The Electron Correlation Problem from a Quantum Information Perspective

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Describing strongly interacting electrons is one of the crucial challenges of modern quantum physics. A comprehensive solution to this electron correlation problem would simultaneously exploit both the pairwise interaction and its spatial decay. By taking a quantum information perspective, we explain how this structure of realistic Hamiltonians gives rise to two conceptually different no- tions of correlation and entanglement. The first one describes correlations be- tween orbitals while the second one refers more to the particle picture. We illustrate those two concepts of orbital and particle correlation and present measures thereof. Our results for different molecular systems reveal that the total correlation between molecular orbitals is mainly classical, raising questions about the general significance of entanglement in chemical bonding. Finally, we also speculate on a promising relation between orbital and particle correlation and explain why this may replace the obscure but widely used concept of static and dynamic correlation.