Model space incompleteness in multireference state-universal and state-selective coupled-cluster theories

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ABSTRACT

The role of the so-called C-conditions, originally introduced in the general model space (GMS), state-universal (SU), coupled-cluster (CC) theory with singles and doubles (GMS SU CCSD) to account for the internal cluster amplitudes that vanish in the case of a complete model space, is explored in the context of the state-selective Mukherjee MR-CC method (MkCCSD). Using three examples that involve a considerable quasidegeneracy we show that the C-conditions can be usefully employed also in the MkCCSD method once an incomplete (or general) model space is used.

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1. Introduction

For nondegenerate closed-shell systems the single-reference (SR) coupled-cluster (CC) method with singles and doubles (CCSD), particularly its perturbatively corrected version for triples CCSD(T), represents the method of choice in molecular electronic structure calculations. Unfortunately, CCSD(T) breaks down once the multireference (MR) character of the state sets in, as is invariably the case when breaking genuine chemical bonds or, generally, for open-shell systems, such as various diradicaloid species (see, e.g., [1–4]). Although in many instances, when the implied quasidegeneracy is not too strong, this breakdown can be to a large extent overcome via the renormalized or completely-renormalized (CR) methods, in particular via the CR-CC(2,3) version [5,6] or via the so-called ΛCCSD(T) method [7–9], a fundamental approach to the quasidegeneracy problem should be based on a multireference (MR) version of the CC formalism (see, e.g., [10–12]).

In contrast to configuration interaction (CI) methods, an extension of SR-CC to a MR-CC case is far from being unambiguous and straightforward. It can be achieved in essentially two ways, depending on whether we strive for a single cluster operator as in the *valence-universal* (VU) or Fock space approaches [13–15] or consider distinct operators for each reference spanning the model space, as in the *state-universal* (SU) or Hilbert space methods [16]. Both of these MR-CC approaches lead to a rather formidable formalism and encounter a number of difficulties, primarily due to the requirement of a complete model space (CMS) and an implied presence of intruder states. For this reason, there has been various

attempts to focus on one state at a time via the so-called *state-selective* or *state-specific* (SS) methods. Since this term has been employed for a whole plethora of approaches, it is important to distinguish at least those that rely on some modification of standard SR-CC methods by accounting, in one way or another, for MR effects via higher-than-pair clusters (see, e.g., active-space SSMRCC-type approaches [17–19]) from those that employ a genuine MR-CC formalism.

From among the SR-based SS approaches we shall employ the so-called reduced multireference (RMR) CCSD method [20–22], which represents an externally corrected (ec) CCSD approach [23] that employs some external source for an information about the most important (primary) triples and quadruples. In the case of RMR-CCSD one employs a modest size MR CISD wave function for this purpose, exploiting the complementarity of CI and CC approaches in their handling of nondynamic and dynamic correlation effects, respectively [24]. The remaining (secondary) triples are then accounted for in a standard perturbative manner via the RMR-CCSD(T) method [25].

The SS-type methods that are based on genuine MR-CC formalism are best represented by the SS version of the MR-SU-CC approaches as formulated by Mukherjee et al. [26,27] (for an excellent review of the SS-type approaches see [28]). These MR-SS-SU CC approaches have recently attracted a considerable attention [29–32]. We shall refer to their SD version by the acronym MkCCSD. Just as the standard MR-SU approaches, the original formulation of the MkCCSD method requires the use of a CMS. Even though the intruders are now largely avoided by considering one state at a time (particularly when focusing on the ground state), similarly as in the Brillouin–Wigner (BW) CCSD [33], the dimension of the model space rapidly increases with the number of active MOs. It is thus desirable, in general, to truncate the model space to an incomplete model space (IMS). For this reason we introduced the general model space (GMS) MR-CC approach [34–40] that

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can employ an arbitrary model space (i.e., not necessarily a sub-space of CMS as implied by some active space of MOs). In such a case, however, a proper care must be taken of the so-called *internal* cluster amplitudes that are associated with excitation operators transforming one reference into another one. These amplitudes vanish in the case of a CMS, but must be properly accounted for via the so-called *C-conditions* [34] (C for constrained or connected), in the GMS case.

