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The Gutzwiller Ansatz: A new Approach J.D. MANCINI, Kingsborough College of CUNY, V. FESSATIDIS, Fordham University, I. DJURIC, Stevens Institute of Technology, S.P. BOWEN, Chicago State University — The search for calculational methods for dealing with strongly correlated electron systems ranging from high Tc superconducting compounds and other transition metal oxide materials to f-electron bearing elements is a long and continuous one. There are a number of well documented failures of such schemes as the local density approximation and the generalized gradient approach. Although these methods partially address the issues related to the strongly correlated electrons, a comprehensive theory is still lacking. The choice of including electrons correlations using the Gutzwiller variational wave function has proved over the years to be a useful one in the interpolation between the strong electron correlation (large U) and weak electron correlation (small U) limits. In this work a novel variational ansatz is applied to strongly correlated systems by using the Gutzwiller wave function as our initial vector, and then systematically constructing a basis by taking derivatives with respect to the variational parameters of the system. The eigenvalues of the Hamiltonian matrix with this basis are then minimized to yield a variational upper bound on the ground state energy.

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