

Elastic scattering and rotational excitation of Li<sub>2</sub> by positron impactEliton P. Seidel<sup>a,\*</sup>, Marcos V. Barp<sup>a</sup>, Wagner Tenfen<sup>b</sup>, Felipe Arretche<sup>a</sup><sup>a</sup> Departamento de Física, Universidade Federal de Santa Catarina, 88040-900 Florianópolis, Santa Catarina, Brazil<sup>b</sup> Departamento de Física, Universidade Federal da Fronteira Sul, 85770-000 Realeza, Paraná, Brazil

## ARTICLE INFO

## Keywords:

Elastic scattering  
Rotational excitation  
Cross section  
Positrons  
Li<sub>2</sub>

## ABSTRACT

We report an *ab initio* and model potential investigation of elastic and rotational excitation cross sections for positron impact with Li<sub>2</sub> 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<sub>2</sub> between 150 and 160 a<sub>0</sub><sup>3</sup>, 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<sub>2</sub> molecule, which usually is experimentally manipulated in the gas phase.

Li<sub>2</sub> is a system with several peculiar characteristics. For example, the internuclear distance in the equilibrium geometry is 5.05 a<sub>0</sub> [7], a value expressively larger than the one found for H<sub>2</sub> (1.400 a<sub>0</sub>) and N<sub>2</sub> (2.068 a<sub>0</sub>). Also, the static dipole polarizability of Li<sub>2</sub> (140–270 a<sub>0</sub><sup>3</sup>) presents a considerable magnitude when compared to the corresponding ones for H<sub>2</sub> (5.4 a<sub>0</sub><sup>3</sup>) and N<sub>2</sub> (11.4 a<sub>0</sub><sup>3</sup>).

Beyond the particular molecular characteristics, Li<sub>2</sub> is a system that invites for a theoretical investigation in the context of positron scattering, mainly in the low energy region. For Li<sub>2</sub>, the inelastic electronic

thresholds are open at relatively small energies when compared to other similar systems. For example, the ionization potential of Li<sub>2</sub> is  $\approx 4.94$  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  $1^1\Sigma_g \rightarrow 1^1\Sigma_u$ , 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  $\approx 1$  eV, such that, a rigorous investigation about the positron-Li<sub>2</sub> scattering should take into account all these collision channels and its couplings.

As far as we know, the only existing calculation for positron-Li<sub>2</sub> 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<sub>2</sub> 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

\* Corresponding author.

E-mail addresses: [e.p.seidel@posgrad.ufsc.br](mailto:e.p.seidel@posgrad.ufsc.br) (E.P. Seidel), [f.arretche@ufsc.br](mailto:f.arretche@ufsc.br) (F. Arretche).

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<sub>2</sub> 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<sub>2</sub>O [22] and positron-H<sub>2</sub>O [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<sub>2</sub> 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

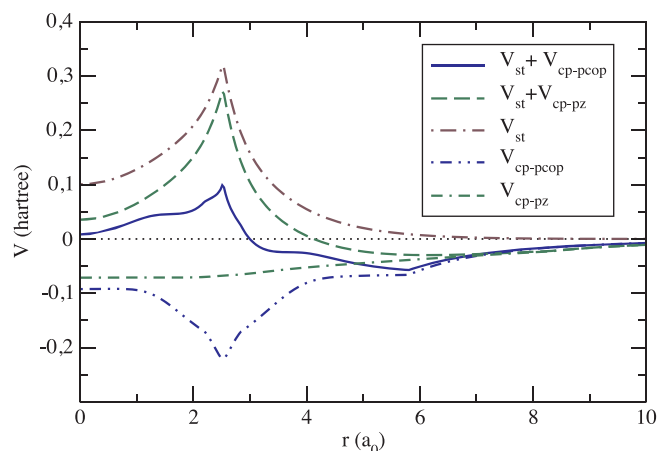


Fig. 1. Spherical component of the positron-Li<sub>2</sub> potential as a function of the positron distance to the center of the molecule. The solid line represents the total interaction in the static plus polarization approximation with PCOP; the dashed line is the same as solid one but for PZ potential; 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].

(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  $\approx 6 a_0$  (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.

As one may observe, in Fig. 1, the correlation component of the PCOP ( $V_{cp-pcop}$ ) has a different shape when compared to the PZ one ( $V_{cp-pz}$ ). Also,  $V_{cp-pcop}$  has a magnitude comparable to the static potential. This is not observed in other molecules such as H<sub>2</sub> and N<sub>2</sub> [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<sub>2</sub> 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:

$$T_{l_f m_f}^{l_i m_i} = -\frac{2}{\pi} \sum_{l_m} [(1 - iK)^{-1}]_{l_f m_f}^{l_i m_i} [K]_{l_m}^{l_i m_i} \quad (1)$$

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

$$\begin{aligned} \sigma^{J_i \rightarrow J_f} &= \frac{1}{4\pi} \frac{k_f}{k_i} \sum_{l_f l_i} \sum_{m_n} (-1)^{m+n} f_{l_f m}^{l_i n} (f_{l_f n}^{l_i m})^* \\ &\times \sum_j C(J_f j J_f; 000)^2 \\ &\times C(l_f l_i j; -m m 0) C(l_f l_i j; -n n 0), \end{aligned} \quad (2)$$

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  $f_{l_f m}^{l_i m}$  are connected to the  $T$  matrix ones by:

Download English Version:

<https://daneshyari.com/en/article/7839272>

Download Persian Version:

<https://daneshyari.com/article/7839272>

[Daneshyari.com](https://daneshyari.com)