It has been shown earlier that the C-conditions may be profitably employed in other MR-CC approaches, specifically in the BW CCSD [41]. In this paper we wish to point out the usefulness of the C-conditions even for the MkCCSD method. Here we must note that so far the exploitations of the MkCCSD method focused almost exclusively on the ground state (or, generally, the lowest state of a given symmetry species), even though, in principle, it should be able to access excited states as well (in contrast to SR-based approaches like RMR-CCSD). In this paper we shall also limit ourselves to the ground states and will consider the problem of excited states elsewhere.

We next present a brief outline of the methods employed and then illustrate the exploitation of the C-conditions and the role they can play in the MkCCSD approach on a few simple examples.

2. Methods

The RMR-CCSD method [20–22,24,40] and its RMR CCSD(T) version corrected for secondary triples [25] are amply documented in the literature. We shall thus focus on those MR-CC methods that are relevant for this work, namely on SS MkCCSD [26–28] and the handling of model space incompleteness via the C-conditions [34–37]. We recall that all genuine MR-CC methods are based on the effective Hamiltonian formalism and a generalized Bloch equation (see, e.g., [12]).

Designating the references spanning the model space $\mathcal{M}_0$ by $|\Phi_i\rangle$, $i = 1, \ldots, M$, and the corresponding target states by $|\Psi_i\rangle$, the MR-SU-CC Ansatz of Jeziorski and Monkhorst [16] takes the form

$$|\Psi_i\rangle = \sum_{j=1}^{M} c_{ij} \exp(T^{[j]}) |\Phi_j\rangle$$
$$= \sum_{j=1}^{M} c_{ij} |\Phi_j\rangle + \sum_{|\Xi_j\rangle \in \mathcal{M}_0^{\perp}} d_{ij} |\Xi_j\rangle, \tag{1}$$

where the coefficients c_{ij}, $\mathbf{C} = ||c_{ij}||$, are given by the eigenvectors of the effective Hamiltonian matrix $\mathbf{H}^{(\text{eff})} = ||H_{ij}^{(\text{eff})}||$,

$$H_{ij}^{(\text{eff})} = \langle \Phi_i | \{H_{N_j} \exp(T^{[j]})\}_C | \Phi_j \rangle. \tag{2}$$

Further, $\mathcal{M}_0^{\perp}$ designates the orthogonal complement of $\mathcal{M}_0$ in the N-electron space implied by a chosen basis set, H_{N_j} stands for the electronic Hamiltonian in the normal product form relative to $|\Phi_j\rangle$ as vacuum, and the subscript C implies the connected part.

We shall consider two types of approaches to the determination of cluster amplitudes, namely the standard SU one and the Mukherjee-type SS approach. In the first one, the amplitude equations that determine $T^{[i]}$ are target-state independent and all the M target states are simultaneously generated by solving the same generalized Bloch equation that takes the form [16,10–12]

$$\langle \Phi_\alpha^\rho[i] | \overline{H}[i] | \Phi_i \rangle = \sum_{j(\neq i)} \Gamma^{ij}(\Phi_\alpha^\rho[i]) H_{ji}^{(\text{eff})}, \tag{3}$$

where $\overline{H}[i]$ is a similarity transformed Hamiltonian $\overline{H}[i] = \exp(-T^{[i]}) H_{N_i} \exp(T^{[i]})$ and $\Gamma^{ij}(\Phi_\alpha^\rho[i])$ represent the coupling coefficients

$$\Gamma^{ij}(\Phi_\alpha^\rho[i]) = \langle \Phi_\alpha^\rho[i] | \exp(-T^{[i]}) \exp(T^{[j]}) | \Phi_j \rangle. \tag{4}$$

Note that the left-hand side of (3) has the standard form of SR CC equations for the reference $|\Phi_i\rangle$, with $|\Phi_\alpha^\rho[i]\rangle \in \mathcal{M}_0^{\perp}$ representing excited configurations defined by the excitation operator $G_\alpha^\rho[i]$, $|\Phi_\alpha^\rho[i]\rangle = G_\alpha^\rho[i] |\Phi_i\rangle$, characterized by the (spin) orbital hole and particle labels relative to $|\Phi_i\rangle$, $\alpha \equiv \{P_1, \ldots, P_m\}$ and $\rho \equiv \{Q_1, \ldots, Q_m\}$, respectively.

