Flexible Wavefunction Ansatze for Strong Electron Correlation

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Abstract:
A flexible ansatz for N-electron wavefunctions that subsumes the wavefunctions used in traditional configuration interaction approaches, coupled cluster methods, geminal-product wavefunctions, electron-group-function approaches, matrix-product states, and tensor-network states is presented. In this approach, desirable properties of wavefunctions (e.g., quasiparticle interpretations; size-consistency) are expressed as properties of a function that determines the coefficients of Slater determinants as (generally nonlinear) functions of the input parameters. Some of these key properties will be presented, allowing us to generate entirely new wavefunction forms that have desirable formal properties and yet, in some cases, are fully applicable to strongly correlated systems. A perturbative form of this approach will also be presented; the perturbative expression is especially useful for generating initial guesses for the wavefunction optimization.