Strong Electronic Correlation with Richardson-Gaudin States

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Weakly-correlated electronic systems are well-described as individual electrons: the wavefunction is a Slater determinant of the occupied orbitals with small corrections from single- and double-excitations. This is not the case for strongly-correlated systems. The wavefunction is very complicated in terms of Slater determinants and thus the correct physical picture is not independent electrons.

For strongly-correlated molecular systems, we have shown that the eigenvectors of reduced Bardeen-Cooper-Schrieffer Hamiltonians, so-called Richardson-Gaudin (RG) states, are a much better starting point. They describe weakly-correlated pairs of electrons. They are tractable variationally and form a basis for the Hilbert space allowing for systematic improvement.

We will show for the isomers of H_{10} that a single RG state is a very good approximation to the wavefunction. Corrections for the remaining weak electronic correlation are obtainable with an approximate functional, or with a short CI expansion in RG states. Thus, the present development is an analogue of both Kohn-Sham DFT and correlated wavefunction theories based on Slater determinant references.