In the second, SS-type approaches, the amplitude equations are target-state dependent (i.e., state-selective), so that only one eigenvalue and eigenvector of the effective Hamiltonian is optimal, even though all target states are still generated in each calculation. Consequently, the SS-MR-CC equations must be solved anew for each target state. The MkCCSD SS version of the MR-SU-CC formalism represents one such approach. Through a suitable manipulation of the Schrödinger equation for a given state using the SU CC Ansatz, resolution of the identity, and the sufficiency conditions (see, e.g., [12]), the MkCCSD equations for the kth target state take the form

$$\langle \Phi_\alpha^\rho[i] | \overline{H}[i] | \Phi_i \rangle c_{ik} = -\sum_{j(\neq i)} \widetilde{\Gamma}^{ij}(\Phi_\alpha^\rho[i]) H_{ij}^{(\text{eff})} c_{jk}, \tag{5}$$

where the coupling coefficients $\widetilde{\Gamma}^{ij}(\Phi_\alpha^\rho[i])$ have now a different form, namely

$$\widetilde{\Gamma}^{ij}(\Phi_\alpha^\rho[i]) = \langle \Phi_\alpha^\rho[i] | \exp(-T^{[i]}) \exp(T^{[j]}) | \Phi_i \rangle. \tag{6}$$

This form of coupling coefficients involves the same reference i in the bra and the ket, facilitating their evaluation.

For a CMS, all excitation operators $G_\alpha^\rho[i]$ are *external* by definition, i.e. $G_\alpha^\rho[i] |\Phi_i\rangle \in \mathcal{M}_0^{\perp}$, so that one directly solves the above given CC equations, Eqs. (3) or (5). However, when a GMS is used, some of the excitation operators may be of an internal kind, i.e., $G_\alpha^\rho[i] |\Phi_i\rangle \in \mathcal{M}_0$, and the corresponding *internal* amplitudes must be properly taken care of.

Now, the cluster operator $\exp(T^{[i]})$ transforms $|\Phi_i\rangle$ into $|\widetilde{\Psi}_i\rangle$ given by a linear combination of target states $|\Psi_j\rangle$,

$$|\widetilde{\Psi}_i\rangle = \exp(T^{[i]}) |\Phi_i\rangle = \sum_{j=1}^{M} (\mathbf{C}^{-1})_{ij} |\Psi_j\rangle$$
$$= |\Phi_i\rangle + \sum_{|\Xi_j\rangle \in \mathcal{M}_0^{\perp}} \tilde{d}_{ij} |\Xi_j\rangle, \tag{7}$$

where now $\widetilde{\mathbf{D}} = ||\tilde{d}_{ij}|| = \mathbf{C}^{-1}\mathbf{D}$, $\mathbf{D} = ||d_{ij}||$, while $\widetilde{\mathbf{C}} = ||\widetilde{C}_{ij}|| = \mathbf{C}^{-1}\mathbf{C} = \mathbf{1}$, which is associated with the model space, becomes the identity. In view of this fact the off-diagonal coefficients $\tilde{c}_\alpha^\rho[i]$ must vanish. This implies that all singly-excited internal cluster amplitudes $t_P^Q[i]$ automatically vanish since, generally, $C_1 = T_1$, while the higher excited ones are given by the requirement that $\tilde{c}_\alpha^\rho[i] \equiv 0$. For example, assuming that $|\Phi_2\rangle = G_{P_1 P_2}^{Q_1 Q_2}[1] |\Phi_1\rangle$, we require that $\tilde{c}_{P_1 P_2}^{Q_1 Q_2}[1] = 0$, implying that

$$t_{P_1 P_2}^{Q_1 Q_2}[1] \equiv -t_{P_1}^{Q_1}[1] t_{P_2}^{Q_2}[1] + t_{P_1}^{Q_2}[1] t_{P_2}^{Q_1}[1]. \tag{8}$$

These relations for the *internal* amplitudes are referred to as the C-conditions [34]. Clearly, the origin of the C-conditions does not involve amplitude Eqs. (3) or (5), so that they apply not only to the GMS-based SU CCSD method, but also to both the BW CCSD [41] and MkCCSD methods.

