# 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**

1. J. Tennyson, L.K. McKemmish and T. Rivlin, *Faraday Disc.* **195**, 31 (2017).
2. T. Rivlin, L.K. McKemmish, K.E. Spinlove and J. Tennyson, *Mol. Phys.* in press, doi 10.1080/00268976.2019.1615143.
3. S.N. Yurchenko, L. Lodi, J. Tennyson and A.V. Stolyarov, *Comp. Phys. Comms.*, **202**, 262 (2019).
4. L.K. McKemmish and J. Tennyson, *Phil. Trans. Royal Soc. London A* (in press).