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Richardson-Gaudin Wavefunctions for Strong Correlation

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Weakly-correlated systems are well-described as individual electrons. The dominant contribution to the wave function 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. Many Slater determinants contribute substantially and thus the correct physical picture is not independent electrons. For molecular systems, we have shown that Richardson-Gaudin (RG) states are a much better starting point. They amount to pair wave functions, but they are tractable and form a basis of the Hilbert space, allowing for systematic improvement. Pair wavefunctions are near synonymous with natural orbital functionals, and we argue that it is easier, and more reasonable physically, to consider the RG states directly.

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