A CANONICAL APPROACH TO GENERATE MULTIDIMENSIONAL POTENTIAL ENERGY SURFACES

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Previously adaptions of canonical approaches were applied to algebraic forms of the classic Morse, Lennard-Jones, and Kratzer potentials. Using the classic Morse, Lennard-Jones, or Kratzer potential as reference, inverse canonical transformations allow the accurate generation of Born-Oppenheimer potentials for $H_2{}^+$ ion, neutral covalently bound H_2, van der Waals bound Ar_2, and the hydrogen bonded 1-dimensional dissociative coordinate in water dimer. This methodology is now extending to multidimensional potential energy surfaces, and as a proof-of-concept, it is applied to the 3-dimensional water molecule potential surface. Canonical transformations previously developed for diatomic molecules are used to construct accurate approximations to the 3-dimensional potential surface of the water molecule from judiciously chosen 1-dimensional planar slices that are shown to have the same canonical shape as the classical Lennard-Jones potential curve. Spline interpolation is then used to piece together the 1-dimensional canonical potential curves, to obtain the full 3-dimensional potential surface of water molecule with a relative error less than 0.008.