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Explicitly Correlated Wavefunctions for Few-Body Problems[1]
FRANK E. HARRIS, Quantum Theory Project, U. of Florida and Dept. of Physics, U. of Utah — Explicitly correlated wavefunctions enable far more compact, yet accurate descriptions of few-body systems than are possible using basis functions built from orbital products. The most efficient functions of this type contain all the interparticle distances as exponentials. Progress in evaluating the matrix elements for such a basis is reviewed for three and four-body systems, with particular attention to the difficult analytical problems posed by the four-body system and the challenges associated with highly singular integrals in the three-body system (which arise in the computation of relativistic effects). An alternative basis is provided by Gaussians in all the interparticle distances; recent contributions toward systematizing the use of such functions are also reported. Application of the exponential basis to the He isoelectronic series is described; the results differ from those reported by others in that their quality does not decrease with increasing nuclear charge Z. This feature permits an improved characterization of the coefficients in the $1/Z$ expansion. Also disscused is the cancellation of divergences in the combinations of individually divergent integrals arising in the treatment of relativistic effects in the He system.

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