AGP decades later: Why revisiting this ansatz?

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AGP is not a great wavefunction for chemistry. Electrons like to form pairs but geminals are rarely the same as in AGP, the number projected BCS wavefunction. We also know that in quantum chemistry, spin projection is much more important than number, a symmetry that does not break spontaneously in mean-field. So why bother with AGP? We have recently shown that AGP and its seniority zero (paired) excitations are a great starting point for describing fancy geminal wave functions with polynomial computational cost. In this talk, I will discuss the structure of the seniority zero Hilbert space based on AGP and how to describe DOCI efficiently based on it. Two recent papers [1,2] discuss some of the formal aspects of the theory. The extension of the model to broken pairs is currently under development.

[1] Geminal-based configuration interaction, T. M. Henderson, and G. E. Scuseria, *J. Chem. Phys.* **151**, 051101 (2019); http://arxiv.org/abs/1906.11361

[2] Efficient evaluation of AGP reduced density matrices, A. Khamoshi, T. M. Henderson, and G. E. Scuseria, *J. Chem. Phys.* **151**, 184103 (2019); https://arxiv.org/abs/1909.06345