Density matrix based methods for bonded and non-bonded interactions

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The postulates of quantum mechanics state that the wave function contains all the possible information about a molecular system. As a consequence, all information about any bonded and non-bonded interaction a system contains or engages in should be derivable from the wave function.

In my tutorial style presentation, I will show how from the first and second order density matrices obtained from any level of theory one can obtain bond indices\(^1\) reflecting the strength of both bonds and non-bonded interactions and how these are connected to the existence of so-called Fermi Holes and domain averaged Fermi hole analysis.\(^2\)