3. Role of C-conditions

The usefulness and, in fact, the necessity of the C-conditions when using incomplete model spaces in the MR-SU-CCSD method has been demonstrated in a number of actual applications [34–36,42–44], which demonstrate that one can avoid a CMS and obtain highly-accurate results using relatively small, yet appropriate, low-dimensional GMSs. An exploitation of the C-conditions in the

Brillouin–Wigner CC approach [33] has also been outlined and demonstrated on an actual example [41].

In this paper we wish to show that the C-conditions may be conveniently exploited in the SS MkCCSD approach as well. For this purpose we have chosen three examples that involve a significant MR character: (i) The water molecule with stretched one or both O–H bonds, (ii) the (2,5)-isomer of pyridynium (or didehydropyridinium) cation, showing a strong diradical character [45], and (iii) an artificial model of H_2O with a strongly truncated virtual MO set that allows only double excitations, so that already CISD and CCSD yield the FCI result. In all these examples, the T_1 amplitudes are large, so that the C-conditions for *internal* doubles are non-negligible [cf. Eq. (8)]. As already pointed out we restrict ourselves in this communication to the ground states. The examples presented below are intended to show the difference between the MkCCSD energies obtained with a CMS and IMS, when in the latter case we use or ignore the C-conditions. To emphasize the effects of quasidegeneracy, we consider models with significantly stretched bond(s) or having a biradical nature. These, of course, represent a rather special cases, so that we must be careful in drawing general conclusions concerning the performance of the studied methods in the entire region of potential energy surfaces.

3.1. Stretched H_2O models

We first consider the H_2O molecule using both the TZ and aug-cc-pVTZ basis sets (the former one resulting by deleting polarization functions from the cc-pVTZ basis) for the two stretched geometries designated as A and B. In geometry A, one O–H bond is stretched to $R_1 = 4.4$ a.u. and the second bond length R_2, as well as the bond angle $\angle HOH$, are optimized at the CCSD/cc-pVTZ level, yielding $R_2 = 1.829$ a.u. and $\angle HOH = 85.4°$. In geometry B, both O–H bonds are symmetrically stretched to $R_1 = R_2 = 3.2$ a.u., while keeping the equilibrium geometry bond angle at $\angle HOH = 104.52°$.

In both cases we employ a simple two-electron/two-orbital active space. The corresponding CMS thus involves four references (4R) assuming that both orbitals belong to the same symmetry species and we rely on a spin–orbital formalism, namely the Hartree–Fock (HF), two singly-excited, and one doubly-excited determinants. A truncated two-dimensional model space (2R) involving only the HF and doubly-excited determinants then represents an IMS. In such a case we require the C-conditions for the internal double-excitations transforming one reference into the other one.

In Table 1 we demonstrate the effect of C-conditions when using the 2R model space in the MkCCSD method rather than the 4R CMS. The case when one ignores the C-conditions in the 2R-MkCCSD method is indicated by the symbol "$C = 0$". In the same table we also give the 4R-MkCCSD results, as well as the SR CCSD, SR CCSD(T), CR-CC(2,3), 4R-RMR-CCSD and 4R-RMR-CCSD(T) results. For the TZ basis set we also present the benchmark FCI energies. Since the 4R-RMR-CCSD(T)/TZ energies are very close to the FCI ones, we can use them as a benchmark in the case of a large aug-cc-pVTZ basis.

We see that the effect of the C-conditions amounts to about $1-2 mE_h$. We also see that in the case of H_2O the 2R-MkCCSD energies are very close to the 4R-MkCCSD results when we exploit the C-conditions. We shall see in the next example that this is not always the case. In all cases, however, the effect of the C-conditions decreases the energy and brings it closer to the FCI result.

