1. Model potential calculation

As previously cited, the only work found on positron scattering by Li_2 in the low energy regime is the one of [9]. These authors calculated the cross sections within the LFCC formulation using the molecular wavefunction of [24] and the correlation-polarization (CP) potential of [25] (PZ). Other models for CP potentials have been proposed (see [26–28]). Among them, the PCOP proposed by [20] (from the positron-electron correlation energy presented by [29]) has been applied with considerable success.

Firstly, we calculated the elastic scattering cross section through the MCF using the PCOP in the same way as [30]. Details about MCF and its application to positron-molecule scattering can be found in that reference. Here, we limit ourselves to say that it is an iterative method that calculates the scattering of a single particle by a given potential $V(\vec{r})$. Since the original work of [9], advances have been made in the development of Gaussian basis sets to generate accurate molecular wavefunctions. Among many possibilities, we decided to work with the Gaussian basis set provided by [31], specially constructed to better represent electronic correlation effects.

Fig. 1 presents the spherical component of the positron-molecule interaction potential. The dashed-dotted line is the static potential obtained by us, which it is very similar to the one presented by [9]. The double-dashed-dotted and dashed-double-dotted lines are the CP potentials of PZ and PCOP, respectively. Curves dashed (PZ) and solid (PCOP) are the total interaction (static plus CP) for each of CP potentials. From this figure, we see that for values of radial coordinate above ≈6 a_0 (cutoff radius) the full interaction potentials provided by both CP models are very similar. From the cutoff radius towards the molecular center, the CP potentials become rather different.

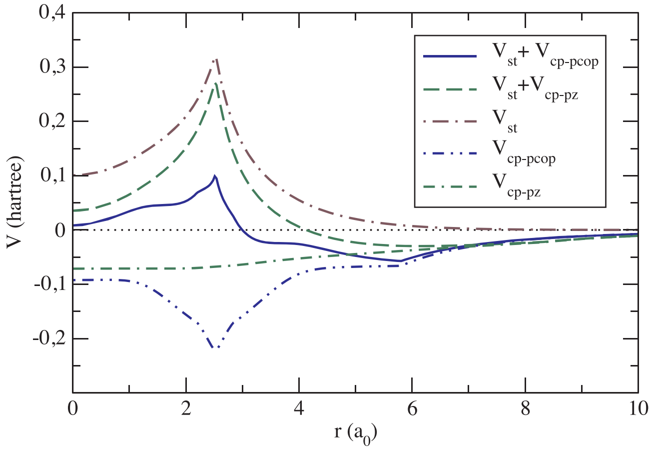

Fig. 1. Spherical component of the positron-Li_2 potential as a function of the positron distance to the center of the molecule. The solid line represents the total interaction in the static plus polarization approximation with PCOP; the dashed line is the same as solid one but for PZ potential; the dash-dotted curve is the static potential; the dash-double-dotted line is the PCOP; double-dashed-dotted one is the PZ-CP potential used by [9].

As one may observe, in Fig. 1, the correlation component of the PCOP ($V_{cp\text{-}pcop}$) has a different shape when compared to the PZ one ($V_{cp\text{-}pz}$). Also, $V_{cp\text{-}pcop}$ has a magnitude comparable to the static potential. This is not observed in other molecules such as H_2 and N_2 [30]. As a consequence, the potential becomes more attractive at the molecular border and the positron penetrates deeper into the molecular field. It indicates that in Li_2 the description of the correlation is central to produce reliable cross sections. Finally, we note that the scattering potential does have a large range. From this, one may expect that this feature produces cross sections of expressive magnitude.

2.1.1. Adiabatic rotational approximation in the method of continued fractions

In order to compare our results to the ones reported by [9], we adapted the MCF to compute the rotational cross sections within the Adiabatic Rotational Approximation (ARA) [32,33]. Here we follow the same implementation presented in [34] and only a brief overview is given.

