Extension of coupled-cluster theory with a non-iterative treatment of connected triply excited clusters to three-body Hamiltonians

Sven Binder,[1,*] Piotr Piecuch,[2,†] Angelo Calci,[1,‡] Joachim Langhammer,[1,§] Petr Navrátil,[3,¶] and Robert Roth[1,**]

[1] *Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany*
[2] *Department of Chemistry, Michigan State University, East Lansing, Michigan 48824, USA*
[3] *TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia, V6T 2A3 Canada*

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We generalize the coupled-cluster (CC) approach with singles, doubles, and the non-iterative treatment of triples termed ΛCCSD(T), to Hamiltonians containing three-body interactions. The resulting method and the underlying CC approach with singles and doubles only (CCSD) are applied to the medium-mass closed-shell nuclei ^{16}O, ^{24}O and ^{40}Ca. By comparing the results of CCSD and ΛCCSD(T) calculations with explicit treatment of three-nucleon (3*N*) interactions to those obtained using an approximate treatment in which they are included effectively via the zero-, one- and two-body components of the Hamiltonian in normal-ordered form, we quantify the contributions of the residual three-body interactions neglected in the approximate treatment. We find these residual normal-ordered three-body contributions negligible for the ΛCCSD(T) method, although they can become significant in the lower-level CCSD approach, particularly when the nucleon-nucleon interactions are soft.

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I. INTRODUCTION

Chiral effective field theory (EFT) provides a systematic link between low-energy quantum chromodynamics (QCD) and nuclear-structure physics [1–9]. In order to make accurate QCD-based predictions using *ab initio* many-body methods employing Hamiltonians constructed within chiral EFT, the inclusion of three-nucleon (3*N*) forces is inevitable [8, 9], affecting various important nuclear properties, such as binding and excitation energies [10–17]. While some many-body approaches, such as the no-core shell model (NCSM) [10, 12, 18–36] and its importance-truncated (IT) extension [33, 37, 38] or the coupled-cluster (CC) theory [39–46] truncated at the singly and doubly excited clusters (CCSD) [38, 47–62] have already been extended to the explicit treatment of 3*N* interactions and were successfully applied to light and medium-mass nuclei [13, 14, 17, 63, 64], other approaches remain to be generalized to the explicit 3*N* case. Among these are the more quantitative CC approaches, including those based on a non-iterative treatment of the connected triply excited clusters on top of CCSD, such as CCSD(T) [63, 65], CR-CCSD(T) [51, 53–56, 66–70], CCSD(2)$_\text{T}$ [71–74], ΛCCSD(T) [17, 60, 64, 75–78], and CR-CC(2,3) [38, 58, 61, 79–82], or the in-medium similarity renormalization group [16, 83].

Considering the substantial cost of *ab initio* many-body computations with 3*N* interactions, it is important to examine how much information about the 3*N* forces has to be included in such calculations explicitly. A common practice in nuclear-structure theory is to incorporate 3*N* forces into the many-body considerations with the help of effective interactions that can provide information about these forces via suitably re-defined lower-particle terms in the Hamiltonian. In particular, the normal-ordering two-body approximation (NO2B), where normal ordering of the Hamiltonian becomes a formal tool to demote information about the 3*N* interactions to lower-particle normal-ordered terms and the residual normal-ordered 3*N* term is subsequently discarded, has led to promising results in NCSM and CCSD calculations for light and medium-mass nuclei [13, 14, 17, 63, 64]. In the case of the IT-NCSM and CCSD approach, contributions from the residual 3*N* interactions have been shown to be small [14, 63, 64], although not always negligible [14, 64]. In many cases one needs to go beyond the CCSD level within the CC framework to obtain a highly accurate quantitative description of several nuclear properties, including binding and excitation energies [38, 51, 53–58, 60, 61, 78]. Thus, a more precise assessment of the significance of the residual 3*N* contribution in the normal-ordered Hamiltonian at the CC theory levels that incorporate the connected triply excited clusters in an accurate and computationally manageable manner, such as CCSD(T), ΛCCSD(T) and CR-CC(2,3), is an important and timely objective. It is nowadays well established that once the connected triply excited clusters are included in the CC calculations, the resulting energies can compete with the converged NCSM, high-level configuration interaction (CI), or other nearly exact numerical data, which is a consequence of the use of the exponential wave function ansatz in the CC considerations, where various higher-order many-particle correlation effects are described via products of low-rank excitation operators (for the examples of the more recent nuclear-structure calculations illustrating this statement, see Refs. [17, 38, 51, 53–58, 60–64, 78]; cf., also, Ref. [84]). This makes the examination of the CC models that account for the connected triply excited clusters, in addition to the singly and

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[*] Corresponding author; Electronic address: `sven.binder@physik.tu-darmstadt.de`

[†] Electronic address: `piecuch@chemistry.msu.edu`

[‡] Electronic address: `angelo.calci@physik.tu-darmstadt.de`

[§] Electronic address: `joachim.langhammer@physik.tu-darmstadt.de`

[¶] Electronic address: `navratil@triumf.ca`

[**] Electronic address: `robert.roth@physik.tu-darmstadt.de`

doubly excited clusters and their products captured by CCSD, and their extensions to $3N$ interactions even more important.

In our earlier work on CC methods with non-iterative treatment of the connected triply excited clusters (called triples) using two-nucleon (NN) interactions in the Hamiltonian, the highest theory level considered thus far was CR-CC(2,3) [38, 61]. The experience of quantum chemistry, where several CC approximations of this type have been developed, indicates that CR-CC(2,3) represents the most complete and most robust form of the non-iterative triples correction to CCSD (cf., e.g., Refs. [79–81, 85–88]), producing results that in benchmark computations are often very close to those obtained with a full treatment of the singly, doubly, and triply excited clusters via the iterative CCSDT approach [89, 90], at a small fraction of the computing cost [79, 80, 88]. However, there also exist other methods in this category, such as the ΛCCSD(T) approach that has been examined in the nuclear context as well [17, 64, 78], which represent approximations to CR-CC(2,3) [79–81, 88] and are almost as effective in capturing the connected triply excited clusters in closed-shell systems, while simplifying programming effort, particularly when $3N$ interactions need to be examined and when efficient angular-momentum-coupled codes have to be developed. Thus, although we would eventually also like to work on an angular-momentum-coupled formulation of the CR-CC(2,3) method for Hamiltonians including $3N$ forces, in this first work on the examination of the role of $3N$ interactions in the CC theory levels beyond CCSD, we focus on the simpler ΛCCSD(T) approach. Following the considerations presented in Ref. [76] for the case of two-body Hamiltonians and those presented in Refs. [79, 80, 82] in the more general CR-CC(2,3) context, which help us to identify additional terms in the equations due to the $3N$ forces, we derive the ΛCCSD(T)-style triples energy correction for three-body Hamiltonians which we subsequently apply to the medium-mass closed-shell nuclei ^{16}O, ^{24}O, and ^{40}Ca. By comparing the CCSD and ΛCCSD(T) binding energies obtained with the explicit treatment of $3N$ interactions with their counterparts obtained within the NO2B approximation, we quantify the contributions of the residual $3N$ interactions that are neglected in the NO2B approximation at two different CC-theory levels, with and without the connected triply excited clusters.

