

Electron-molecule scattering dynamics under the influence of polarization and multichannel coupling effects

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Synopsis The Schwinger multichannel method was designed to account for exchange, polarization and electronic multichannel coupling effects in the low-energy region of electron scattering from molecules with arbitrary geometry. The applications of the method became more ambitious with availability of computer power combined with parallel processing, use of norm-conserving pseudopotentials and improvement of target description. As will be discussed, the latest applications involving 33, 45 and 63 electronically open channels for phenol, ethylene and furfural molecules, represent good examples of the present status of the method.

The description of the many-body dynamics in electron-molecule collisions is, at least at the fixed-nuclei approximation, strongly affected by the inclusion and also by a proper balanced treatment of exchange, polarization and multichannel coupling effects. At sufficiently low impact energies, only the elastic channel is open (i.e., it is the only channel that is energetically accessible to the system) and the collision process is dominated by the description of the distortion of the target's electronic cloud due to the presence of the incident electron, an effect which is taken into account by allowing virtual excitations (closed channel space) from the ground state. This effect combined with the proper solution of the scattering problem, including the exchange interaction, is known as the static-exchange-plus-polarization (SEP) approximation. As the electron impact energy increases, several discrete and continuum states (above the ionization threshold) become accessible giving rise to what is called as the multichannel coupling effect. This means that all states that become energetically allowed to the target during the collision process represent possible final states that compete for the flux that defines the cross section and must therefore be treated as open channels. In practice, however, the intrinsic many-body character of the electron-molecule collision problem imposes the use of approximations and this occurs at both, bound state and scattering calculations. According to our experience, a good description of the target states combined with the use of a suitable strategy to minimize the open channel space represent a crucial step towards a computationally feasible choice for the level of multichannel coupling to be used in the scattering calculations. Having these questions in mind, we have developed the so called minimal orbital basis for single configuration interaction (MOBSCI) strategy [1]. Through the use of the MOBSCI strategy, we

constructed an open channel space composed by a set of hole-particle orbitals which is capable of reproducing the spectrum of excitation energies obtained with a full single configuration interaction (FSCI) calculation for energies below a previously defined cutoff energy value. At the same time, within this approach, the number of pseudo states is minimized and the open channel space becomes as compact as possible.

Recent applications of the Schwinger multichannel method with pseudopotentials [2] involving small polyatomic molecules provided a clear indication that: (i) inclusion of polarization effects for description of the electronic excitation process is important in circumstances under which the target has excited states opening up at the low-energy domain and resonances in the elastic channel that are located near to the threshold of these low-lying excited states and (ii) a very large number (i.e., a much bigger number than the ones considered in the previous studies reported in the literature) of electronic states should be included in the expansion of the open channel space in order to achieve (or, at least, move towards obtaining) converged elastic and electronic excitation cross sections. In this talk we will illustrate these findings by presenting results for ethylene, phenol and furfural molecules [3], each one of them obtained in calculations in which the multichannel coupling effect was treated in a growing level of complexity.

References

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