Electronic Excitation of Molecules by Electron Impact with the Schwinger Multichannel Method with Pseudopotentials (SMCPP): How far has it gone?

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The Schwinger variational method for scattering calculations uses Green's functions with proper boundary conditions for allowing a continuum wave function to be expanded in a square integrable basis set (known as a L^2 method). The method works well as long as the chosen basis set is sufficiently complete within the scattering potential range. The Schwinger Multichannel method incorporated this strategy for a much more complicated system, the electron scattering by molecules, a many body target involving electrons and nuclei. Born Oppenheimer approximation followed by proper averaging over fixed nuclei geometries, allow the theoreticians to focus only in the many-body character of the electronic part. The SMCPP methods accounts for the static-exchange-plus-polarization interactions and for the electronic excitations by electron impact for molecules with arbitrary geometries. The fixed nuclei approximation works for many applications as long as the scattering electron is fast enough compared with the times involved in the nuclei motion. Norm conserving pseudopotentials allows cutting down the number of electrons to a not so many-body problem and it helps to exploit molecular systems composed by any atom of the periodic table. In my presentation, I will discuss the progress done with this L^2 method for obtaining cross sections for electronic excitation of molecules by electron impact, considering that the molecular target imposes many challenges as an infinite number of bound states (replaced by a proper choice of a finite number of states) and a continuum band of states from several ionization potentials (completely disregarded by the method).