II. THEORY

A. Brief synopsis of coupled-cluster theory

The CCSD and ΛCCSD(T) approaches examined in this study, and the CR-CC(2,3) counterpart of ΛCCSD(T) used in our considerations as well, are examples of approximations based on the exponential ansatz of single-reference CC theory, in which the ground state $|\Psi\rangle$ of an A-particle system is represented as [39–46]

$$|\Psi\rangle = e^{T}|\Phi\rangle, \tag{1}$$

where $|\Phi\rangle$ is the reference determinant (in the computations reported in this paper, the Hartree-Fock state) and

$$T = \sum_{n=1}^{A} T_n \tag{2}$$

is a particle-hole excitation operator, defined relative to the Fermi vacuum $|\Phi\rangle$ and referred to as the cluster operator, whose many-body components

$$T_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1,\ldots,i_n \\ a_1,\ldots,a_n}} t_{i_1\ldots i_n}^{a_1\ldots a_n}\, a_{a_1}^{\dagger} \cdots a_{a_n}^{\dagger} a_{i_n} \cdots a_{i_1} \tag{3}$$

generate the connected wave-function diagrams of $|\Psi\rangle$. The remaining linked, but disconnected contributions to $|\Psi\rangle$ are produced through the various product terms of the T_n operators resulting from the use of Eqs. (1)–(3). Here and elsewhere in this article, we use the traditional notation in which $i_1, i_2, \ldots$ or $i,\ j, \ldots$ are the single-particle states (orbitals) occupied in $|\Phi\rangle$, $a_1,\ a_2, \ldots$ or $a,\ b, \ldots$ are the single-particle states unoccupied in $|\Phi\rangle$, and $p, q, \ldots,\ p_1,\ p_2, \ldots,$ or $q_1,\ q_2, \ldots$ represent generic single-particle states.

Typically, the explicit equations for the ground-state energy E, which can be written as

$$E = E_{\text{ref}} + \Delta E, \tag{4}$$

where

$$E_{\text{ref}} = \langle\Phi|H|\Phi\rangle \tag{5}$$

is the independent-particle-model reference energy and ΔE its correlation counterpart, and the cluster amplitudes $t_{i_1\ldots i_n}^{a_1\ldots a_n}$ defining the many-body components T_n of T, are obtained by first inserting the ansatz for the wave function $|\Psi\rangle$, Eq. (1), into the Schrödinger equation, $H_N|\Psi\rangle = \Delta E|\Psi\rangle$, where

$$H_N = H - E_{\text{ref}} \tag{6}$$

is the Hamiltonian in normal-ordered form relative to $|\Phi\rangle$. Then, premultiplying both sides of the resulting equation on the left by e^{-T} yields the connected cluster form of the Schrödinger equation [42, 43],

$$\overline{H_N}|\Phi\rangle = \Delta E|\Phi\rangle, \tag{7}$$

where

$$\overline{H_N} = e^{-T}\, H_N\, e^{T} = (H_N\, e^{T})_C \tag{8}$$

is the similarity-transformed Hamiltonian or, equivalently, the connected product of H_N and e^{T} (designated by the subscript C). Finally, both sides of Eq. (7) are projected on the reference determinant $|\Phi\rangle$ and the excited determinants

$$|\Phi_{i_1\ldots i_k}^{a_1\ldots a_k}\rangle = a_{a_1}^{\dagger} \cdots a_{a_k}^{\dagger} a_{i_k} \cdots a_{i_1}|\Phi\rangle \tag{9}$$

that correspond to the particle-hole excitations included in T. The latter projections result in a nonlinear system of the explicitly connected and energy-independent equations for the cluster amplitudes $t^{a_1 \dots a_k}_{i_1 \dots i_k}$ [42–45] (cf., e.g., Refs. [38, 41, 46, 70, 88, 91–95] for review information),

$$\langle \Phi^{a_1 \dots a_n}_{i_1 \dots i_n} | \overline{H_N} | \Phi \rangle = 0, \quad i_1 < \cdots < i_n, \; a_1 < \cdots < a_n, \tag{10}$$

where $\overline{H_N}$ is defined by Eq. (8) and $n = 1, \dots, A$, whereas the projection of Eq. (7) on $|\Phi\rangle$ results in the CC correlation energy formula,

$$\Delta E = \langle \Phi | \overline{H_N} | \Phi \rangle. \tag{11}$$

If one is further interested in properties other than energy, which require the knowledge of the ket state $|\Psi\rangle$ and its bra counterpart

$$\langle \tilde{\Psi} | = \langle \Phi | (1 + \Lambda) e^{-T}, \tag{12}$$

which satisfies the biorthonormality condition $\langle \tilde{\Psi} | \Psi \rangle = 1$, and where

$$\Lambda = \sum_{n=1}^{A} \Lambda_n, \tag{13}$$

with

$$\Lambda_n = \left(\frac{1}{n!} \right)^2 \sum_{\substack{i_1, \dots, i_n \\ a_1, \dots, a_n}} \lambda^{i_1 \dots i_n}_{a_1 \dots a_n} \, a^\dagger_{i_1} \cdots a^\dagger_{i_n} a_{a_n} \cdots a_{a_1}, \tag{14}$$

is the hole-particle deexcitation operator generating $\langle \tilde{\Psi} |$, we also have to solve the linear system of the so-called Λ equations [38, 88, 91, 93–99],

