Abstract Submitted
for the DAMOP06 Meeting of
The American Physical Society

Atomic Spectral Methods for Molecular Electronic Structure Calculations ROBERT HINDE, Univ. of Tennessee, JERRY BOATZ, Air Force Research Laboratory, PETER LANGHOFF, Univ. of California, San Diego — Progress is reported in development and implementation of atomic spectral methods for electronic structure and excitation-energy calculations on molecules and other atomic aggregates. The approach presented defers enforcement of wave function antisymmetry subsequent to construction of the Hamiltonian matrix in a formally complete atomic spectral-product basis, affording a number of conceptual and potential computational advantages over more conventional currently employed methods. Progress in implementation reported includes development of methods for isolating the totally antisymmetric representation of the aggregate symmetric group in the presence of non-Pauli states, avoidance of large-dimension Hamiltonian matrices and the attainment of closure by incorporation of explicitly antisymmetric atomic-pair information obtained from largely conventional diatomic calculations, and associated enforcement of appropriate wave function behavior in dissociation limits. These issues are illustrated with explicit calculations on simple diatomic and triatomic molecules and comparisons with results obtained for these systems using conventional electronic structure methods.

Robert Hinde
Univ. of Tennessee

Date submitted: 27 Jan 2006 Electronic form version 1.4