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Constructing Multi-Slater-Jastrow Wavefunctions via Reduced Density Matrix Covariance KIEL WILLIAMS, LUCAS WAGNER, Univ of Illinois - Urbana — The multi-determinant Slater-Jastrow ansatz wavefunction is a powerful tool for conducting ab initio electronic structure calculations in strongly correlated systems. We illustrate a new method of systematically constructing multi-determinant expansions by analyzing the covariance of elements of the two-body reduced density matrix (2RDM) with respect to the local energy distribution for a Slater-Jastrow wave function. By ordering the elements of the 2RDM with respect to their computed mean and associating each matrix element with a new determinant, we construct new multi-determinant expansions. We show that the energies of an H2 and stretched N2 molecule converge more rapidly with respect to the number of included determinants using this technique than in conventional configuration interaction calculations. This suggests that our analysis of the 2RDM captures qualitative differences between the single Slater determinant and the Slater-Jastrow wave function. This method provides a new way of diagnosing and correcting the deficiencies of certain trial wavefunction types in quantum Monte Carlo calculations. This work was supported by NSF DMR 12-06242.

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