$$\begin{aligned} \langle \Phi | (1 + \Lambda) \, \overline{H_N} | \Phi^{a_1 \dots a_n}_{i_1 \dots i_n} \rangle \; &= \; \Delta E \, \lambda^{i_1 \dots i_n}_{a_1 \dots a_n}, \\ & i_1 < \cdots < i_n, \; a_1 < \cdots < a_n, \end{aligned} \tag{15}$$

obtained by substituting Eq. (12) into the adjoint form of the Schrödinger equation, $\langle \tilde{\Psi} | H_N = \Delta E \langle \tilde{\Psi} |$. System (15) can be further simplified into the energy-independent form

$$\begin{aligned} \langle \Phi | (1 + \Lambda) \, (\overline{H_N})_{\text{open}} | \Phi^{a_1 \dots a_n}_{i_1 \dots i_n} \rangle \; &= \; 0, \\ & i_1 < \cdots < i_n, \; a_1 < \cdots < a_n, \end{aligned} \tag{16}$$

where

$$(\overline{H_N})_{\text{open}} = \overline{H_N} - (\overline{H_N})_{\text{closed}} = \overline{H_N} - \Delta E \tag{17}$$

is the open part of $\overline{H_N}$, defined by the diagrams of $\overline{H_N}$ that have external Fermion lines. Clearly, the only diagrams of $\overline{H_N}$ that enter the CC system given by Eq. (10) are the diagrams of $(\overline{H_N})_{\text{open}}$, whereas the only diagrams that contribute to ΔE, Eq. (11), are the vacuum (or closed) diagrams that have no external lines. We discuss the Λ or left-eigenstate CC equations, Eq. (15) or (16), for the deexcitation amplitudes $\lambda^{i_1 \dots i_n}_{a_1 \dots a_n}$ here, since they are one of the key ingredients of ΛCCSD(T) and the related CR-CC(2,3) considerations below. It is worth pointing out, though, that by examining these equations in the context of the ΛCCSD(T)/CR-CC(2,3) considerations for the three-body Hamiltonians, we are at the same time helping future developments in the area of CC computations of nuclear properties other than binding energy, extending the relevant formal considerations to the case of $3N$ interactions. For example, the Λ operator obtained by solving Eq. (16) can be used to determine the CC one-body reduced density matrices,

$$\gamma^q_p \equiv \langle \tilde{\Psi} | (a^\dagger_p a_q) | \Psi \rangle = \langle \Phi | (1 + \Lambda) \overline{(a^\dagger_p a_q)} | \Phi \rangle, \tag{18}$$

where we define $\overline{(a^\dagger_p a_q)}$ as

$$\overline{(a^\dagger_p a_q)} = e^{-T} \, (a^\dagger_p a_q) \, e^{T} = [(a^\dagger_p a_q) \, e^{T}]_C, \tag{19}$$

and determine expectation values of one-body operators in the usual manner as

$$\langle \tilde{\Psi} | \Theta | \Psi \rangle = \sum_{p,q} \theta^p_q \, \gamma^q_p \equiv \theta^p_q \, \gamma^q_p, \tag{20}$$

where $\Theta = \sum_{p,q} \theta^p_q a^\dagger_p a_q$ is a one-body property operator of interest. In writing Eq. (20), the Einstein summation convention over repeated upper and lower indices in product expressions of matrix elements has been assumed. We will exploit this convention throughout the rest of this article.

The above is the exact CC theory, which is equivalent to the exact diagonalization of the Hamiltonian within the full CI approach and is, for practical reasons, limited to small few-body problems. Thus, in all practical applications of CC theory, one truncates the many-body expansion for T, Eq. (2), at some, preferably low, m-particle–m-hole excitation level T_m. In this study, we focus on the CCSD approach in which T is truncated at the doubly excited clusters T_2, and the ΛCCSD(T) method, which allows to correct the CCSD energy for the dominant effects due to the triply excited clusters T_3 in a computationally feasible manner, avoiding the prohibitively expensive steps of full CCSDT, in which one has to solve for T_1, T_2 and T_3 in an iterative fashion. The final form of the CC amplitude and energy equations also depends on the Hamiltonian used in the calculations, since the length of the many-body expansion of the resulting similarity-transformed Hamiltonian $\overline{H_N}$, Eq. (8), which can also be written as

$$\begin{aligned} \overline{H_N} \; &= \; H_N + \sum_{n=1}^{2k_{\max}} \frac{1}{n!} \underbrace{\big[\dots \big[}_{n \text{ times}} H_N, \underbrace{T \big], \dots, T \big]}_{n \text{ times}} \\ &= \; \sum_{n=0}^{2k_{\max}} \frac{1}{n!} (H_N T^n)_C, \end{aligned} \tag{21}$$

depends on $k_{\max}$, where $k_{\max}$ is the highest many-body rank of the interactions in H_N or H ($k_{\max} = 2$ for $2N$ interactions, $k_{\max} = 3$ for $3N$ interaction terms, etc.). In this article we focus on the $k_{\max} = 3$ case, emphasizing the differences between the more familiar CCSD and ΛCCSD(T) equations for two-body Hamiltonians, which can be found, in the most compact, factorized form using recursively generated intermediates, in Refs. [47, 52, 97, 100] for CCSD and [76] for ΛCCSD(T), and their extensions to the three-body case. The key ingredients of the CCSD and ΛCCSD(T) approaches for $3N$ interactions in the Hamiltonian are discussed in the next two subsections. We begin with the Hamiltonian.

B. Normal-ordered form of the Hamiltonian with three-body interactions and the NO2B approximation

As shown in the previous subsection, the single-reference CC equations for the cluster amplitudes $t^{a_1\ldots a_n}_{i_1\ldots i_n}$ defining T, their deexcitation counterparts $\lambda^{i_1\ldots i_n}_{a_1\ldots a_n}$ defining Λ, and the correlation energy ΔE can be conveniently expressed in terms of the Hamiltonian in normal-ordered form relative to the Fermi vacuum $|\Phi\rangle$, transformed with e^T, as in Eqs. (8) and (21). For Hamiltonians with up to three-body interactions,

$$H = H_1 + H_2 + H_3, \tag{22}$$

where

$$H_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{p_1,\ldots,p_n \\ q_1,\ldots,q_n}} h^{p_1\ldots p_n}_{q_1\ldots q_n}\, a^\dagger_{p_1} \cdots a^\dagger_{p_n} a_{q_n} \cdots a_{q_1} \tag{23}$$

