Open problems in low energy interaction of positrons with molecules: theoretical

F. Arretche, D.P. Almeida, W. Tenfen, D.E. Zanellato, and S.E. Michelin
Departamento de Física, Universidade Federal de Santa Catarina, 88040-900, Florianópolis, Santa Catarina, Brazil.

A.C.F. Santos
Instituto de Física, Universidade Federal do Rio de Janeiro, 21945-900, Rio de Janeiro, Rio de Janeiro, Brazil.

J.B.P. Diaz
Departamento de Ciencias Físicas y Matemáticas, Universidad Arturo Prat, Casilla 121, Iquique, Chile.

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We present a brief discussion about two problems in the low energy scattering of positrons by molecules. Recent measured total cross sections present appreciably higher magnitude in low energies compared to other similar data. The status of such question is presented. Also, experimental absolute cross sections were measured and these were not described by theoretical calculations yet. The status of such questions is presented paying attention to future opportunities in theoretical positron-molecule research.

Keywords: Positron scattering; cross sections.

Presentamos una breve discusión acerca de dos problemas en la dispersión de baja energía de positrones por moléculas. Secciones transversales recientemente medidas presentan magnitudes considerablemente mayores a bajas energías comparadas con datos similares. Se presenta el estado de tal pregunta. También, se midieron secciones transversales absolutas que no han sido descritas por cálculos teóricos aún. El estado de tales preguntas se presenta llamando la atención a futuras oportunidades en la investigación teórica de positrón-molécula.

Descriptores: Dispersión de positrones; sección transversal.

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1. Introduction and motivation

The objective of this article is to present and briefly discuss some of the problems concerning the positron interaction with molecules. A first good question on the subject would be, why study positron physics? In solid state physics, positrons are used as tools to identify defects and vacancies in crystalline arrays [1]. The Doppler broadening of the annihilation radiation brings information about the velocity of the electrons in the solid. In astrophysics, the modelling of positron interaction with the interstellar medium [2] can be used as a tool to analyse the sources of annihilation radiation observed in the cosmos, like the center of our galaxy for example [3]. The interaction of positrons with biological molecules if of interest in order to improve the comprehension of positron emission tomography technique [4]. This is a medical technique that permits the visualization of the inner structure of a living organism without destructing it. Finally, due to technological advances, low energy antihydrogen atoms are now being produced [5]. Such antimatter experimental projects, wish to study, among other problems, the gravitational behaviour of antimatter [6] and possible violations of the CPT theorem [7]. The synthesis of antihydrogen is based in the trapping of positrons and antiprotons in a given volume. This way, the knowledge of the positron cross sections with atoms and molecules is welcome, since some molecular gases are used along the experimental procedure as buffer gases to dissipate the positron energy.

2. Open problems

In this section, we discuss two specific open problems concerning the scattering of low energy positrons ($\approx \text{eV}$) by molecules.

2.1. Total cross sections in the low energy limit

Recent measurements of the total cross section (TCS) for $\text{H}_2$, $\text{N}_2$ [8] and $\text{CO}_2$ [9] present higher magnitudes compared to other similar data reported previously for energies below 1 eV. Specifically, Karwasz et al. [8] discuss the “forward scattering error” as a key point to measure TCS’s with the correct magnitude. If the total cross section is written as

$$\sigma = 2\pi \left( \int_0^{\eta} \frac{d\sigma}{d\Omega} \sin \theta d\theta + \int_{\eta}^{\pi} \frac{d\sigma}{d\Omega} \sin \theta d\theta \right)$$

(1)

the angular resolution error happens when positrons scattered into forward angles below the cut-off angle $\eta$ are not counted. If such thing occur, the measured TCS is underestimated. Karwasz et al. argue that the use of narrow slits in the entrance and exit of the scattering cell suppress considerably this source of error. They used the differential cross sections reported by de Carvalho et al. [10] to estimate the correction in their TCS for $\text{e}^+\cdot\text{N}_2$. In a recent measurement for $\text{e}^+\cdot\text{CO}_2$ scattering, Zecca et al. [9] observed the same
kind of tendency. These authors explicitly state that the data for energies lower than 0.5 eV should be taken with caution because the energy resolution of the positron beam used was \(\approx 0.3\) eV. So, in the low energies, the uncertainty is of the order of the own positron kinetic energy.