We also note that for the given geometries, the SR CCSD and CCSD(T) methods still provide reasonable results, since only single-bonds are involved. Yet, we see already the trend of CCSD(T) to overestimate the correlation energy and, eventually, to break down completely. Indeed, for a symmetrically stretched geometry B, we find already the CCSD(T) energy below the FCI one by

Table 1
Role of C-conditions in the SS MkCCSD method with a truncated model space for two geometries A[a] and B[b] of the stretched H_2O molecule using a TZ[c] and aug-cc-pVTZ basis sets. See the text for details.

Method	Geometry A		Geometry B	
	TZ	aug-cc-pVTZ	TZ	aug-cc-pVTZ
CCSD	−76.00361	−76.13360	−75.95343	−76.06752
2R-MkCCSD ($C = 0$)[d]	−76.00809	−76.14256	−75.95193	−76.06695
2R-MkCCSD	−76.00971	−76.14505	−75.95335	−76.06837
ΔE[e]	0.00162	0.00249	0.00142	0.00142
4R-MkCCSD	−76.00935	−76.14512	−75.95335	−76.06856
4R RMR-CCSD	−76.01323	−76.15003	−75.95855	−76.07276
CCSD(T)	−76.01845	−76.16026	−75.96530	−76.08909
CR-CC(2,3)	−76.01575	−76.15536	−75.96475	−76.08669
4R-RMR-CCSD(T)	−76.01574	−76.15816	−75.96552	−76.08927
FCI	−76.01603		−75.96506	

[a] Geometry A: $R_1 = 4.4$ a.u., $R_2 = 1.829$ a.u., $\angle HOH = 85.4°$.
[b] $R_1 = R_2 = 3.2$ a.u., $\angle HOH = 104.52°$.
[c] TZ basis results from cc-pVTZ by deleting polarization functions.
[d] $C = 0$ implies that the C-conditions were ignored.
[e] ΔE gives the energy difference between the 2R-MkCCSD energies as obtained with and without the C-conditions.

$0.24 mE_h$. With an additional stretch to $R_1 = R_2 = 4$ a.u. (geometry C; general results not shown for the sake of brevity), the CCSD(T) energy is lower than the FCI one by $25 mE_h$. At the level of quasidegeneracy in our models, the breakdown of CCSD(T) is rather nicely corrected by the CR-CC(2,3) method, which, however, also overshoots FCI by $3.82 mE_h$ at the geometry C. In fact, even SR CCSD has a tendency to fail at these geometries, the corresponding energy being below that of 2R-MkCCSD ($C = 0$) one by $2.2 mE_h$ and by $7.5 mE_h$ for the geometry C. Even 4R RMR-CCSD(T) overshoots the FCI energy, since the 4R model space becomes inadequate for severely stretched geometries, in which case a larger 7R space is required (e.g., for the C geometry, we find six two-body amplitudes larger than 0.2; the corresponding 7R RMR-CCSD(T) then provides a good approximation to FCI differing by only $2.2 mE_h$).

3.2. Pyridynium cation

Among the (m, n)-isomers of pyridynium cation $C_5NH_4^+$ the (2,5) isomer shows the strongest MR character as already implied by the fact that it may be regarded as an analog of *para*-benzyne with one C–H group replaced by the (N–H)$^+$ group. Moreover, it shows the smallest singlet–triplet splitting of all the six isomers and a very large CCSD t_1 amplitude amounting to 0.31. Our earlier study of this system [45] also showed the failure of CCSD(T) in this case, predicting too low an energy for the singlet ground state.

The results in Table 2 show a similar behavior as in the preceding case, except that now even 2R-MkCCSD with the C-conditions differs significantly from 4R-MkCCSD by almost $7 mE_h$, the latter one being very close to the 4R-RMR-CCSD result. The SR CCSD(T) method again overestimates the correlation energy due to triples, while CR-CC(2,3) is closest to 4R RMR-CCSD, the $4.5 mE_h$ difference being likely due to quadruples that are neglected in the former approach.