is the n-body contribution to H, and the normal-ordered Hamiltonian H_N, Eq. (6), which provides information about the many-particle correlation effects beyond the mean-field level represented by $|\Phi\rangle$, can be represented in the form

$$H_N = F_N + V_N + W_N. \tag{24}$$

The one-, two-, and three-body components F_N, V_N and W_N in Eq. (24) are defined as

$$F_N = \sum_{p,q} f^p_q\, N[a^\dagger_p a_q], \tag{25}$$

$$V_N = \tfrac{1}{4} \sum_{p,q,r,s} v^{pq}_{rs}\, N[a^\dagger_p a^\dagger_q a_s a_r], \tag{26}$$

and

$$W_N = \tfrac{1}{36} \sum_{p,q,r,s,t,u} w^{pqr}_{stu}\, N[a^\dagger_p a^\dagger_q a^\dagger_r a_u a_t a_s], \tag{27}$$

where $N[\ldots]$ designates normal ordering relative to $|\Phi\rangle$ and the matrix elements f^p_q, v^{pq}_{rs} and w^{pqr}_{stu} are given by

$$f^p_q = h^p_q + \sum_i h^{pi}_{qi} + \tfrac{1}{2} \sum_{i,j} h^{pij}_{qij}, \tag{28}$$

$$v^{pq}_{rs} = h^{pq}_{rs} + \tfrac{1}{4} \sum_i h^{pqi}_{rsi}, \tag{29}$$

and

$$w^{pqr}_{stu} = h^{pqr}_{stu}, \tag{30}$$

repectively. The corresponding reference energy E_{ref}, Eq. (5), which one needs to add to the correlation energy ΔE to obtain the total ground-state energy E, is calculated via

$$E_{\text{ref}} = \sum_i h^i_i + \tfrac{1}{2} \sum_{i,j} h^{ij}_{ij} + \tfrac{1}{6} \sum_{i,j,k} h^{ijk}_{ijk}. \tag{31}$$

When the Hamiltonian is used in the normal-ordered form, information about the three-body interaction in H enters in two fundamentally different ways: effectively, via the reference energy E_{ref}, Eq. (31), and the normal-ordered one- and two-body matrix elements f^p_q and v^{pq}_{rs}, Eqs. (28) and (29), which define the F_N and V_N components of H_N, and explicitly, via the genuinely three-body residual term W_N, Eq. (27), which captures those $3N$ contributions to the Hamiltonian that cannot be demoted to the lower-rank F_N and V_N operators or the reference energy E_{ref}. Considering the fact that the F_N and V_N components of H_N combined with the reference energy E_{ref} contain the complete information about pairwise interactions and much of the information about the $3N$ forces, it is reasonable to consider the NO2B approximation, discussed in Refs. [14, 17, 63, 64], in which the three-body residual term W_N is neglected in H_N. The main goal of this study is to compare the CCSD and ΛCCSD(T) results obtained with a full representation of the normal-ordered Hamiltonian H_N in which the residual three-body term W_N is retained in the calculations, with their counterparts obtained using the truncated form of H_N that defines the NO2B approximation, in which Eq. (24) is replaced by the simplified expression

$$H_{N,2\text{B}} = F_N + V_N \tag{32}$$

containing only the one- and two-body components of H_N defined by Eqs. (25)–(26) and (28)–(29).

The NO2B approximation offers several advantages over the full treatment of $3N$ forces. First of all, it allows to reuse the conventional CC equations derived for two-body Hamiltonians, which one can find for CCSD in Refs. [47, 52, 97, 100] and for ΛCCSD(T) in Ref. [76], by replacing the f^p_q and v^{pq}_{rs} matrix elements in these equations with their values determined using Eqs. (28) and (29). Clearly, the three-body interactions are not ignored when the NO2B approximation is invoked, since the reference energy E_{ref}, Eq. (31), the one-body operator F_N, defined by Eqs. (25) and (28), and the two-body operator V_N, defined by Eqs. (26) and (29), contain information about the $3N$ forces in the form of the integrated $\frac{1}{6}\sum_{i,j,k} h^{ijk}_{ijk}$, $\frac{1}{2}\sum_{i,j} h^{pij}_{qij}$ and $\frac{1}{4}\sum_i h^{pqi}_{rsi}$ contributions to E_{ref}, f^p_q and v^{pq}_{rs}. Secondly, the NO2B approximation leads to major savings in the computational effort, since the most expensive terms in the CC equations that are generated by the three-body residual interaction W_N are disregarded when one uses Eq. (32) instead of Eq. (24). Our objective is to examine if neglecting these residual terms, particularly at the more quantitative ΛCCSD(T) level, does not result in a substantial loss of accuracy in the description of the $3N$ contributions to the resulting binding energies.

The above discussion implies that in order to compare the CCSD and ΛCCSD(T) energies corresponding to the full treatment of $3N$ forces with their counterparts obtained using the NO2B approximation, as defined by Eq. (32), one has to augment the existing CCSD and ΛCCSD(T) equations derived for Hamiltonians with up to two-body components in H_N, reported, for example, in Refs. [47, 52, 76, 97, 100], by terms generated by the residual W_N interaction, while adjusting matrix elements of the F_N and V_N operators in the resulting equations through the use of Eqs. (28) and (29). This has been done for the CCSD case in Ref. [63], but none of the earlier nuclear CC works have dealt with the explicit and complete incorporation of $3N$ interactions in modern post-CCSD considerations. The present study addresses this concern by extending the considerations reported in Ref. [63] to the triples energy correction of ΛCCSD(T) and also the ΛCCSD equations, which one has to solve prior to the determination of the ΛCCSD(T) correction. Since, as discussed in Sec. II A, the CC amplitude and energy equations and their left-eigenstate Λ counterparts rely on the similarity-transformed form of H_N, designated by $\overline{H_N}$, Eq. (8), the most convenient way to incorporate the additional terms due to the presence of W_N into the CC considerations is by partitioning $\overline{H_N}$ as

$$\overline{H_N} = e^{-T}(H_{N,2\text{B}} + W_N)\, e^{T} = \overline{H_{N,2\text{B}}} + \overline{W_N}, \tag{33}$$

where

$$\overline{H_{N,2\text{B}}} = e^{-T} H_{N,2\text{B}}\, e^{T} = (H_{N,2\text{B}}\, e^{T})_C \tag{34}$$

is the similarity-transformed form of $H_{N,2\text{B}}$ and

$$\overline{W_N} = e^{-T} W_N\, e^{T} = (W_N\, e^{T})_C \tag{35}$$

is the similarity-transformed form of W_N. In this way, we can split the CC equations Eqs. (10), (11) and (16) into the NO2B contributions expressed in terms of $\overline{H_{N,2\text{B}}}$, which, with the exception of the f^p_q and v^{pq}_{rs} matrix elements that define F_N and V_N, have the same algebraic structure as the standard CC equations derived for two-body Hamiltonians, and the W_N-containing terms that provide the rest of the information about $3N$ contributions neglected by the NO2B approximation.

