

# Quantum Dissection of a Covalent Bond

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Theoretical analysis of covalent bonding is quite successful in many regards, but leaves open many mysteries even for simple diatomic molecules. We develop a framework for analyzing bonds which uses ideas from the field of quantum entanglement. The main development involves the creation of tools that break up a many body wave function into real space pieces. This includes a recent algorithm that we developed that is able to calculate the entanglement spectrum with quantum Monte Carlo. We are able to address the controversial  $C_2$  molecule with these tools, and demonstrate its bonding properties, which includes an inverted fourth bond. With this analysis we also consider bonding in Hartree-Fock wave functions and find simple additions to text book molecular orbital theory that can easily be incorporated into molecular hybridization diagrams. The ideas considered in this work have the potential to provide a significantly more detailed picture of bonding than allowed by previous techniques.