Abstract Submitted
for the DAMOP07 Meeting of
The American Physical Society

B-splines in variational atomic structure theory CHARLOTTE FROESE FISCHER, National Institute of Standards and Technology — Many of the problems associated with the use of finite differences for the solution of variational Hartree-Fock or Dirac-Hartree-Fock equations are related to the orthogonality requirement and the need for node counting to control the computed solution of a two-point boundary value problem with many solutions. By expanding radial functions in a B-spline basis, the differential equations can be replaced by non-linear systems of equations of eigenvalue type. Hartree-Fock orbitals become solutions of generalized eigenvalue problems where orthogonality requirements can be dealt with through projection operators applied to the matrix that preserve the symmetry of the matrix. When expressed as banded systems of equations, all orbitals may be improved simultaneously using singular value decomposition or the Newton-Raphson method for faster convergence. Computational procedures will be outlined for non-relativistic multiconfiguration Hartree-Fock variational methods and extensions to the calculation of Rydberg series. It will also be shown how tensor products of B-splines can be applied to the calculation of two-electron pair-correlation functions where high-order partial waves improve the short-range electron-electron cusp condition at $\mathbf{r_1} = \mathbf{r_2}$.

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Date submitted: 31 Jan 2007 Electronic form version 1.4