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On the basis size problem in ultracold molecular scattering: Approximate hyperfine cross sections from hyperfine-free calculations[1]

MAYKEL LEONARDO GONZALEZ-MARTINEZ, Laboratoire Aime Cotton, CNRS, Universite Paris-Sud XI, Bat. 505, Campus d'Orsay, 91405 Orsay, THEOMOL TEAM — Understanding (ultra)cold collisions is crucial to assess both the prospects of cooling techniques that rely on thermalization and trapping lifetimes. However, brute-force application of the coupled-channel method to many low-temperature scattering problems finds two main obstacles: (1) the need for large basis sets that are computationally intractable, and (2) the need to explore a multidimensional parametric space in order to tackle questions concerning real experimental conditions. The basis size problem arises because many interactions that are negligible at thermal temperatures become comparable to, or larger than, the collision energies involved. Taking all such terms into account significantly increases the size of the basis needed for convergence, with dramatic effects on the computing effort. Here, I discuss an approximate method to account for the effect of hyperfine interactions in ultracold molecular scattering. The method naturally resolves the effects discussed by Gonzalez-Martinez and Hutson in calculations on Mg+NH, and may be combined with those by Tscherbul et al. and Croft et al. to tackle problems which are computationally intractable to date. Depending on the system, the proposed method may lead to one to four orders-of-magnitude savings in computing times.

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