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Abstract for an Invited Paper for the MAR13 Meeting of the American Physical Society

Variational methods with all-particle explicitly correlated Gaussians SERGIY BUBIN, Vanderbilt University

Accurate treatment of electron correlation in quantum systems of various nature remains an important challenge for modern theoretical and computational approaches. The variational method in conjunction with explicitly correlated Gaussian (ECG) basis sets is one of the most capable, accurate, and conceptually simple methods for calculating the ground, excited, and even scattering state properties of small quantum systems. I will review the basic theoretical foundations, recent advances, and the applications of the ECG method to Coulomb systems such as atoms, molecules, and systems containing positrons. I will also discuss some of the most important challenges that need to be overcome in order to extend the current range of applicability of the method.