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Wave Function Functional via the Normalization Constraint XIAO-YIN PAN, VIRAHT SAHNI, LOU MASSA, The Graduate School, CUNY
— In this paper we extend our prior work [1] on the construction of approximate wave function functionals $\Psi = \Psi[\chi]$ for the ground state of the He atom by attempting to expand the space of variations of the functional. As in our prior work, we assume $\Psi[\chi] = \Phi\{\phi_i\}[1 - f(\chi)]$, where $\Phi\{\phi_i\}$ is a normalized Slater determinant of the orbitals $\phi_i(\mathbf{x})$, $\mathbf{x} = \mathbf{r}\sigma$, and $f(\chi)$ a correlation factor, and employ normalization as the constraint to determine the function χ. However, we expand the space of variations from $\chi = \chi(s)$ to $\chi = \chi(st)$, where $s = r_1 + r_2, t = r_1 - r_2$. Although the constrained search over the entire requisite (st) space is not achieved, two solutions of the integral equation for the function χ have been obtained. These two wave functions have the properties that they are normalized independent of the prefactor, with the density being that of the prefactor. The significance of these attributes of the wave function functionals will be discussed.
1 . X.-Y. Pan et al, Phys. Rev. Lett. **93**, 130401 (2004)

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