The main result of a MCF calculation is the *K*-matrix in body-frame, in the angular momentum representation: *K*(*l*, *m*;*l′*, *m′*). From the *K*-matrix the corresponding *T*-matrix is obtained through:

$$T^{l_i\,m_i}_{l_f\,m_f} = -\frac{2}{\pi}\sum_{l\,m}\,[(1-\mathrm{i}\,\mathrm{K})^{-1}]^{l\,m}_{l_f\,m_f}\,[K]^{l_i\,m_i}_{l\,m} \tag{1}$$

where $K = K[\vec{k_f};\,\vec{k_i}]$ and $T = T[\vec{k_f};\,\vec{k_i}]$. From the *T*-matrix, the corresponding rotational cross section is calculated by

$$\begin{aligned}\sigma^{J_i\to J_f} &= \tfrac{1}{4\pi}\tfrac{k_f}{k_i}\textstyle\sum_{l_f\,l_i}\sum_{m\,n}(-1)^{m+n}f^{l_i m}_{l_f m}\,(f^{l_i\,n}_{l_f\,n})^{*}\\ &\times\ \textstyle\sum_j C(J_i\,j\,J_f;\,0\,0\,0)^2\\ &\times\ C(l_f\,l_i\,j;\,-m\,m\,0)\,C(l_f\,l_i\,j;\,-n\,n\,0),\end{aligned} \tag{2}$$

where the *C′s* are the usual Clebsch–Gordan (CG) coefficients, k_f and k_i are the absolute value of the final and initial positron wave vectors, J_f and J_i are the final and initial rotational states of the molecule and the amplitude coefficients $f^{l_i m}_{l_f m}$ are connected to the *T* matrix ones by:

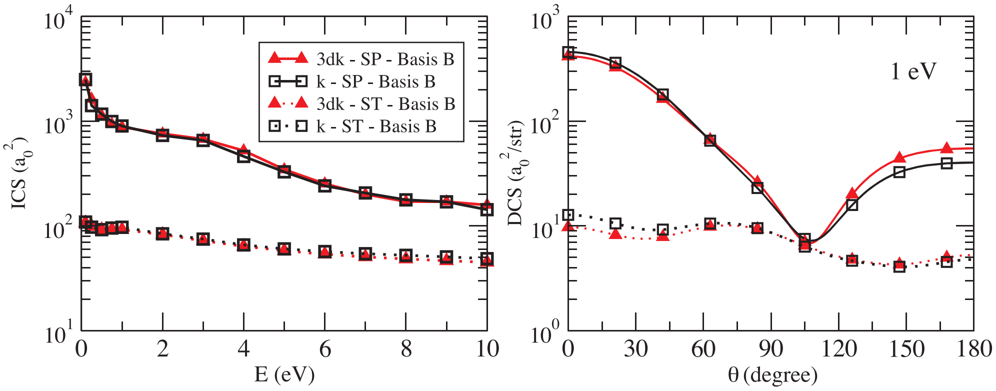

Fig. 2. Left: Integral cross sections for basis B (see Section 3) calculated by SMC. Static approximation (ST): dotted line with triangles for 3dk insertion and dotted line with squares for k insertion. Static plus polarization approximation (SP): solid line with triangles for 3dk insertion and solid line with squares for k insertion. Right: same as left, but for differential cross section for 1 eV.

$$f^{l_i m}_{l_f m} = -(2\pi)^2 \frac{i^{l_i - l_f}}{k_i} T^{l_i m}_{l_f m}. \tag{3}$$

2.2. *Ab initio calculations*

The *ab initio* calculations were performed with the Schwinger Multichannel Method (SMC) [19]. In this method, the variational expression for the scattering amplitude is given by:

$$f\,[\vec{k}_f, \vec{k}_i] = -\frac{1}{2\pi}\sum\nolimits_{\rm m\,n} \left\langle S_{\vec{k}_f}|V|\chi_m \right\rangle (d^{-1})_{\rm mn} \left\langle \chi_n|V|S_{\vec{k}_i} \right\rangle \tag{4}$$

where

$$d_{\rm mn} = \langle \chi_m|{\rm PVP} + Q\hat{H}Q - {\rm VG}_P^{(+)}V|\chi_n\rangle. \tag{5}$$

In the expressions above $S_{\vec{k}}$ is a solution of the unperturbed Hamiltonian (molecular Hamiltonian plus the kinetic energy operator for the incident positron), P and Q are projectors onto energetically open and closed states of the target, V is the scattering potential, $\hat{H}$ is the total energy minus the scattering Hamiltonian, $G_P^{(+)}$ is the projected Green's function and $\{\chi_{m\equiv\mu\nu}\}$ are the $(N+1)$-particle trial scattering functions which have the form

$$\chi_{m\equiv\mu\nu} = \Phi_\mu(\vec{r_j}) \times \varphi_\nu(\vec{x}) \tag{6}$$

with $\Phi_\mu(\vec{r_j})$ and $\varphi_\nu(\vec{x})$ being the μth state of the target and the νth positron scattering orbital respectively.

