

Post-AGP Methods for Seniority-Breaking Systems

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The antisymmetrized geminal power (AGP) wavefunction is a good starting point for describing strong pairing correlations where conventional electronic structure methods fail. Closely related to symmetry-projected methods, this post-AGP approach is also promising for strongly correlated seniority-breaking systems that do not conserve the number of pairs. We here present AGP-based correlated methods such as configuration interaction, Lie algebra similarity transformation, and random phase approximation. We also explore solving a seniority-conserving Hamiltonian that is mapped from a seniority-breaking one.