Multiple Ionic Channel Formulation for Strong Field Single Ionization of Multielectron Targets

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Synopsis We present a novel approach to calculating strong field ionization dynamics of multielectron molecular targets. Adopting a multielectron wavefunction ansatz based on field-free *ab initio* neutral and ionic multielectron states, a set of coupled time-dependent single-particle Schrödinger equations describing the neutral amplitude and continuum electron are constructed. These equations, amenable to direct numerical solution or further analytical treatment, allow one to study multielectron effects during strong field ionization, recollision, and high harmonic generation.

Present theoretical tools for calculating strong field ionization fall into two categories, 1) semianalytical theories based the Strong Field Approximation, often with improvements over the traditional formulation, and 2) direct time-dependent numerical solution of the Schrödinger equation. The first category suffers from approximations necessary to allow a semianalytical treatment, most notably the neglect of the binding potential of the molecular core on the ionization, continuum, and recollision dynamics. The second category has the shortcoming that full numerical treatment becomes impossible as the number of degrees of freedom increases. Time-dependent numerical solutions of the Schrödinger equation including a strong laser field is only feasible for one or two particle systems.

In this work we address both the problems of including the binding potential consistently throughout the strong field dynamics as well as the problem of accounting for multielectron effects. Our approach to strong field ionization of multielectron targets combines *ab initio* quantum chemistry multielectron wavefunctions with single particle time-dependent numerical solutions. Our derived equations coupling the neutral to the continuum electron follow directly from the multielectron Schrödinger equations and contain no adjustable parameters.

Figure 1 shows preliminary calculation and experimental results for the angle-dependent ionization yields from CO_2, where the angle is the angle between the molecular axis and polarization vector of the linearly polarized strong laser field. The theoretical plots show the ionization yield for different final states of the CO_2^+ cation (colored curves) as well as the total yield summed over all these channels (black curve). The experimental curves show analogous angle-dependent ionization yields. In the experimental plots, the red line is the measured yield for a distribution of aligned CO_2 molecules and the green curve shows the molecular frame angle-dependent yields obtained by deconvolving the measure yields from the distribution of molecular alignment. Comparison should be made between the black theoretical curves and the green experimental curves. The theoretical calculations capture the symmetries and trends seen in experimental yields as the intensity is varied. In our formulation it is necessary to include multiple final ion states (i.e. the multielectron nature of the problem) in order to approach the experimental results.

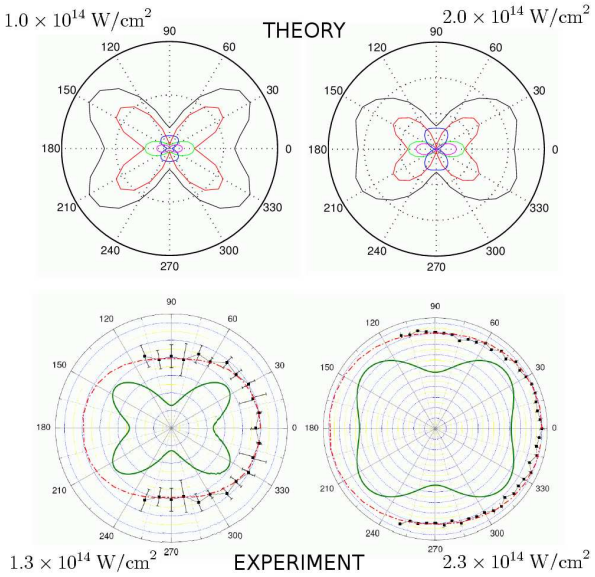

Fig. 1. Theoretical and experimental angle-dependent ionization yields for CO_2.

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