ELECTRONIC EXCITATION OF H_2 BY POSITRON IMPACT

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In this work, we apply Schwinger Multichannel method (SMC) [1] to calculate the electronic excitation cross section of H_2 by positron impact. Specifically, we considered the $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$, $X^1\Sigma_g^+ \rightarrow E,F^1\Sigma_g^+$ and $X^1\Sigma_g^+ \rightarrow C^1\Pi_u$ electronic transitions in the energy range from 13.5 to 30.0 eV.

In recent applications of SMC, the presence of spurious resonances was detected [2] in electronic excitation cross sections for N_2. These structures were generated by intrinsic problems with the basis set employed in the calculation. To overcome the problem, a technique based on direct comparison with the first Born approximation (FBA) was developed.

This procedure is called "Basis Set Born Approximation" (BSBA) because when correlation ($Q\hat{H}Q$) and Green's function ($VG_P^{(+)}V$) terms are switched off in the working expression for the SMC scattering amplitude, the results provided by the variational scattering basis set ($\{\chi_m\}$) should be identical to the FBA ones (nearly basis-set independent). The configurations weakly coupled to the scattering potential are then draw back until the BSBA cross section becomes similar to the FBA result.

In a first application of SMC to electronic excitation, the $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ electronic excitation of H_2 was considered in a "two state level of approximation" [3]. Due to the problems found in the works with N_2, the results presented before became uncertain. The main motivation for this work is to verify the reliability of the old results, and to verify the power of the BSBA technic to predict electronic excitation cross sections. In figure 1, we present the new results with the old ones and also with the experimental data o Sullivan *et al* [4]. We hope this work motivate experimentalists to realize new measurements with H_2 and other molecular targets in near future.

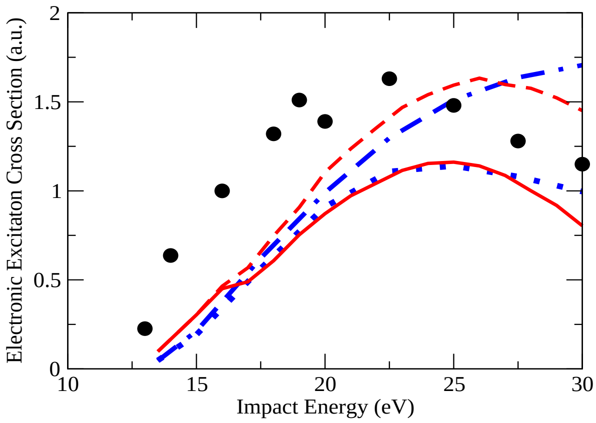

Fig. 1. $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ electronic excitation cross section. Circles: experimental data of Sullivan *et al.* [4]. Red full line: old SMC results [3]. Red dashed line: old Born-SMC results [3]. Blue points: new SMC results. Blue dashed-point line: new Born-SMC results.

References

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