Abstract Submitted
for the DAMOP14 Meeting of
The American Physical Society

Adiabatic Hyperspherical Study of One-dimensional Hydrogen Molecule[1] YOULIANG YU, YUJUN WANG, BRETT ESRY, J. R. Macdonald Laboratory, Kansas State University, Manhattan, Kansas, 66506 — We present a calculation of the adiabatic hyperspherical potentials for one-dimensional H_2. Although the adiabatic hyperspherical representation has proven very useful in understanding atomic systems, especially highly correlated states like doubly excited states, it has not yet been applied to the electronic and nuclear degrees of freedom for a molecule more complicated than H_2^+. We thus present the first such calculation, albeit for a one-dimensional model of H_2. Our model, however, is chosen to exactly reproduce the three-dimensional H_2 and H_2^+ ground Born-Oppenheimer potentials. One of our goals is to identify and understand the role of doubly excited states — which can be readily identified in the adiabatic hyperspherical representation, unlike standard quantum chemistry. We illustrate the method with an application to attosecond physics. We also want to take advantage of the fact that the adiabatic hyperspherical representation produces well defined and discrete effective potentials for all ionization channels to help understand processes like strong-field dissociative ionization. These topics, and others, will be discussed.

[1]Supported by the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy

Youliang Yu
J. R. Macdonald Laboratory, Kansas State University,
Manhattan, Kansas, 66506

Date submitted: 31 Jan 2014 Electronic form version 1.4