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Wave Function Functionals via the Constraint of the Expectations of Hermitian Single-Particle Operators MARLINA SLAMET, Sacred Heart University, XIAO-YIN PAN, VIRAH T SAHNI, The Graduate School, CUNY — Recently, the idea [1] of expanding the space of variations in calculations of the energy by considering the approximate wave function Ψ to be a functional of functions χ , $\Psi = \Psi[\chi]$, rather than a function, has been proposed. A constrained search over all functions χ such that $\Psi[\chi]$ satisfies a physical constraint or leads to a known value of an observable, is performed. A rigorous upper bound to the energy is then obtained via the variational principle. In this paper we extend this work on the ground state of the He atom by imposing the constraint that $\Psi[\chi]$ reproduce the exact expectations of the Hermitian single-particle operators $W = \sum_i r_i^n, n = -2, -1, 1, 2$, and $W = \sum_i \delta(\mathbf{r}_i)$. By employing the form $\Psi[\chi] = \Phi[1-f(\chi)]$, where Φ is a prefactor and $f(\chi)$ a correlation factor, two solutions to the resulting integral equation for the functions χ are determined for each operator W . In each case, the two wave function functionals lead to upper bounds to the energy that differ minimally from those of [1] in which only the constraint of normalization is imposed, while simultaneously reproducing the exact expectation of the operator W .

1. X.-Y. Pan, et al, Phys. Rev. Lett. **93**, 130401 (2004)

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