

# Structure of the One-electron Reduced Density Matrix in Quantum Mechanics from the Generalized Pauli Exclusion Principle

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The Pauli exclusion principle requires that the occupations of the orbitals lie between zero and one. These Pauli conditions hold for one-electron reduced density matrices (1-RDMs) from both open and closed quantum systems. More than 40 years ago, it was recognized that there are additional conditions on the 1-RDM for closed quantum systems. In this lecture we will discuss the structure of the 1-RDM from the generalized Pauli exclusion principle in many-electron atoms and molecules [1], the violation of the generalized Pauli principle as a sufficient condition for the openness of a many-electron quantum system [2], as well as connections to 1-RDM and geminal functional theories.

[1] R. Chakraborty and D. A. Mazziotti, "Generalized Pauli conditions on the spectra of one-electron reduced density matrices of atoms and molecules," *Phys. Rev. A* **89**, 042505 (2014).

[2] R. Chakraborty and D. A. Mazziotti, "Sufficient condition for the openness of a many-electron quantum system from the violation of a generalized Pauli exclusion principle," *Phys. Rev. A* **91**, 010101(R) (2015).