The partitioning of $\overline{H_N}$ represented by Eqs. (33)–(35) reflects the obvious fact that the normal-ordered form of the Hamiltonian including three-body interactions, Eq. (24), is a sum of the NO2B component $H_{N,2\text{B}}$, Eq. (32), and the three-body residual W_N term.

As implied by Eq. (21), $\overline{H_{N,2\text{B}}}$ terminates at the quadruply nested commutators or terms that contain the fourth power of T, since one can connect up to four vertices representing T operators to the diagrams of $H_{N,2\text{B}}$. Similarly, $\overline{W_N}$ terminates at the T^6 terms, since the diagram representing W_N has six external lines. As a result, the complete many-body expansions of $\overline{H_{N,2\text{B}}}$ and $\overline{W_N}$, i.e.,

$$\overline{H_{N,2\text{B}}} = \sum_n \overline{H}_{n,2\text{B}}, \tag{36}$$

where

$$\begin{aligned}\overline{H}_{n,2\text{B}} \;=\; & \left(\frac{1}{n!}\right)^2 \sum_{\substack{p_1,\ldots,p_n\\ q_1,\ldots,q_n}} \overline{h}^{p_1\ldots p_n}_{q_1\ldots q_n}(2\text{B}) \\ & \times a^{\dagger}_{p_1}\cdots a^{\dagger}_{p_n} a_{q_n}\cdots a_{q_1},\end{aligned} \tag{37}$$

and

$$\overline{W_N} = \sum_n \overline{W}_n, \tag{38}$$

where

$$\overline{W}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{p_1,\ldots,p_n\\ q_1,\ldots,q_n}} \overline{w}^{p_1\ldots p_n}_{q_1\ldots q_n}\, a^{\dagger}_{p_1}\cdots a^{\dagger}_{p_n} a_{q_n}\cdots a_{q_1}, \tag{39}$$

respectively, are quite complex, even at the lower levels of CC theory, such as CCSD, where T is truncated at T_2. Indeed, it is easy to demonstrate that when the cluster operator T is truncated at the doubly excited T_2 component, the resulting $\overline{H_{N,2\text{B}}}$ operator contains up to six-body terms. The corresponding operator $\overline{W_N}$ is even more complex, containing up to nine-body terms. Fortunately, as shown in the next subsection, by the virtue of the projections on the subsets of determinants that enter the CCSD and ΛCCSD(T) considerations, the final amplitude and energy equations used in the CCSD and ΛCCSD(T) calculations do not utilize all of the many-body components of $\overline{H_{N,2\text{B}}}$ and $\overline{W_N}$. For example, the highest many-body components of $\overline{H_{N,2\text{B}}}$ and $\overline{W_N}$ that have to be considered in the CCSD and ΛCCSD(T) calculations are selected types of three-body ($\overline{H_{N,2\text{B}}}$) or four-body ($\overline{W_N}$) terms, which greatly simplifies these calculations. The CCSD and ΛCCSD(T) equations, with emphasis on the additional terms beyond the NO2B approximation, are discussed next.

C. The CCSD and ΛCCSD(T) approaches for the Hamiltonians with three-body interactions

As mentioned in the introduction, the residual $3N$ interaction, represented by the W_N component of the normal-ordered Hamiltonian H_N, although generally small [14, 63, 64], may not always be negligible, particularly when the basic CC theory level represented by the CCSD approach is considered [14, 64]. Considering the fact that one has to go beyond the CCSD level within the CC framework to obtain a more quantitative description of nuclear properties [14, 17, 38, 51, 53–58, 60, 61, 64, 78], it is imperative to investigate how significant the incorporation of the residual three-body interactions in the Hamiltonian is when the connected triply excited (T_3) clusters are included in the calculations, in addition to the singly and doubly excited clusters, T_1 and T_2, included in CCSD. Ideally, one would prefer to examine this issue using the full CCSDT approach, in which one solves the system (10) of coupled nonlinear equations for the T_1, T_2, and T_3 cluster components in an iterative manner. Unfortunately, the full CCSDT treatment is prohibitively expensive and thus limited to small few-body problems, even at the level of pairwise interactions. When the residual $3N$ interactions are included in the CC considerations, the situation becomes even worse. For this reason we resort to the approximate treatment of the T_3 clusters via the non-iterative energy correction added to the CCSD energy defining the ΛCCSD(T) approach, which is capable of capturing the leading T_3 effects at the small fraction of the cost of the full CCSDT computations. A few remarks about the closely related CR-CC(2,3) method, which contains ΛCCSD(T) as the leading approximation and which also captures the T_3 effects, will be given too, since the CR-CC(2,3) expressions provide a transparent and pedagogical mechanism for identifying terms in the ΛCCSD(T) equations that result from adding the $3N$ interactions to the Hamiltonian. Considering the relatively low computational cost of the ΛCCSD(T) approach while providing information about the T_3 clusters, we can for medium-mass nuclei compare the results of the CC calculations describing the T_1, T_2, and T_3 effects using the complete representation of the three-body Hamiltonian including the residual W_N term with their counterparts relying on the NO2B truncation of H_N.

The determination of the ΛCCSD(T) (or CR-CC(2,3)) energy, which has the general form

$$E = E^{(\mathrm{CCSD})} + \delta E^{(\mathrm{T})}, \tag{40}$$

where

$$E^{(\mathrm{CCSD})} = E_{\mathrm{ref}} + \Delta E^{(\mathrm{CCSD})} \tag{41}$$

is the total CCSD energy and $\delta E^{(\mathrm{T})}$ the energy correction due to the connected T_3 clusters, consists of four steps: First, as in all many-body computations, we generate the appropriate single-particle basis, which in our case will be obtained from Hartree-Fock calculations. In the next two steps, which we discuss in Sec. II C 1, we solve the CCSD equations and their left-eigenstate Λ counterparts, and determine the CCSD correlation energy $\Delta E^{(\mathrm{CCSD})}$. The $\delta E^{(\mathrm{T})}$ correction, discussed in Sec. II C 2, is calculated in the fourth step using the information resulting from the CCSD and ΛCCSD calculations.

