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A new Variational Approach to the Hydrogen Atom I. DJURIC, F.A. CORVINO, Stevens Institute of Technology, V. FESSATIDIS, Fordham University, J.D. MANCINI, Kingsborough College of CUNY — Over a decade ago, a systematic scheme for improving the variational wave functions and corresponding energy levels for quantum systems was developed. By expanding the wave function around a variational parameter value(s), a family of independent functions may be systematically generated. The eigenstates are then obtained by diagonalizing the Hamiltonian basis and optimized with respect to variational parameter(s). In this work we wish to apply this scheme to the well studied and understood ground state of the hydrogen atom. For a trial (starting vector) state we make two choices: $e^{-\alpha r}$ and $e^{-\beta r}$ where α and β are variational parameters. Our two (variational) basis are then constructed by taking derivatives with respect to these parameters. We then choose a linear combination of the two states $e^{-\alpha r}$ and $e^{-\beta r}$ as our initial state and minimize with respect to both parameters. This leads to questions of the optimal number of each derivative $\partial_{\alpha}^p, \partial_{\beta}^q$, which will yield the lowest ground state energy for a given basis size N ($p + q = N$).

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