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How competitive are expansions in orbital products with explicitly correlated expansions

KRZYSZTOF SZALEWICZ, University of Delaware

Helium dimer potential is of great importance for metrology since several future measurement standards will be based on helium gas. Such potential can be used to predict all thermodynamic properties of diffuse helium gas (nonadditive three-body potential is needed for higher densities). The accuracy required by these standards is so high, that in the past work of our group we had to include nonadiabatic, relativistic, and quantum electrodynamics effects. The current state is that the largest contribution to the uncertainty of the helium dimer potential is due to the Born-Oppenheimer (BO) part of this potential. This uncertainty was reduced and became comparable to other uncertainties in the new calculations that will be presented. These calculations used explicitly correlated Gaussian (ECG) basis sets and represent nearly exact solutions of the Schrödinger equation in the BO approximation. Similar calculations were also performed in orbital basis sets using a multilevel approach up to the full configuration interactions level. Largest existing basis sets were used at each level so that our calculations represent the best results that can currently be obtained using orbitals. These results will be critically compared with those obtained using ECG bases.