Abstract Submitted
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Adiabatic hyperspherical study of one-dimensional H_2[1] YOULIANG YU, J.R. Macdonald Laboratory, Kansas State University — 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 are rigorously defined in the adiabatic hyperspherical representation, unlike standard quantum chemistry. We are especially interested in understanding their role in strong-field and attosecond processes. We also want to take advantage of the fact that the adiabatic hyperspherical representation produces rigorously 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.

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