1. *The CCSD and left-eigenstate CCSD equations for three-body Hamiltonians*

We begin our considerations with the key elements of the CCSD approach, where the cluster operator T defining the ground-state wave function $|\Psi\rangle$ using Eq. (1) is truncated at the doubly excited clusters, so that (cf. Eqs. (2) and (3))

$$T \approx T^{(\mathrm{CCSD})} = T_1 + T_2, \tag{42}$$

with

$$T_1 = \sum_{i,a} t_i^a \, a_a^\dagger a_i = \sum_{i,a} t_i^a \, N[a_a^\dagger a_i] \tag{43}$$

and

$$T_2 = \tfrac{1}{4} \sum_{i,j,a,b} t_{ij}^{ab} \, a_a^\dagger a_b^\dagger a_j a_i = \tfrac{1}{4} \sum_{i,j,a,b} t_{ij}^{ab} \, N[a_a^\dagger a_i a_b^\dagger a_j], \tag{44}$$

and the left-eigenstate counterpart of CCSD, where the deexcitation operator Λ defining the bra ground state $\langle\tilde{\Psi}|$, Eq. (12), is approximated using the expression (cf. Eqs. (13) and (14))

$$\Lambda \approx \Lambda^{(\mathrm{CCSD})} = \Lambda_1 + \Lambda_2, \tag{45}$$

with

$$\Lambda_1 = \sum_{i,a} \lambda_a^i \, a_i^\dagger a_a = \sum_{i,a} \lambda_a^i \, N[a_i^\dagger a_a] \tag{46}$$

and

$$\Lambda_2 = \tfrac{1}{4} \sum_{i,j,a,b} \lambda_{ab}^{ij} \, a_i^\dagger a_j^\dagger a_b a_a = \tfrac{1}{4} \sum_{i,j,a,b} \lambda_{ab}^{ij} \, N[a_i^\dagger a_a a_j^\dagger a_b]. \tag{47}$$

In addition to being useful in their own right, the CCSD and left-eigenstate CCSD calculations provide the singly and doubly excited cluster amplitudes, t_i^a and t_{ij}^{ab}, and their deexcitation λ_a^i and λ_{ab}^{ij} analogs, which are needed to construct the non-iterative corrections to the CCSD energy via the ΛCCSD(T), CR-CC(2,3), and similar techniques. The CCSD equations for three-body Hamiltonians have been discussed in Ref. [63], but their left-eigenstate ΛCCSD analogs have not been examined so far. Since the regular CCSD and ΛCCSD considerations cannot be separated out, we first summarize the CCSD amplitude and energy equations for the case of $3N$ interactions.

The CCSD equations are obtained by replacing T in Eqs. (10) and (11) by $T^{(\mathrm{CCSD})}$, and by limiting the projections on the excited determinants $|\Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n}\rangle$ in Eq. (10) to those that correspond to the singly and doubly excited cluster amplitudes t_i^a and t_{ij}^{ab} we want to determine, so that the number of equations matches the number of unknowns [38, 47–62]. Assuming that the Hamiltonian of interest contains three-body interactions, we obtain the system of equations for t_i^a and t_{ij}^{ab} [63]

$$\langle \Phi_i^a | \overline{H_N}^{(\mathrm{CCSD})} | \Phi \rangle = \Theta_i^a(2\mathrm{B}) + \Theta_i^a(W_N) = 0, \tag{48}$$

$$\langle \Phi_{ij}^{ab} | \overline{H_N}^{(\mathrm{CCSD})} | \Phi \rangle = \Theta_{ij}^{ab}(2\mathrm{B}) + \Theta_{ij}^{ab}(W_N) = 0, \tag{49}$$

where

$$\overline{H_N}^{(\mathrm{CCSD})} = e^{-T_1 - T_2} \, H_N \, e^{T_1 + T_2} = (H_N \, e^{T_1 + T_2})_C \tag{50}$$

is the similarity-transformed Hamiltonian of CCSD and $|\Phi_i^a\rangle$ and $|\Phi_{ij}^{ab}\rangle$ are the singly and doubly excited determinants relative to $|\Phi\rangle$. The $\Theta_i^a(2\mathrm{B})$, $\Theta_i^a(W_N)$, $\Theta_{ij}^{ab}(2\mathrm{B})$, and $\Theta_{ij}^{ab}(W_N)$ terms entering Eqs. (48) and (49) are defined as

$$\Theta_i^a(2\mathrm{B}) = \langle \Phi_i^a | \overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})} | \Phi \rangle, \tag{51}$$

$$\Theta_i^a(W_N) = \langle \Phi_i^a | \overline{W_N}^{(\mathrm{CCSD})} | \Phi \rangle, \tag{52}$$

$$\Theta_{ij}^{ab}(2\mathrm{B}) = \langle \Phi_{ij}^{ab} | \overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})} | \Phi \rangle, \tag{53}$$

and

$$\Theta_{ij}^{ab}(W_N) = \langle \Phi_{ij}^{ab} | \overline{W_N}^{(\mathrm{CCSD})} | \Phi \rangle. \tag{54}$$

The operators $\overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})}$ and $\overline{W_N}^{(\mathrm{CCSD})}$ appearing in Eqs. (51)–(54) are defined as

$$\overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})} = e^{-T_1 - T_2} \, H_{N,2\mathrm{B}} \, e^{T_1 + T_2} = (H_{N,2\mathrm{B}} \, e^{T_1 + T_2})_C \tag{55}$$

and

$$\overline{W_N}^{(\mathrm{CCSD})} = e^{-T_1-T_2}\, W_N\, e^{T_1+T_2} = (W_N\, e^{T_1+T_2})_C, \qquad (56)$$

and represent the similarity-transformed forms of the $H_{N,2\mathrm{B}}$ and W_N operators, Eqs. (34) and (35), adapted to the CCSD case, which obviously add up to $\overline{H_N}^{(\mathrm{CCSD})}$,

$$\overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})} + \overline{W_N}^{(\mathrm{CCSD})} = \overline{H_N}^{(\mathrm{CCSD})}. \qquad (57)$$