The ground state target wavefunction $\Phi_0(\vec{r_j})$ is a Restricted Hartree–Fock (RHF) one obtained from a Self Consistent Field (SCF) calculation. As usual, the molecular orbitals are formed by linear combination of atomic orbitals, in this case, Cartesian–Gaussian functions (CGF's). The set of positron scattering orbitals $\{\varphi_\nu(\vec{x})\}$ is taken as the set of occupied and virtual orbitals generated in the SCF calculation.

If we turn-off the $Q\hat{H}Q$ and $VG_P^{(+)}V$ terms in Eq. (5), the SMC scattering amplitude becomes similar to the one computed in the first Born approximation (FBA), i.e., $f^{SMC} \approx f^{FBA}$ under the condition that $\sum_m |\chi_m\rangle\langle\chi_m| \approx \hat{1}$. In this case the SMC scattering amplitude reduces to what is called the Basis Set Born Approximation (BSBA).

2.2.1. *Gaussian basis sets selection*

The cross sections computed with SMC depend on the initial set of CGF's used to describe the target wavefunction and the positron scattering orbitals. Here, we used the same criteria adopted in the article of [34]. These are:

1. $Z_{\rm eff}^{\rm BSBA} \approx Z$: when the annihilation parameter Z_{eff} is computed considering a scattering basis set expansion that mimics the first Born approximation (FBA) we must find $Z_{\rm eff}^{\rm BSBA} \approx Z$, where Z is the number of electrons of the target [35–37];
2. $\sigma^k \approx \sigma^{3dk}$: the cross sections must be converged when compared to the method used to compute the Green's function matrix elements (k-insertion and 3dk-insertion methods) [38].

The calculation of the Green's function has shown to be a challenging point along the development of the SMC method. Briefly, the original technique to compute it was founded in the spectral decomposition of a plane wave in a CGF basis:

$$\left|\vec{k}\right\rangle = \sum_\alpha \left|\alpha\right\rangle \left\langle \alpha\middle|\vec{k}\right\rangle, \tag{7}$$

where the $\{|\alpha>\}$'s were the own CGF's used to describe the molecular target. Analysis of the unitary property of the S matrix suggested that, even after the insertion of a huge number of CGF's, completeness was still questionable. To overcome such difficulty, an hybrid approach was considered, where the residue component was computed numerically and the principal value was still calculated using the α-insertion procedure. This technique is known as the k-insertion method, and the cross section computed within such implementation are here called σ^k. As observed in [38], considering the numerical calculation of both residue and principal value terms, introduced the independence of spectral decomposition of the plane wave. Cross sections computed within this approach are called σ^{3dk}. It is possible to demonstrate that when $\sigma^k \approx \sigma^{3dk}$ we have, in fact, completeness in the CGF ($\sum_\alpha |\alpha\rangle\langle\alpha| \approx \hat{1}$) and in the trial scattering basis set ($\sum_m |\chi_m\rangle\langle\chi_m| \approx \hat{1}$).

Fig. 2 shows the typical integral and differential elastic cross sections obtained considering the criteria listed above. It is important to highlight that we demanded the $\sigma^k \approx \sigma^{3dk}$ convergence to be respected in the static (ST) and static plus polarization approximations (SP). We easily see from this figure that within the limitation of each Gaussian basis set, the cross sections reported here are the best results SMC can produce within this implementation and the criteria here adopted.

Before presenting our results, we state that all basis sets associated to SMC calculations provide satisfactory values for the total energy when compared to the Hartree–Fock limit reported by Jensen [39]. We also only consider the basis sets which gives a satisfactory description of the quadrupole moment Q, for which the values varies from ≈ 8 to ≈ 11 ea$_0^2$ [40], and of the dipole polarizability α_0, for which the value varies from $\approx 140a_0^3$ [41] up to $\approx 270a_0^3$ [42].

3. Results and discussion

Fig. 3 shows our results for the elastic cross sections. The dashed line is the cross section calculated with the PCOP using the basis of [31] while the double dotted-dashed line are the data of [9] obtained within the LFCC formulation with the PZ-CP. Both exhibit the typical behavior of a positron-molecule elastic cross section in the low energy domain. The PCOP cross section have the same energy dependence found in LFCC, but with a systematic larger magnitude for all energies. These two cross sections are the ones that come from model potential calculations.

