Abstract Submitted
for the DAMOP14 Meeting of
The American Physical Society

Quantum defect theory with full close-coupling method at short-range: Applications to ro-vibrational transitions in ultracold H_2-H_2 collisions and beyond[1] JISHA HAZRA, N. BALAKRISHNAN, University of Nevada Las Vegas, Las Vegas, NV 89154, BRANDON P. RUZIC, JOHN L. BOHN, JILA, University of Colorado and National Institute of Standards and Technology, Boulder, CO 80309 — An accurate characterization of both short-range dynamics and long-range physics continues to be a major challenge in describing ultracold collisions. While quantum close-coupling (CC) is the preferred approach, it is computationally intractable for many systems of current experimental interest. A well-tested and computationally tractable approach for ultracold collisions is multi-quantum defect theory (MQDT). It is adept in handling both long-range forces and external field dependencies. Here we describe a hybrid approach that uses explicit CC method at short-range and the MQDT formalism at long range. The CC calculations needs to be carried out only at one energy, essentially at zero collision energy, to yield a short-range K-matrix from which accurate cross sections can be evaluated for energies up to a kelvin using the MQDT formalism. We illustrate the approach for the benchmark case of rovibrational transitions in H_2-H_2 collisions. Potential applicability of the approach to reactive collisions is discussed.

[1]This work was supported in part by NSF grant PHY-1205838 (N.B.) and ARO MURI grant No. W911NF-12-1-0476 (N.B, J.L.B).

Balakrishnan Naduvalath
University of Nevada Las Vegas, Las Vegas, NV 89154

Date submitted: 29 Jan 2014 Electronic form version 1.4