Ultra low energy scattering and chemistry with the R-matrix

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New developments in experimental methods allow for the routine production of ultracold (microkelvin) atoms and molecules. This has facilitated the study of chemical reactions involving only a small number of partial waves, allowing for unprecedented control over elastic and inelastic collisions and ultracold chemical reactions. We are developing a new program, RmatReact, which uses the R-matrix and associated methodology to accurately simulate heavy particle collision events at these ultracold temperatures [1]. The method divides space into an inner and outer region along the reaction coordinate. The only input required is a suitable potential energy function. Information about the bound rovibrational states in the inner region, specifically eigenenergies and wavefunctions, which are generated from variational nuclear motion programs built for high-accuracy spectroscopy, is used to generate information about the scattering event in the outer region. The results which are produced are scattering observables such as the scattering length, the S-matrix and the cross sections for different processes. With this method, calculations can be done inexpensively at many different scattering energies, allowing for high-resolution plots of these observables and the characterisation of long-lived quasi-bound states (resonances). Initial results generated using this code have concentrated on atom-atom collision such as Ar – Ar [2] and O – He using code Duo [3] for the inner region. Development of the method for atom – diatom collisions, including reactive one, is also in progress [4].

References