In order to find a recommended positron-Li$_2$ elastic cross section

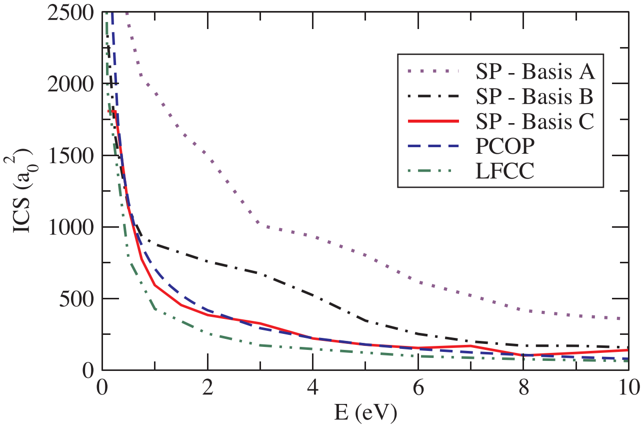

Fig. 3. Elastic cross sections. Dotted line: SMC cross section for static plus polarization potential for basis A calculated through 3dk-insertion; Dash-dotted line: the same, but for basis B; solid line: the same, but for basis C; dashed line: results obtained with PCOP interaction model; dashed-double-dotted line: results reported by [9] with PZ correlation potential.

from an *ab initio* approach, we firstly tried to calculate it with [31] basis in the same way as performed with PCOP. This basis is composed by 156 Gaussian functions. It is a huge number for our computation capabilities and it took several weeks to produce any results. Unfortunately, it contains several diffuse functions and these generated spurious resonances in the elastic cross section. Even after removal of trial scattering vectors from the variational basis [37] this kind of undesirable structures could not be removed. Because of that, the elastic SMC cross section associated with this basis is not shown in Fig. 3.

One of the main conditions to obtain reliable cross sections within SMC is the property of completeness of the scattering basis sets ($\Sigma_m|\chi_m\rangle\langle\chi_m| \approx 1$). Therefore, we decided to run a preliminary calculation with modest sized basis sets. We elected the basis formed by Gaussians I, II and IV given in Table 1 of the article of [8], originally applied to very low energy electron-Li_2 scattering. This basis set has 54 functions, a small number that provided us the elastic cross section called basis A and represented by the dotted line in Fig. 3. As one may observe, it presents a magnitude much larger than the ones obtained by model potential calculations. The structures from 1 up to 8 eV does not present the typical shape of an elastic positron-molecule cross section. It is important to state that the results reported for this basis were treated in the same fashion as described in [37], i.e, spurious trial scattering vectors were removed until the criteria given in Section 2.2.1 were satisfied. In this scenario, in spite of satisfying the criteria mentioned in Section 2.2.1, this basis set seems to be not complete.

We then decided to amplify the number of Gaussian functions used in the basis, but still keeping a manageable size to produce results in a reasonable time. Inspired in the basis reported by [8], we developed basis B. Essentially, the same set of Gaussian exponents used to represent the Li atom were used (but now, all of them uncontracted). [8] call attention to the fact that when trying to model electron-Li_2 collisions, the use of additional Gaussian functions at the chemical bond (CB) improved the flexibility of the trial scattering wave function. This idea was also previously observed by [43], who called attention to the fact that Li_2 resembles much more a molecule like CO_2 than a familiar diatomic like H_2 or N_2. The Gaussian functions used at the CB were chosen in order to satisfy the criteria listed above. The elastic cross section obtained with this basis is given by the dashed-dotted line in Fig. 3. We immediately recognize that the results obtained with this basis set are very similar to the PCOP ones for energies bellow ≈1 eV and above ≈7 eV. The structure between 1 and 7 eV suggests that some lack of correlation is still present in this basis.

Finally, we decided to work with different basis sets (not the ones inspired in the work of [8]) keeping the total number of Gaussian basis functions, but removing functions from the CB. We were able to find a basis, which we call basis C, that fulfilled the criteria. The results obtained with this basis set are presented in Fig. 3 by the solid line. We observe that the elastic *ab initio* and model potential cross sections become relatively well converged when such basis was considered. This is the positron-Li_2 elastic cross section we recommend for reference in future works. It is important to observe that the convergence between the elastic cross sections was achieved for $\alpha_0 = 150\ a_0^3$ in the MCF calculation, and $\alpha_0 = 160\ a_0^3$ for SMC, a value considerably lower than the experimental one reported by [44]. The basis sets used in this investigation are listed in the Appendix A.

