

Abstract Submitted
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Wave Function Functionals for the Density MARLINA SLAMET, Sacred Heart University, XIAOYIN PAN, Ningbo University, VIRAHT SAHNI, Brooklyn College, CUNY — In recent work we have developed¹ a constrained-search variational method for the construction of wave functions that are functionals of a function $\chi : \Psi = \Psi[\chi]$. These wave function functionals are *simultaneously* normalized, reproduce the *exact* expectation of either single- or two-particle operators, and lead to rigorous upper bounds to the energy. In this paper we extend this method to the construction of wave function functionals $\Psi[\chi]$ that are simultaneously normalized, reproduce the density *exactly*, and lead to rigorous upper bounds to the energy. We apply the method to the ground state of the He atom to obtain wave function functionals that reproduce the density of an accurate correlated wave function. The wave function functionals as expected give rise to the exact expectation of non-differential single particle operators, and lead to accurate two-particle expectations and highly accurate energies.

¹Pan, Slamet, and Sahni, Phys. Rev. A **81**, 042524 (2010).

Viraht Sahni
Brooklyn College, CUNY

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