Abstract Submitted
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Entanglement spectrum and covalent bonding DAVID YANG, NORM TUBMAN, Univ of Illinois - Urbana — We present an approach for computing the entanglement spectrum with quantum Monte Carlo for both continuum and lattice Hamiltonians. This method provides direct access to the matrix elements of the spatially reduced density matrix, using a generalization of the SWAP operator. We apply this method to several diatomic molecules and describe how the spatial entanglement spectrum encodes a covalent bond that includes all the many-body correlations. Of particular focus is the C_2 molecule, which has been subject to recent controversy. Our results suggest that entanglement-based methods can lead to more realistic analysis of covalent bonds than possible before.

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