Sturmian Approach To Single Photoionization of CH_4

C. M. Granados-Castro[(a),(b)], L. U. Ancarani[(a)], G. Gasaneo[(b),(d)] D. Mitnik[(c),(d)]

[(a)] Equipe TMS, SRSMC, UMR CNRS 7565, Université de Lorraine, 57078 Metz, France
[(b)] Departamento de Física, Universidad Nacional del Sur, 8000 Bahía Blanca, Buenos Aires, Argentina
[(c)] Instituto de Astronomía y Física del Espacio (IAFE) and Universidad de Buenos Aires, C1428EGA Buenos Aires, Argentina
[(d)] Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina

The study of ionization and photoionization phenomena in atoms and molecules has been a subject of active research, and has a direct impact in other fields such as plasma, atmospheric, medical and astrophysics. The quantal description of ionization processes in molecular systems (even simple ones) is highly complex.

To a good approximation, the molecular structure can be described in the *self-consistent field* [1] approach which uses a spherically symmetric potential for individual electrons. Generally, this leads to a reasonable agreement between calculated and experimental cross sections, in particular when the molecular systems possess a high degree of symmetry, as in the case of CH_4 [2]. This encourages us to use central potentials, as a first approximation, to study photoionization in CH_4. We start with an angular averaged model potential $U_i(r)$ [3], which is calculated from the independent particle model (see figure 1), considering one active electron placed in the molecular orbital (MO) i of the ground state. For each MO we use the wave functions provided by Moccia [4].

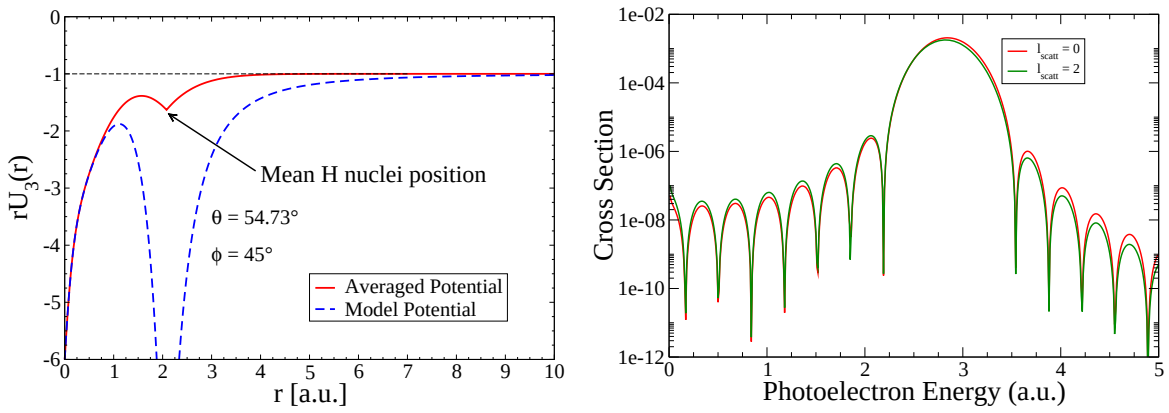

Figure 1: Left panel: Angular averaged (in red) potential and molecular model non-averaged (at indicated angles, in blue), multiplied by r (effective charge) for the $1T_{2z}$ state of CH_4. Right panel: Calculated photoionization cross sections from $1T_{2z}$ state of CH_4 for the two possible final states, with $l_{\text{scatt}} = 0$ (red) and 2 (green), using a short laser pulse with a central frequency $\omega_0 = 3.37$ a.u. and a pulse duration of 450 as.

In the first part of this work, we solve the time-independent Schrödinger equation (TISE) in a first order perturbation theory, with the dipolar operator in the velocity gauge, and

for an ultrashort laser pulse with different central frequencies. We use $U_i(r)$ and an initial MO ground state, and the final state is expanded in a generalized Sturmians basis, with correct asymptotic behavior [5, 6]. From the scattering solution of the corresponding driven equation, we extract the photoionization cross sections (see figure 1) and compare them with previous calculations and available experimental data, as in [2, 7, 8] and references there in.

In a second step, we use a more realistic potential, which includes all the nuclei and other electrons interaction as in [3]. We solve again the TISE which, in this case, is an angular-coupled set of equations. The results are compared with our previous (averaged potential) results.

The second part of this work concentrates in the study of the collision of electrons with the CH4 molecule, starting with the angular averaged potential $U_i(r)$, and comparing our results with previous works [8, 9].

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E-mail: ugo.ancarani@univ-lorraine.fr