Application of the Schwinger Multichannel Method in the Study of the Electronic Excitation of H_2 molecules by Electron-Impact: Development of the Minimal Orbital Basis for Single Configuration Interactions (MOB-SCI) Strategy

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It has been pointed out by several authors that the electronic excitation of molecules by impact of slow electrons strongly affects the reaction dynamics in discharge environments [1, 2, 3]. For instance, detailed information concerning such inelastic process is essential for the modeling of plasma processing gases, largely used in the semiconductor manufacturing. As a result of the increasing number in applications of the plasma based technologies, it has yielded a strident demand for the compilation of a reliable cross section database. In spite of this fact, the effort undertaken by experimentalists and theorists to generate the required data has attained just a moderate degree of success. Due to the difficulties to produce and characterize excited species with sufficient accuracy, experimental measurements on the electronic excitation by electron-impact were performed for few molecular systems and have covered only a limited range of impact energies [4]. From the theoretical point of view, the challenge has been to develop strategies for the close-coupling expansion or, in more words, how to define the number and the type of energetically open channels that should be included in the scattering calculations. As a matter of the fact, the actual capacity of providing calculated cross sections for plasma modeling is still not reliable since there are no molecular systems for which the results obtained by different theoretical methods display a systematic agreement in terms of the multichannel convergence. Having these considerations in mind, we have proposed a new scheme for the study of the electron-molecule electronic excitation problem. Our scattering amplitudes were calculated using the Schwinger multichannel method [5, 6, 7] within the so-called minimal orbital basis for single configuration interaction (MOB-SCI) level of approximation. More specifically, we have chosen a minimal orbital basis that, for the first singlet and triplet states of a given symmetry representation, generates the small(est) configuration space equivalent to the full single configuration one. The intention was to provide an alternative technique beyond the two-channel approach, with a minimum number of states used in the composition of the active configuration space as possible. The identification and remotion of spurious structures of numerical linear dependence nature were also addressed through the use of a check procedure similar to those proposed in Refs. [8, 9]. In this talk we report integral and differential cross sections for the electronic excitation of H_2 molecules by electron-impact. Our study includes the $\mathrm{X}^1\Sigma_g^{(+)} \rightarrow \mathrm{b}^3\Sigma_u^{(+)}$, $\mathrm{B}^1\Sigma_u^{(+)}$; $\mathrm{X}^1\Sigma_g^{(+)} \rightarrow \mathrm{a}^3\Sigma_g^{(+)}$, $\mathrm{E,F}^1\Sigma_g^{(+)}$; and $\mathrm{X}^1\Sigma_g^{(+)} \rightarrow \mathrm{c}^3\Pi_u$, $\mathrm{C}^1\Pi_u$ electronic transitions for impact energies up to 30 eV. The results obtained by means of the MOB-SCI technique, combined with the analysis of the numerical stability of the present calculations, show a significant improvement towards experimental data in comparison with previous two-channel close-coupling calculations, as can be notice from Figure 1. Calculations for the electronic excitation of N_2 molecules by impact of low-energy electrons are also underway. In this case, the implementation of the MOB-SCI strategy is more sophisticated, since transitions may come from different particle-orbitals. A discussion on what is, and possibly not is, working in this study will be included in the presentation.

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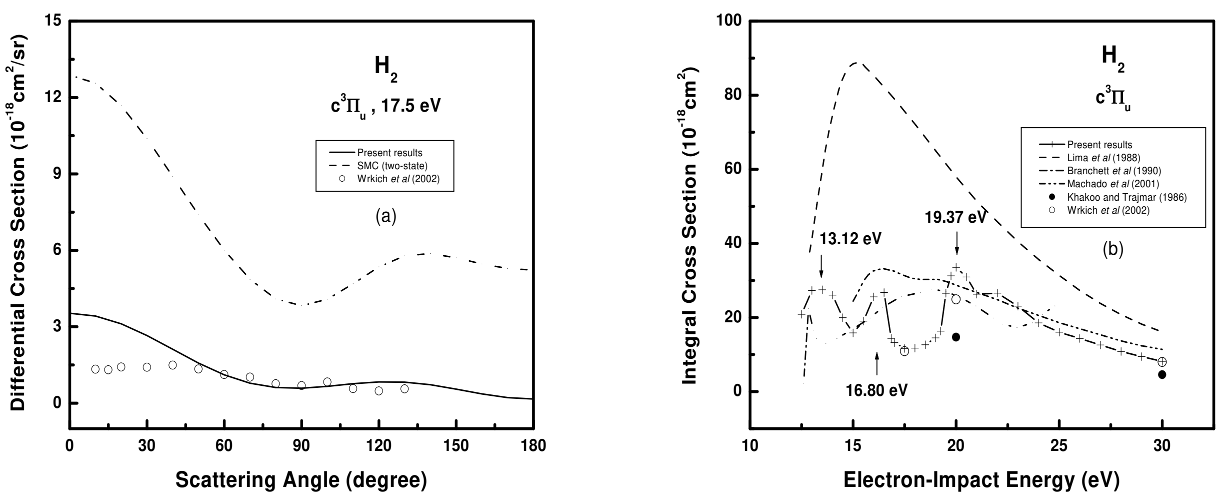

Figure 1: Differential and Integral cross sections for the $X^1\Sigma_g^{(+)} \rightarrow c^3\Pi_u$ electronic transition of the H_2 molecule: (a) DCS at 17.5 eV and (b) ICS. Solid line: present results; dashed line: SMC two-state results from Lima *et al* [10]; dash-dotted line: R-Matrix seven-state results from Branchett *et al* [11]; dash-dot-dotted line: Continued Fractions four-state results from Machado *et al* [12]; full circles and open circles: experimental results from Khakoo and Trajmar [13] Wkrich *et al* [14], respectively.