Abstract Submitted
for the DAMOP18 Meeting of
The American Physical Society

Non-adiabatic quantum reactive scattering in hyperspherical coordinates[1] BRIAN K. KENDRICK, Los Alamos Natl Lab — A new methodology for performing electronically non-adiabatic quantum reactive scattering calculations in hyperspherical coordinates is presented for A + B_2 $\leftrightarrow$ AB + B and AB + B $\rightarrow$ AB + B reactive systems. The methodology accurately treats all six degrees of freedom relative to the center of mass on two coupled Born-Oppenheimer electronic potential energy surfaces which exhibit a conical intersection (degeneracy). The non-adiabatic coupling between the two electronic states is equivalent to a U(2) non-abelian gauge potential and a particular choice of gauge is shown to remove the troublesome singularities which occur at the conical intersection. The new methodology is applied to ultracold collisions of H/D with vibrationally excited HD(v=4, j=0). For high vibrational excitation of HD, the H/D + HD system is a barrierless exoergic reaction which exhibits significant reactivity in the Wigner threshold regime. The total, vibrationally, and rotationally resolved reaction rate coefficients are reported as a function of collision energy between 1uK and 100K. Interesting constructive and destructive quantum interference effects are shown to alter the ultracold reaction rates by several orders of magnitude which confirm recently reported results for this system.

[1]Funding acknowledgment: DOE LANL project LDRD20170221ER

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Date submitted: 25 Jan 2018 Electronic form version 1.4