Implications of pinned occupation numbers for natural orbital expansions

Abstract: The ground state of a non-interacting quantum system of many fermions is a single Slater determinant consisting of the eigenfunctions of the corresponding single-electron Hamiltonian. The Hartree-Fock method assumes that the wavefunction an interacting multifermion system has the form of a Slater determinant where the single-electron orbitals are found via the variational optimisation approach. However, the description of the subtle properties of interacting quantum systems requires superposing many Slater determinants — a subject of the so-called post Hartree- Fock methods. These include the variational multi configurational ansatz methods exploiting the concept of active spaces where the computations are simplified by assuming certain orbitals to be effectively inactive (not occupied by fermions) or occupied by a “frozen” fermion (their occupation number being fixed to one). In other words, these ansatz wavefunctions saturate one or more Pauli constraints which state that the occupation numbers of a fermionic quantum system take values between zero and one. In my talk, I will present a systematic generalisation of the concept of active spaces based on the generalised Pauli constraints which are inequalities involving linear combinations of different occupation numbers. I will explain and illustrate that the saturation of any such constraint by the fermionic occupation numbers characterises a distinctive set of active multi fermion configurations. The use of such generalised active spaces has the potential to provide a more accurate description of quantum correlations as it allows one to increase the number of active orbitals while maintaining a low number of multi fermion configurations. Finally, the structure of the related generalised Pauli polytope sheds light on the systematic and possibly efficient way of identifying the optimal ansatz states.

[1] Schilling, C., Benavides-Riveros, C., L., Lopes, A., Maciążek, T., Sawicki, A. (2020), Implications of pinned occupation numbers for natural orbital expansions: I. Generalizing the concept of active spaces, New Journal of Physics 22 (2), 023001

[2] Maciążek , T., Sawicki, A., Gross, D., Lopes, A., Schilling, C. (2020), Implications of pinned occupation numbers for natural orbital expansions. II: Rigorous derivation and extension to non-fermionic systems, New Journal of Physics 22 (2), 023002