3.3. Truncated H_2O model

As a final illustration of the role of the C-conditions we employ a truncated H_2O model in which we correlate ten electrons in a six orbital space. In other words, in addition to the five occupied MOs of the HF reference we have only one virtual MO, all other virtual MOs being frozen, so that the model admits at most double excitations. This enables us to recover the FCI result at the

Table 2
Role of C-condition in the SS MkCCSD method with truncated model space for (2,5)-pyridinium cation $C_5NH_4^+$ using a cc-pVDZ basis set and the (2,5) geometry of Ref. [45].

Method	Energy
CCSD	−246.51446
2R-MkCCSD ($C = 0$)[a]	−246.52721
2R-MkCCSD	−246.52809
ΔE[b]	0.00088
4R-MkCCSD	−246.53486
4R RMR-CCSD	−246.53475
CCSD(T)	−246.58980
CR-CC(2,3)	−246.57317
4R-RMR-CCSD(T)	−246.57776

[a] $C = 0$ implies that the C-conditions were ignored.
[b] ΔE gives the energy difference between the 2R-MkCCSD energies as obtained with and without the C-conditions.

Table 3
Ten-electron/six-orbital model of H_2O for the two geometries A and B (see Table 1 and the text) using a TZ basis set. See the text for details.

Method	Geometry A	Geometry B
2R-MkCCSD ($C = 0$)[a]	−75.8744840	−75.7367099
2R-MkCCSD	−75.8756611	−75.7416133
ΔE[b]	0.0011771	0.0049034
4R-MkCCSD	−75.8756611	−75.7416133
FCI	−75.8756611	−75.7416133

[a] $C = 0$ implies that the C-conditions were ignored.
[b] ΔE gives the energy difference between the 2R-MkCCSD energies as obtained with and without the C-conditions.

one- and two-body cluster level. Thus, both SR CISD and CCSD will be equivalent to FCI, yielding the exact result for this model. Otherwise, the same geometries are used as in Section 3.1.

The results in Table 3 clearly indicate that indeed we obtain the FCI energies using either the 4R CMS, or an incomplete 2R space with the C-conditions, while without the C-conditions the 2R-MkCCSD energies differ from the "exact" ones by up to about 5 mE_h. Using the C-conditions, we achieve a full nine digit (or 10^{-7} a.u.) accuracy. Although the present example is rather contrived, it shows very clearly the role of the C-conditions, since it enables us to recover the FCI result at the full cluster level even when relying on an incomplete model space. Unfortunately, we are unable to carry out a similar test employing more than one virtual orbital, since that would require handling of up to four-body clusters. This facility is not available in our current implementation of the MkCCSD codes.

4. Conclusions

The C-conditions have been originally introduced in the GMS-SU-CCSD methods to account for the internal cluster amplitudes that are associated with excitation operators transforming one reference into another one. While these amplitudes exactly vanish when we employ a CMS, they must be properly accounted for when an IMS is used, such as a GMS, in order to keep the connected cluster character of the MR-CC formalism. The usefulness of these conditions was also exploited in the Brillouin–Wigner version of the MR-CC method [41].

In this paper we show that the C-conditions can also be advantageously employed in the SS version of the SU-CC method as formulated by Mukherjee et al. [26,27] and usually referred to by the acronym MkCCSD [28]. We demonstrate on several examples, all involving a considerable quasidegeneracy due to a MR or diradical nature of the states considered, that the use of C-conditions when employing an IMS always improves the performance, bringing the result closer to that obtained with the CMS. This is particularly clearly demonstrated by our last example that involves at most pair cluster amplitudes.

In general, the C-conditions are given in terms of products of lower-order cluster amplitudes, so that their importance depends on the magnitude of such amplitudes. In the case of two-body clusters, the C-conditions are given by products of t_1 amplitudes. Clearly, if these t_1 amplitudes are small, say $< 10^{-2}$, their products will be of the order $< 10^{-4}$, so that these conditions will have only a marginal effect on the final energies. However, as we have seen above, in the case of the (2,5)-pyridinium cation, the largest t_1 amplitude is ∼0.3 and the effect is significant. The same will hold, of course, for higher order cluster amplitudes, particularly when the effect of connected quadruples will be non-negligible.

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