

# When two is better than one: the seniority scheme as a new tool to build wave functions

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Strong quantum correlation is one of the unsolved problems of electronic structure theory. It was recently observed [1] that the *seniority* scheme offers a much better partitioning of the Hilbert space than the conventional particle-hole scheme to capture strong static correlations. This scheme organizes the electron configurations into electron *pairs*, rather than in single-particle excitations on top of a reference state. It was found that full Configuration Interaction (fCI) calculations limited to the fully paired space only (or Doubly-Occupied Configuration Interaction), were able to describe bond-breaking processes with very high accuracy. Unfortunately, as a fCI method, the computational scaling of DOCI remains exponential, and hence impractical for large systems.

The mean-field picture associated with electron pairing is known as the theory of Antisymmetric Product of Interacting *Geminals*<sup>1</sup> (APIG). This ties in with the intuitive Lewis picture of chemical bonding, however the exponentially scaling computational cost of an APIG wavefunction hardly trumps DOCI. A recent breakthrough in APIG theory came with the connection with Richardson-Gaudin (RG) integrable systems [2, 3], in which we have identified a new family of APIG states with mean-field like computational cost and the same accuracy as DOCI.

In this presentation, I will discuss recent research from the Ghent-McMaster collaboration on the seniority scheme, APIG theory and its connection to Richardson-Gaudin integrability.

## References

- [1] Bytautas L, Henderson T M, Jimenez-Hoyos C A, Ellis J K and Scuseria G E 2011 *J. Chem. Phys.* **135** 044119
- [2] Johnson P A, Ayers P W, Limacher P A, De Baerdemacker S, Van Neck D and Bultinck P 2013 *Comp. Theor. Chem.* **1003** 101
- [3] Limacher P A, Ayers P W, Johnson P A, De Baerdemacker S, Van Neck D and Bultinck P 2013 *J. Chem. Theor. Comp.* **9** 1394

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<sup>1</sup>*Geminus*: [Latin] double, paired (substantive) one who is a twin.