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On the Non-Pauli Electronic States of Atoms and Molecules PETER LANGHOFF, UCSD, JEFFREY MILLS, AFRL — Schrödinger's equation for atoms and molecules supports solutions that are not totally antisymmetric under electron coordinate permutations. These non-Pauli eigenstates are generally regarded as unphysical, with interest in them centered largely on their role as possible "contaminants" in physical solutions constructed by methods that provide only approximate antisymmetry, such as exchange perturbation theories, many-body diagrammatic approaches, and variational methods in the absence of precise prior enforcement of basis-state antisymmetry. Here we report atomic and molecular non-Pauli Schrödinger solutions employing largely pedestrian methods as an alternative to the more complicated Wigner-Weyl approach based on theory of the symmetric group. Using the non-relativistic Hamiltonian operator and spin-orbital product representations in variational calculations, we show that every antisymmetric Schrödinger eigenstate of an n electron atom or molecule is accompanied by 2^n-1 degenerate non-Pauli "ghost" solutions. As a consequence of this degeneracy, admixtures of non-Pauli states are always present in Pauli solutions having only approximate antisymmetry. These can significantly affect calculated expectation values, even in the face of precise energy predictions.

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