Some comments must be done when comparing the elastic integral cross section obtained by us when compared to the one reported by [9]. This last one was computed with a CP formulation originally developed to treat electron-molecule scattering. Fig. 3 shows that our result has similar energy dependence and magnitude slightly higher. In a given sense it seems that using electron or positron CP model does not appreciably affects the ICS. It is well known in literature that electron CP potentials work reasonably well in the positron case for some systems. This point was explicitly discussed in the articles of [27,45]. More stringent tests, nonetheless, show that the apparent insensitivity of the elastic ICS's, in fact, hide deficiencies in the description of the differential cross sections and annihilation rates. Indeed, those were the motivations that leaded [45] to propose a genuine positron CP model, i.e., the PCOP. It leads us to conjecture that the similarity between the PZ and PCOP ICS's is more fortuitous than physical. Similar situation has already been reported in literature. In [46] the positron-N_2 elastic ICS calculated with PCOP and ECOP (electron correlation-polarization potential) provided alike elastic results, in spite of being generated from very different potentials, as can be seen in Fig. 1 of that reference.

In Fig. 4 we present the rotational cross section associated to the quadrupolar transition $J_i = 0 \rightarrow J_f = 2$ computed in the ARA with the PCOP compared to the previous calculation of [9]. These authors report a structure around 0.5 eV which is not present in our results. Also, the $J_i = 0 \rightarrow J_f = 2$ cross section reported in the present work is higher in magnitude than the corresponding LFCC results for positron energies bellow 3 eV. Above this energy, we can see complete convergence between the two different approaches. In our calculations, the rotational constant of Li_2 molecule was taken as 8.1705×10^{-5} eV.

The uncertainty principle tell us that there is a time $\tau_{rot}(j)$

$$\tau_{\text{rot}}(j) \approx \frac{1}{(4j+6)B_{\text{rot}}} \tag{8}$$

associated to quadrupole transitions ($j \rightarrow j + 2$). The effective radius of the quadrupole interaction can be estimated by:

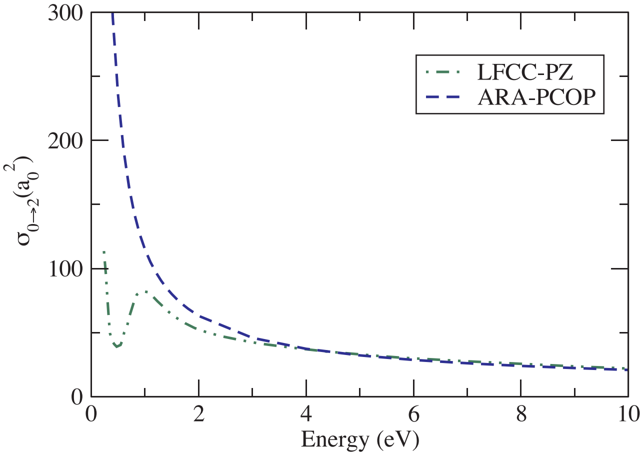

Fig. 4. Rotational excitation cross sections for the transition 0 → 2. Legends are the same as in Fig. 3. The ARA-PCOP cross section becomes practically equal to the LFCC-PZ for energies above ≈3 eV.

Table 1
Total and rotational cross sections obtained within the PCOP approach compared to the data of [9] which adopted the PZ-CP. The cross sections are given in a_0^2.

Energy (eV)	$\sigma^{0\to0}$		$\sigma^{0\to2}$		$\sigma^{0\to4}$		σ^{tot}	
	PCOP	PZ	PCOP	PZ	PCOP	PZ	PCOP	PZ
0.1	2618.8	1632.0	879.7	321.2	0.59	0.06	3501.3	1954.0
0.5	937.9	731.7	234.5	39.09	0.81	0.54	1173.2	777.3
1.0	596.0	344.3	114.9	82.56	1.26	0.92	712.2	427.8
2.0	358.4	200.7	62.99	52.78	2.30	1.48	423.7	254.9
3.0	252.3	127.9	45.86	43.16	2.67	1.86	300.8	172.9
6.0	129.6	64.2	28.64	30.26	2.90	2.65	161.2	97.12
8.0	95.29	47.46	23.96	25.85	3.00	2.81	122.4	76.30
10.0	73.51	38.49	20.80	22.80	3.06	2.90	97.60	64.19

Table 2
Cartesian-Gaussian basis set B used in SMC calculations. CB denotes center of bond and it is situated at the origin of the coordinate system.

