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Lowest Order Relativistic Corrections of the Helium Atom and the Hydrogen Molecule Computed Using Monte Carlo Methods S.A. ALEXANDER, Southwestern University, SUMITA DATTA, S.N. Bose National Centre for Basic Sciences, R.L. COLDWELL, University of Florida — We have calculated the lowest order relativistic effects for the three lowest states of the helium atom with symmetry ^{1}S, ^{1}P, ^{1}D, ^{3}S, ^{3}P and ^{3}D using variational Monte Carlo methods and compact, explicitly correlated trial wavefunctions. Our results are in excellent agreement with those of Drake and Yan (Phys. Rev. A **46**, 2378, 1992). We have also calculated the lowest order relativistic effects for the ground state of the hydrogen molecule with symmetry $X^1\Sigma_g^+$, $B^1\Sigma_u^+$, $a^3\Sigma_g^+$, $b^3\Sigma_u^+$, $I^1\Pi_g$, $C^1\Pi_u$, $i^3\Pi_g$, $c^3\Pi_u$, $J^1\Delta_g$ and $j^3\Delta_g$ using these same methods and a new set of compact, explicitly correlated trial wavefunctions. Our values are in excellent agreement with earlier calculations on the $X^1\Sigma_g^+$ and $B^1\Sigma_u^+$ states. For the other states, our work provides the first evaluation of these properties. Finally, we discuss the extension of these methods to larger atoms and molecule.

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