

Abstract Submitted
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Nearly exact calculations of small atomic and molecular systems using explicitly correlated gaussians¹ SERGIY BUBIN, KALMAN VARGA, Vanderbilt University, LUDWIK ADAMOWICZ, University of Arizona — We demonstrate how very precise (virtually exact) solutions of various quantum mechanical problems can be obtained using the variational method with explicitly correlated Gaussian basis functions (ECGFs). As examples we consider several benchmark systems, such as few-electron atoms and molecules, as well as Coulomb systems containing exotic particles. We also discuss the evaluation of relativistic corrections in the framework of ECGFs.

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