CORRELATION EFFECTS IN MODEL SYSTEMS: THE HOOKEAN AND HOOKE-CALOGERO H_2 MOLECULE

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Abstract

We consider the exact non-Born-Oppenheimer Schrödinger equation for the Hookean and Hooke-Calogero models of the diatomic molecule H_2. The former is a two-proton, two-electron system where the electron-proton interaction is harmonic while the proton-proton and electron-electron interactions are Coulombic. The latter is the same as the Hookean model, but with an inverse square proton-proton interaction. The Schrödinger equations for these systems decouple into equations for the relative motion of the electrons, the relative motion of the nuclei, the motion of a collective mode representing a three-dimensional harmonic oscillator and the motion of a coordinate proportional to the center of mass. Exact closed-form analytic solutions have been found for all these equations. However, for the Hookean model, solutions for the relative motion of electrons or nuclei occur only for discrete and disjoint values of the coupling parameters. Hence, the choice of a closed-form analytic solution for one of them implies that only an approximate wavefunction is found for the other.

Properties of the electronic and nuclear intracule densities for the Hookean model are examined at different values of the coupling constant. The nuclear motion occurs in a highly correlated regime which leads in a natural way to spatial localization of the nuclei, akin to Wigner crystallization. In addition the exact nuclear and electronic extracular non-Born-Oppenheimer densities have been examined and the salient features of these complex nodal functions are discussed. Results for the Hooke-Calogero model are compared to those of the Hookean model as well as to the exact Coulombic one. The electron Coulomb holes for these systems are seen to be quite similar.

References

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