Basis Generator Method Calculations for Charge-Transfer Collisions Involving Few-Electron Systems

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The basis generator method (BGM) has been developed over many years with the objective to devise a general method for the solution of the time-dependent Schrödinger equation (TDSE) [1, 2]. It is based on the idea that completeness of a basis is not a necessary criterion for converged results. Rather, if the basis used to expand the state vector has the ability to adapt dynamically to the problem at hand, a relatively small basis size may be sufficient to obtain accurate (in principle, exact within numerical accuracy) results. The BGM has been applied most extensively and successfully to ion-atom and, more recently, ion-molecule collisions over broad ranges of impact energies [3, 4]. In its two-center (TC) implementation [5] it is similar to the more traditional atomic orbital close coupling method in that atomic bound states (with electron translation factors) and a set of pseudostates are used to represent the solution of the TDSE. It is in the way the pseudostates are constructed in which it differs.

In this talk, I will give a (necessarily brief) overview of recent TC-BGM collision calculations. The focus will be on charge-transfer reactions involving few-electron systems such as the noble gas atoms and water and methane molecules. The multi-electron problem is dealt within an independent particle model which is inspired by density functional theory. This implies that in addition to uncertainties associated with numerical and/or convergence issues model uncertainties have to be assessed. The only currently known way of doing this is via extensive comparisons of different model variants with experimental data and other theoretical results. It will be demonstrated that this is a useful procedure that provides qualitative, albeit not quantitative, information on the achieved accuracy.

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