From the above definitions it is apparent that $\Theta_i^a(W_N)$ and $\Theta_{ij}^{ab}(W_N)$, due to their origin of W_N, do only contribute when the residual $3N$ interaction is included in the calculations, whereas the NO2B contributions $\Theta_i^a(2\mathrm{B})$ and $\Theta_{ij}^{ab}(2\mathrm{B})$ are present in any case. As in the most common case of two-body Hamiltonians (see, e.g., Refs. [38, 47–50, 95]), it is easy to demonstrate, using Eq. (21) for $k_{\max} = 2$ and the above definitions of $\Theta_i^a(2\mathrm{B})$ and $\Theta_{ij}^{ab}(2\mathrm{B})$, that the NO2B contributions to the CCSD amplitude equations do not contain higher–than–quartic terms in T, i.e.,

$$\begin{aligned}\Theta_i^a(2\mathrm{B}) &= \langle \Phi_i^a | [H_{N,2\mathrm{B}}\, (1 + T_1 + T_2 + \tfrac{1}{2} T_1^2 \\ &\quad + T_1 T_2 + \tfrac{1}{6} T_1^3)]_C | \Phi \rangle \qquad (58)\end{aligned}$$

and

$$\begin{aligned}\Theta_{ij}^{ab}(2\mathrm{B}) &= \langle \Phi_{ij}^{ab} | [H_{N,2\mathrm{B}}\, (1 + T_1 + T_2 + \tfrac{1}{2} T_1^2 \\ &\quad + T_1 T_2 + \tfrac{1}{6} T_1^3 + \tfrac{1}{2} T_2^2 + \tfrac{1}{2} T_1^2 T_2 \\ &\quad + \tfrac{1}{24} T_1^4)]_C | \Phi \rangle. \qquad (59)\end{aligned}$$

For the $\Theta_i^a(W_N)$ and $\Theta_{ij}^{ab}(W_N)$ contributions to the CCSD amplitude equations due to the residual three-body interaction term W_N, we can write [63]

$$\begin{aligned}\Theta_i^a(W_N) &= \langle \Phi_i^a | [W_N\, (T_2 + \tfrac{1}{2} T_1^2 + T_1 T_2 + \tfrac{1}{6} T_1^3 \\ &\quad + \tfrac{1}{2} T_2^2 + \tfrac{1}{2} T_1^2 T_2 + \tfrac{1}{24} T_1^4)]_C | \Phi \rangle \qquad (60)\end{aligned}$$

and

$$\begin{aligned}\Theta_{ij}^{ab}(W_N) &= \langle \Phi_{ij}^{ab} | [W_N\, (T_1 + T_2 + \tfrac{1}{2} T_1^2 + T_1 T_2 + \tfrac{1}{6} T_1^3 \\ &\quad + \tfrac{1}{2} T_2^2 + \tfrac{1}{2} T_1^2 T_2 + \tfrac{1}{24} T_1^4 + \tfrac{1}{2} T_1 T_2^2 \\ &\quad + \tfrac{1}{6} T_1^3 T_2 + \tfrac{1}{120} T_1^5)]_C | \Phi \rangle, \qquad (61)\end{aligned}$$

respectively, i.e., the highest power of T that needs to be considered is 5, not 6, as Eq. (21) for the $k_{\max} = 3$ case would imply, since diagrams of the $(W_N T^6)_C$ type entering $\overline{W_N}$ have more than four external lines and, as such, cannot produce non-zero expressions when projected on $|\Phi_i^a\rangle$ and $|\Phi_{ij}^{ab}\rangle$.

The detailed m-scheme-style expressions for the NO2B-type $\Theta_i^a(2\mathrm{B})$ and $\Theta_{ij}^{ab}(2\mathrm{B})$ contributions to the CCSD amplitude equations, in terms of the one- and two-body matrix elements of the normal-ordered Hamiltonian f_q^p and v_{rs}^{pq}, and the singly and doubly excited cluster amplitudes t_i^a and t_{ij}^{ab}, which lead to efficient computer codes through the use of recursively generated intermediates that allow to utilize fast matrix multiplication routines, can be found in Refs. [47, 52, 97, 100]. The analogous m-scheme-type expressions for the $\Theta_i^a(W_N)$ and $\Theta_{ij}^{ab}(W_N)$ contributions to the CCSD equations, in terms of the w_{stu}^{pqr} matrix elements defining W_N and the t_i^a and t_{ij}^{ab} amplitudes can be found in Ref. [63]. In using the CCSD equations presented in Refs. [47, 52, 97, 100], originally derived for two-body Hamiltonians, as expressions for $\Theta_i^a(2\mathrm{B})$ and $\Theta_{ij}^{ab}(2\mathrm{B})$ in the context of the calculations including $3N$ interactions, one only has to use definitions Eqs. (28) and (29) for the matrix elements f_q^p and v_{rs}^{pq} of the normal-ordered Hamiltonian, which contain the effective $\frac{1}{2} \sum_{i,j} h_{qij}^{pij}$ and $\frac{1}{4} \sum_i h_{rsi}^{pqi}$ contributions due to the $3N$ interactions. All of the remaining details are, however, the same. Following our earlier studies [14, 17, 64], in performing the CCSD calculations for the closed-shell nuclei reported in this work, we use an angular-momentum-coupled formulation of CC theory discussed in Ref. [78], which employs reduced matrix elements for all of the operators involved, allowing for a drastic reduction in the numbers of matrix elements and cluster amplitudes entering the computations, and in a substantial reduction in the number of CPU operations, compared to a raw m-scheme description used in earlier nuclear CCSD work [38, 51–58, 61], enabling us to tackle medium-mass nuclei and larger numbers of oscillator shells in the single-particle basis set.