Center and type	Exponent
Li, 9s	921.30000, 138.70000, 31.940000 9.3530000, 3.1580000, 1.1570000 0.4446000, 0.0766600, 0.0286400
Li, 4p	1.4880000, 0.2667000, 0.0720100 0.0237000
Li, 1d	0.2500000
CB, 2s	1.0000000, 0.02214942
CB, 2p	0.2000000, 0.00110747
CB, 6d	2.2500000, 0.77734266, 0.268560 0.0927838, 0.03205549, 0.011074

$$E \approx \frac{Q}{R^3}, \tag{9}$$

where Q is the molecular quadrupole moment. The crossing time associated to the effective radius of the quadrupole interaction is:

$$t_{\text{cross}} = \frac{1}{\sqrt{2}}\frac{Q^{1/3}}{E^{5/6}}. \tag{10}$$

The ARA is based on the idea that $t_{cross}/\tau_{rot}(j) \ll 1$. This leads us to the following condition of application of the ARA:

$$E \gg \left(\frac{4j+6}{\sqrt{2}}Q^{1/3}B_{\text{rot}}\right)^{6/5}. \tag{11}$$

Since B_{rot} is considerably small, the ARA is certainly valid for positron energies greater than 0.1 eV for this molecule.

We find important to report that when choosing different parameters in the present model calculation, i.e., molecular polarizabilities, we were not able to verify any similar structure as the one present in the $J_i = 0 \to J_f = 2$ cross section as seen in the LFCC calculation. This suggests that the structure seen in the low energy $0 \to 2$ cross section comes from the different treatment of the correlation effects. Comparable situation has been registered by [46], regarding positron-N_2. These authors observed that the quadrupolar transition calculated using positron and electron CP potentials (PCOP and ECOP) are quite similar, the exception being towards low energies where the differences become considerable (see Fig. 4 of such reference). This behavior is also seen in Fig. 4 in the present work, and it justifies an investigation using a proper positron CP potential.

Unfortunately, the calculation of the rotational cross sections is much more delicate in SMC because it depends on the balance between the p–p and s–d components of the scattering amplitude (see Table 1 of [34]) The results obtained for the $0 \to 2$ transition with SMC were not satisfactory and are not reported here.

Table 1 summarizes the total and rotational cross sections in a selected set of energies, compared to those of [9]. We can see numerically the convergence in higher energies between the cross sections listed, with some discrepancies in lower energies as discussed before. We call attention to the $J_i = 0 \to J_f = 4$ transition cross sections, which are in a reasonable agreement with the LFCC calculation, what suggests that the hexadecapole component of both potentials are similar.

4. Conclusions

We calculated elastic and rotational excitation cross sections for positron-Li_2 scattering for energies below 10 eV. The elastic cross section was computed with two independent approaches. The first one was the *ab initio* variational Schwinger Multichannel method (SMC). The second one was the single-body positron correlation-polarization potential (PCOP). Higher magnitude and slightly similar energy dependence were observed compared to the previous calculation of [9].

The elastic calculation shows that functions at the center of bond are not a mandatory condition to produce reasonable cross sections, as previously suggested in literature. In the same fashion, the values for the spherical polarizability obtained with MCF and SMC suggest a value of ≈150–160 a_0^3, a value considerably lower than the experimental one reported by [44].

The analysis of the rotational cross sections shows good agreement for the quadrupolar transition for energies greater than ≈3 eV. The divergence for lower energies comes from the use of a correlation-polarization potential properly developed to treat positron-molecule scattering. The comparison between the hexadecapolar transition have reasonable concordance with minor magnitude discrepancies.

We kindly suggest a future experimental verification of the positron scattering cross section for this molecule, in order to stimulate theoretical work in systems with huge polarizabilities.

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Table 3
The same as Table 2 but for Basis C.

Center and type	Exponent
Li, 10s	270.87720, 40.763780, 9.2075190 2.4906830, 0.7337280, 0.0751640 0.0302950, 0.0162118, 0.0086755 0.0046425
Li, 7p	1.3500000, 0.6750000, 0.3375000 0.1687500, 0.0084375, 0.0323198 0.0123801
Li, 3d	2.0250000, 0.4599198, 0.1044574

Appendix A

In this appendix, we show the set of cartesian Gaussian functions used to construct the trial scattering basis sets in Tables 2 (basis B) and 3 (basis C).

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