ELECTRONIC EXCITATION OF N_2 MOLECULES BY ELECTRON-IMPACT: APPLICATION OF THE MINIMAL ORBITAL BASIS FOR SINGLE CONFIGURATION INTERACTIONS (MOB-SCI) STRATEGY

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Collisions between slow electrons and N_2 molecules play a key role for the understanding of a variety of natural phenomena that occurs in the Earth's upper atmosphere as well as in other planetary atmospheres and in the interstellar media [1]. The knowledge of the cross sections related to collisional processes involving molecular nitrogen is also essential for the modeling of chemically active plasmas used in the fabrication of microelectronics devices [2]. In special, it has been pointed out in several publications that the electronic excitation processes strongly affects the reaction dynamics in such discharge environments [3]. In spite of the great interest in the compilation of reliable cross section data base for this collision process, the number of theoretical studies concerning the electronic excitation of nitrogen molecules by impact of low-energy electrons is still very scarce. Besides, the agreement among measured data and the results obtained by different methods is still far from satisfactory.

Motivated by this context we have decided to perform a study for the e^--N_2 electronic excitation by means of the Schwinger multichannel method [4]. Our scattering amplitudes are obtained within the minimal orbital basis for single configuration interactions (MOB-SCI) level of approximation [5]. Specific issues addressed by the present work may be summarized as follows:

(i) the representation of the target is improved by a CI-singles description of the excited states;

(ii) through the use of the MOB-SCI strategy we have investigated the coupling effects among ground state and first singlet and triplet states of the same symmetry representation, while keeping the pseudo-state associated space as minimum as possible;

(iii) the numerical stability of our scattering calculations is analyzed through the use of a check procedure similar to those developed by Chaudhuri and co-workers [6];

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