Figure 1 present the TCS’s for \(\text{H}_2\), \(\text{N}_2\) and \(\text{CO}_2\). For \(\text{H}_2\), panel a), the Gianturco et al. [13] calculation has the better agreement with the recent data of Karwasz et al. [8] in spite of being not extended to lower energies. The Schwinger variational calculation of Lino et al. [14] basically matches the data of Hoffman et al. [11]. Other theoretical works for \(\text{e}^+ - \text{H}_2\) exist in literature, but we prefer to compare the experimental data with the results provided by these methods because the Gianturco approach deals with a one-body calculation, i.e., the many-body aspect of the problem is incorporated in the interaction potential, while the Schwinger one treats the many-body aspect explicitly. In the \(\text{N}_2\) case, see panel b), both methods have smaller magnitude than the experimental points, except for energies above \(\approx 6\) eV. For \(\text{CO}_2\), panel c), the Zecca’s data [9] present greater magnitude compared to the others for a great energy range. Gianturco’s calculation [17] have good agreement with these for energies above 1 eV. The recent Schwinger variational calculation of Sanchez [16], in spite of does not having the same magnitude of Zecca et al. data, also grows as the energy diminishes.

\(\text{H}_2\), \(\text{N}_2\) and \(\text{CO}_2\) are benchmark systems. Before trying to stablish the positron TCS for other systems, it would be desirable to have good precision on them. In the theoretical frontier, since the problem lies towards low energies, if these experimental points are absolutely correct, there are two options: to improve the description of correlation-polarization effects in the available methods or search for other physical effects not present in the collisional models yet.

2.2. Absolute differential cross sections

The first absolute differential cross sections (DCS’s) for positron-molecule scattering were measured by Sullivan et al. [18] for \(\text{H}_2\) at 0.5 eV and 6.75 eV for \(\text{CO}\).

Figure 2 show the carbon monoxide differential cross section compared to the relative differential cross section reported by Przybyla et al. [19] and the recent calculation of Arretche et al. [20].

For \(\text{H}_2\) (see Fig. 3a of [18]), neither the Kohn variational calculation [21] or the distributed positron model (DPM) [22] were able to reproduce the experimental data. At such low energy, it is expected that the s-wave scattering still be dominant, i.e., practically the same probability for scattering the positron in any given direction, as can be seen in the theoretical calculations. These present a small anisotropy towards the forward direction, and this can be expected due to other contributions of higher partial waves different of \(l=0\). It is hard to imagine what effect could cause great such deviation from the s-wave behaviour. If these experimental data are absolutely correct, it reinforces the idea that other physical effects must be added to the physical scattering models in order to explain them.

**Figure 1.** Total cross sections for \(\text{e}^+ + \text{H}_2\) (panel a), \(\text{e}^+ + \text{N}_2\) (panel b) and \(\text{e}^+ + \text{CO}_2\) (panel c). Panel (a): squares, recent data of Karwasz et al. [8]; triangles, Hoffman et al. [11]; crosses, Charlton et al. [12]; solid line, Gianturco et al. [13]; dot-dashed line, Lino et al. [14]. Panel (b): squares and triangles, the same as in panel (a); circles, data of Sueoka and Hamada [15]; solid line, Gianturco et al. [13]; dot-dashed line, de Carvalho et al. [10]. Panel (c): diamonds, data of Zecca et al. [9]; triangles and circles, the same as in panel (b), solid line, Gianturco and Paoletti [17]; dot-dashed line, recent calculation of Sanchez et al. [16].

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3. Conclusions

In this article, we made a brief discussion about two basic problems in low energy scattering of positrons by molecules. In the first part, we commented about the recent total cross sections reported for \( \text{H}_2, \text{N}_2 \) and \( \text{CO}_2 \). Two different research groups obtained much higher cross sections than the available ones in limit of very small energy. More efforts to understand such discrepancies are necessary, both theoretical and experimental. In the same fashion, the absolute DCS’s data were not reproduced by theory until now. If these experimental data prove to be correct, the theoretical models will have to be improved, through the refining the description of the positron-molecule interaction dynamics.

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