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Particle-number-projected Bogoliubov coupled cluster theory: formalism and first application to the Richardson pairing Hamiltonian.

While coupled cluster theory accurately models weakly correlated quantum systems, it often fails in the presence of strong correlations where the standard mean-field picture is qualitatively incorrect. In many cases, these failures can be largely ameliorated by permitting the mean-field reference to break physical symmetries. Symmetry-broken coupled cluster, e.g. Bogoliubov coupled cluster, theory can indeed provide reasonably accurate energetic predictions, but the broken symmetry can compromise the quality of the resulting wave function and predictions of observables other than the energy.
Merging symmetry projection and coupled cluster theory is therefore an appealing way to describe strongly correlated systems. One indeed expects to inherit and further improve the energetic accuracy of broken-symmetry coupled cluster while retaining proper symmetries. We present the novel particle-number-projected Bogoliubov coupled cluster (PBCC) formalism that consistently allows to do so. While the present focus is on U(1) symmetry associated with particle number conservation, a similar formalism is already available to deal with SU(2) symmetry associated with angular momentum. Next, results obtained by testing PBCC on the solvable Richardson pairing Hamiltonian are shown. The very high quality of those results indicates that symmetry-projected coupled cluster is a promising method that can accurately describe both weakly (e.g. doubly closed-shell nuclei) and strongly (e.g. singly and doubly open-shell nuclei) correlated finite many-fermion systems.

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