Reconstructing magnetic Feshbach resonances of highly anisotropic alkali-like diatom + atom systems with unconverged rotational basis

Marcin Welter [1], **Michał Tomza** [1], **Jeremy M. Hutson** [2]

[1]Faculty of Physics, University of Warsaw, ul. Pasteura 5, 02-093 Warszawa, Poland
[2]Department of Chemistry, Durham University, South Road, Durham, DH1 3LE, United Kingdom

We explore a computation scheme for calculating magnetic Feshbach resonances of highly anisotropic, alkali-like diatom + atom systems. The calculation is done in a smaller, unconverged rotational basis, and aims to reconstruct the results yielded from the converged basis. When dealing with highly anisotropic systems, it is usually needed to include a large number of rotational states to converge. Even in rigid rotor approximation and in the total rotational angular momentum (TRAM) basis, it might require on the order of hundreds of rotational states to converge the energies of the last few bound states and converge the scattering length. With inclusion of spins in the system, the basis size increases substantially. This high computational cost hinders tuning the Feshbach resonances spectrum by for example scaling the potentials. Showing that the smaller basis can reproduce the same results is, thus, of great interest. We work with SrF + Rb system as an example. The idea of our scheme is to scale the triplet and singlet potential surfaces independently, in such a way that each surface's calculated last few bound state spectrum in the unconverged basis best reproduces the spectrum, calculated in the converged basis. We then explore how well the magnetic Feshbach resonances are reconstructed when using those scaled potentials surfaces.