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Highly compact wavefuntions for He-like systems FRANK E. HARRIS, University of Utah and University of Florida — Wavefunctions which are compact, but still quite accurate, are extremely valuable as tools for gaining understanding of quantum systems. Here we study the ground electronic states of the three-body systems comprising the He isoelectronic series, using spatial wavefunctions that depend exponentially on all the interparticle distances, i. e. built from a basis whose members are of the form $\phi_i = (1 + \mathsf{P}_{12}) \exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12})$, where r_1 and r_2 are the electron nuclear distances, r_{12} is the electron-electron separation, and P_{12} permutes the electron coordinates. When the nonlinear parameters α_i, β_i, γ_i are carefully optimized (a nontrivial task), this type of basis is found to be extraordinarily efficient; using as few as four basis functions, it is found that nonrelativistic energies are reproduced to within 38 microhartrees of the exact values, an error far less than for compact wavefunctions previously proposed by others. Other properties, including those totally dependent upon the electron correlation, are also well represented.
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