Pauli Shielding and Breakdown of Spin Statistics in Multielectron, Multi-Open-Shell Dynamical Atomic Systems

I Madesis[1,2], A Laoutaris[1,2], E P Benis[3], T J M Zouros[1†], J W Gao[4] and A Dubois[5*]

[1]Department of Physics, University of Crete, GR-70013 Heraklion, Greece
[2]Tandem Accelerator Laboratory, INPP, NCSR "Demokritos", GR-15310 Ag. Paraskevi, Greece
[3]Department of Physics, University of Ioannina, GR-45110 Ioannina, Greece
[4]Sichuan University, 610064 Chengdu, China
[5]Sorbonne Université, CNRS, Laboratoire de Chimie Physique-Matière et Rayonnement, F-75005 Paris, France

Synopsis State-resolved cross sections of electron capture in collisions of swift $C^{4+}(1s2s\ ^3S)$ ions with He and H_2 are determined to investigate the formation of doubly excited $C^{3+}(1s2s2p)\ ^4P$ and $^2P_\pm$ states and the ratio R of their cross sections as a measure of spin statistics. Using ZAPS measurements and semiclassical close-coupling calculations, a long-standing puzzle and controversy on the value of R and the effect of cascades is resolved invalidating the frozen core approximation generally used in the past when considering electron capture in multielectron, multi-open-shell quantum systems.

We provide experimental results for the $1s2s2p\ ^4P/^2P_\pm$ line ratio R for single electron capture in fast collisions of $C^{4+}(1s2s\ ^3S)$ with helium and hydrogen targets [1]. Our measured R values shown in Fig. 1 are seen to be close to 2, in contrast to previous findings. In parallel, the ratio R calculated using a sophisticated multielectron close-coupling approach (3eAOCC) [2] is found to be in agreement, for the first time, with experiment, when postcollisional radiative cascades [3] are also taken into account. These results draw attention to the limited predictive power of the frozen core approximation regarding spin statistics in highly correlated dynamical atomic systems. To better understand our findings, we propose an elegant Pauli shielding mechanism related to strong exchange effects which selectively (and counter-intuitively) obstructs specific reaction channels. Systematic isoelectronic studies should further validate these conclusions in a more general context.

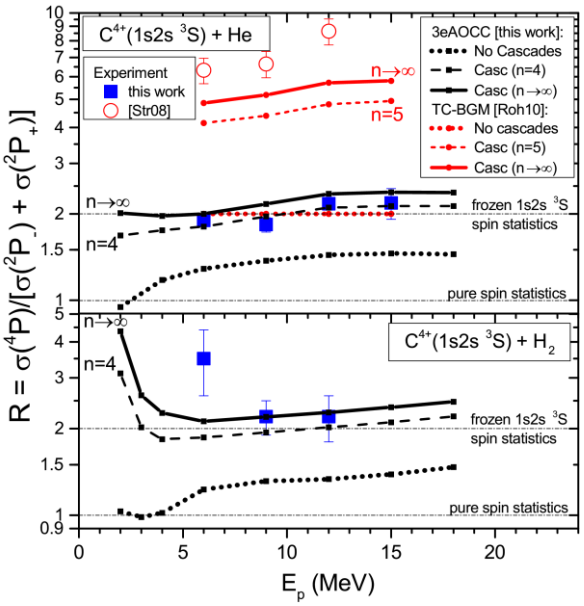

Figure 1. Ratio R for $C^{4+}(1s2s\ ^3S)$ collisions with He (top) and H_2 (bottom) as a function of projectile energy [1]. Experiment (ZAPS): Squares (this work), circles [4]. Theory: Black lines (3eAOCC), red lines [5]. Results without (dotted) and with radiative cascades from 1s2snl ^4L states up to the indicated n (dashed) and extrapolated to $n \to \infty$ (solid) are shown. The frozen 1s2s ^3S core spin statistics and pure spin statistics values are indicated.

References

[1] Madesis I *et al* 2020 *Phys. Rev. Lett.* **124** 113401
[2] Gao J W *et al* 2017 *Phys. Rev. A* **96** 052703
[3] Zouros T J M *et al* 2020 *Atoms* **8** 61
[4] Strohschein D *et al* 2008 Phys. Rev. A **77** 022706
[5] Röhrbein D *et al* 2010 Phys. Rev. A **81** 042701

We acknowledge support of this work by the project "Cluster of Accelerator Laboratories for Ion-Beam Research and Applications - CALIBRA" (MIS 5002799) implemented under the Action "Reinforcement of the Research and Innovation Infrastructure", funded by the Operational Programme "Competitiveness, Entrepreneurship and Innovation" (NSRF 2014-2020) and co-financed by Greece and the European Union (European Regional Development Fund).

* E-mail: alain.dubois@sorbonne-universite.fr
† E-mail: tzouros@physics.uoc.gr