Calculation of ultra cold collisions and temperature-dependent photodissociation cross sections using bound state nuclear motion programs

Jonathan Tennyson[1,2]*
*presenter
[1] Physics and Astronomy, University College London, UK; email: j.tennyson@ucl.ac.uk
[2] Institute for Nuclear Research, 4001 Debrecen, Hungary

Variational bound-state nuclear motion programs such as Duo (diatomics), DVR3D (triatomics) and TROVE (polyatomics) are being used is to perform calculations on both ultracold collisions and photodissociation of small molecules.

For the ultracold collisions the procedure involves dividing space into an inner region where detailed nuclear motion calculations need to be made and an outer region where the particles feel only the long-range potentials. Only the outer region calculations depend on the scattering energy. The nuclear motion codes are used so solve the inner region for each J (and symmetry) of the problem. Cross sections and other scattering parameters (such as resonance positions) are found by propagating R-matrices constructed at the boundary between two regions to large separations [1].

Similar ideas are being used to compute fully vibration-rotation (and potentially hyperfine) resolved photodissociation cross sections. However in this case we are using a simplified procedure which dispenses with need to explicitly treat the long-range part of the dissociative wavefunction [2]. This makes the computation of cross sections (and rates) which depend on the the temperature of the initial target molecule straightforward. Use of this method for astronomical applications is being explored as a function of the dependence on molecular temperature and assumed radiation field with some unexpected results [3].

[1] T. Rivlin, L.K. McKemmish, K.E. Spinlove and J. Tennyson, *Mol. Phys.,* **117**, 3158 (2019).
[2] M. Pezzella, S.N. Yurchenko and J. Tennyson, *Phys. Chem. Chem. Phys.*, **23**, 16390 (2021).
[3] M. Pezzella, S.N. Yurchenko and J. Tennyson, Mon, Not. Roy. Astr, Soc. (submitted).