Positron scattering by molecules: recent applications of the Schwinger multichannel method.

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Positron physics have many applications in fundamental science, technology, and biology. Thus, the knowledge of basics interactions between positrons and molecules is a key aspect to understand the underlying physics of these applications. Despite the advance of theoretical methodologies, availability of powerful computational tools, and the significant experimental advancements have greatly revitalized the field of positron-molecule studies, both theoretical and experimental groups have faced challenges in fully characterizing low-energy (typically below 10 eV) positron scattering, even when dealing with simple non-polar molecules.

In experiments, limitations in the angular resolution of different experimental apparatus seem to be responsible for the discrepancy among the results. On the other hand, in theoretical studies, the challenges arise from accurately considering positron-molecule correlation-polarization interactions, particularly within ab initio methods that rely on virtual single excitations for their description. These challenges likely explain the lack of agreement between theoretical and experimental data and the limited consistency among different theoretical approaches.

In this talk, we will discuss our latest findings concerning positron-molecule scattering, obtained within the Schwinger multichannel method. In particular, we will present some of our recent ab-initio results, which have been achieved through the utilization of our parallelized version [2,3] of the SMC method, which has allowed us to greatly increase the number of single excitations used in the expansion of the scattering wave function. Further, we will focus on a polarization scheme based on a model potential [2] employed to describe positron-molecule polarization and correlation. This model potential seems to allow us to obtain at good estimates of scattering cross sections for bigger systems, which our current ab-initio methodology does not allow.

References

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2. F. F. Frighetto, A. Souza Barbosa, S. d'A. Sanchez, Phys Rev. A **108**, 012818 (2023).
3. F. F. Frighetto, S. d'A. Sanchez, A. Souza Barbosa, to be submitted soon.