Iterative schemes for solving the coupled-cluster equations

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The coupled-cluster (CC) scheme for energy correlation calculations provides a set of nonlinear equations for cluster amplitudes and the energy expression. The set is usually solved using Jacobi-type iterative schemes combined with additional procedures for speeding up the convergence. An alternative route towards solving the CC equations that has been shown employs the intermediate Hamiltonian scheme. The method is known as the size-consistent self-consistent configuration interaction (CI) approach. The CC wave function is partitioned into the linear and nonlinear components and contributions from the latter one are incorporated through modification (dressing) of the CI matrix. Solution is obtained by diagonalization of the dressed matrix but that must be done in a self-consistent manner since the dressing depends on the matrix eigenvector. A possible generalization of this approach can be obtained by approaching the problem of solving the CC equations in more formal way. The set of the standard CC amplitude equations does not depend on the CC energy that is calculated after determining the cluster amplitudes, however, simple manipulations can make the equations energy dependent. .A further rearrangement of the CC equations shows that diagonalization techniques can be employed to solve them. Again the problem requires a self-consistent procedure since the diagonalized matrix depend on cluster amplitudes but this can be built into a Davidson-type procedure for solving an eigenvalue problem of non-symmetric matrix (Hirao-Nakatsuji). The scheme is quite flexible so even Newton-Raphson scheme can used within this framework. Some numerical examples showing the convergence of different iterative methods are presented.