Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Construction of Wave Function Functionals MARLINA SLAMET, Sacred Heart University, XIAO-YIN PAN, Ningbo University, VIRAHT SAHNI, The Graduate School, CUNY — We recently proposed [1] 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. A constrained search is first performed over all functions χ such that $\Psi[\chi]$ satisfies a physical constraint or leads to a known value of an observable. A rigorous upper bound to the energy is then obtained via the variational principle. In this paper we apply this idea to the ground state of the He atom by constructing $\Psi[\chi]$ that reproduce the exact expectations of the Hermitian single- and two-particle operators $W = \sum_i r_i^n, n = -2, -1, 1, 2$; $W = \sum_i \delta(\mathbf{r}_i)$; $W = |\mathbf{r}_1 - \mathbf{r}_2|^m, m = -1, -2, 1, 2$. The functionals are of the form $\Psi[\chi] = \Phi[1 - f(\chi)]$, where Φ is a prefactor and $f(\chi)$ a correlation factor. The $\Psi[\chi]$ (i) lead to the exact expectation value of W; (ii) are automatically normalized; and (iii) provide a rigorous upper bound to the energy.
[1] X.-Y. Pan, *et al*, PRA **72**, 032505 (2005).

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Date submitted: 25 Nov 2007 Electronic form version 1.4