Once the cluster amplitudes t_i^a and t_{ij}^{ab} are determined by solving the non-linear system represented by Eqs. (48) and (49), the CCSD correlation energy $\Delta E^{(\mathrm{CCSD})}$, which is subsequently added to the reference energy E_{ref}, Eq. (31), in order to obtain the total energy $E^{(\mathrm{CCSD})}$, as in Eq. (41), is calculated using Eq. (11), where we replace $\overline{H_N}$ by $\overline{H_N}^{(\mathrm{CCSD})}$. We obtain

$$\Delta E^{(\mathrm{CCSD})} = \Delta E_{2\mathrm{B}}^{(\mathrm{CCSD})} + \Delta E_{3\mathrm{B}}^{(\mathrm{CCSD})}, \qquad (62)$$

where

$$\Delta E_{2\mathrm{B}}^{(\mathrm{CCSD})} = \langle \Phi | \overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})} | \Phi \rangle \qquad (63)$$

and

$$\Delta E_{3\mathrm{B}}^{(\mathrm{CCSD})} = \langle \Phi | \overline{W_N}^{(\mathrm{CCSD})} | \Phi \rangle. \qquad (64)$$

Again, in analogy to the standard two-body Hamiltonians, it is easy to show that the NO2B contribution to the CCSD correlation energy, $\Delta E_{2\mathrm{B}}^{(\mathrm{CCSD})}$, can be calculated using the expression

$$\begin{aligned}\Delta E_{2\mathrm{B}}^{(\mathrm{CCSD})} &= \langle \Phi | [H_{N,2\mathrm{B}}\, (T_1 + T_2 + \tfrac{1}{2} T_1^2)]_C | \Phi \rangle \\ &= f_a^i t_i^a + v_{ab}^{ij} (\tfrac{1}{4} t_{ij}^{ab} + \tfrac{1}{2} t_i^a t_j^b), \qquad (65)\end{aligned}$$

where f_a^i and v_{ab}^{ij} are determined using Eqs. (28) and (29). For the $\Delta E_{3\mathrm{B}}^{(\mathrm{CCSD})}$ component of the CCSD correlation energy due to the residual three-body interaction term W_N, we can write [63]

$$\begin{aligned}\Delta E_{3\mathrm{B}}^{(\mathrm{CCSD})} &= \langle \Phi | [W_N\, (T_1 T_2 + \tfrac{1}{6} T_1^3)]_C | \Phi \rangle \\ &= w_{abc}^{ijk} (\tfrac{1}{4} t_i^a t_{jk}^{bc} + \tfrac{1}{6} t_i^a t_j^b t_k^c). \qquad (66)\end{aligned}$$

As in the case of Eq. (20) and other similar expressions shown in the rest of this section, we have used the Einstein summation convention over the repeated upper and lower indices in the above energy formulas.

We now move to the left-eigenstate or ΛCCSD equations, which one solves after the determination of the T_1 and T_2 clusters and the CCSD energy, and which have to be solved prior to the determination of the ΛCCSD(T) (or CR-CC(2,3)) energy correction $\delta E^{(\mathrm{T})}$, since, as further elaborated on below, the T_1, T_2, Λ_1 and Λ_2 operators enter the $\delta E^{(\mathrm{T})}$ expressions. We examine the ΛCCSD equations in full detail here, since the programmable form of these equations for the case of $3N$ interactions in the Hamiltonian has never been considered before.

The left-eigenstate CCSD equations for the λ_a^i and λ_{ab}^{ij} amplitudes defining Λ_1 and Λ_2 are obtained by replacing the exact Λ and $\overline{H_N}$ operators in Eq. (16) by their truncated CCSD counterparts, $\Lambda^{(\mathrm{CCSD})}$ and $\overline{H_N}^{(\mathrm{CCSD})}$, Eqs. (45) and (50), and by limiting the right-hand projections on the excited determinants $|\Phi_{i_1\ldots i_n}^{a_1\ldots a_n}\rangle$ in Eq. (16) to the singly and doubly excited determinants $|\Phi_i^a\rangle$ and $|\Phi_{ij}^{ab}\rangle$. This leads to the following linear system for the Λ_1 and Λ_2 amplitudes (cf., e.g., Refs. [38, 88, 91, 93–95, 98, 99]):

$$\langle\Phi|(1+\Lambda_1+\Lambda_2)\,(\overline{H_N}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi_i^a\rangle = 0, \tag{67}$$

$$\langle\Phi|(1+\Lambda_1+\Lambda_2)\,(\overline{H_N}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi_{ij}^{ab}\rangle = 0. \tag{68}$$

If we further split the similarity-transformed Hamiltonian of CCSD, $\overline{H_N}^{(\mathrm{CCSD})}$, into the NO2B and W_N contributions $\overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})}$ and $\overline{W_N}^{(\mathrm{CCSD})}$, we can rewrite the ΛCCSD equations (67) and (68) for Hamiltonians including three-body interactions as

$$\Xi_a^i(2\mathrm{B}) + \Xi_a^i(W_N) = 0, \tag{69}$$

$$\Xi_{ab}^{ij}(2\mathrm{B}) + \Xi_{ab}^{ij}(W_N) = 0, \tag{70}$$

where we define the corresponding NO2B and residual $3N$ contributions as

$$\Xi_a^i(2\mathrm{B}) = \langle\Phi|(1+\Lambda_1+\Lambda_2)\,(\overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi_i^a\rangle, \tag{71}$$

$$\Xi_a^i(W_N) = \langle\Phi|(1+\Lambda_1+\Lambda_2)\,(\overline{W_N}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi_i^a\rangle, \tag{72}$$

$$\Xi_{ab}^{ij}(2\mathrm{B}) = \langle\Phi|(1+\Lambda_1+\Lambda_2)\,(\overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi_{ij}^{ab}\rangle, \tag{73}$$

and

$$\Xi_{ab}^{ij}(W_N) = \langle\Phi|(1+\Lambda_1+\Lambda_2)\,(\overline{W_N}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi_{ij}^{ab}\rangle. \tag{74}$$

After identifying the non-vanishing terms in the above formulas and expressing them in terms of the individual n-body components of the $\overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})}$ and $\overline{W_N}^{(\mathrm{CCSD})}$ operators, designated in analogy to Eqs. (36) and (38) by $\overline{H}_{n,2\mathrm{B}}$ and $\overline{W}_n$, we can write

$$\begin{aligned}\Xi_a^i(2\mathrm{B}) \;=\; & \langle\Phi|\{[(1+\Lambda_1)\overline{H}_{1,2\mathrm{B}}]_C + [(\Lambda_1+\Lambda_2)\overline{H}_{2,2\mathrm{B}}]_C \\ & +(\Lambda_2\overline{H}_{3,2\mathrm{B}})_C\}|\Phi_i^a\rangle,\end{aligned} \tag{75}$$

$$\begin{aligned}\Xi_{ab}^{ij}(2\mathrm{B}) \;=\; & \langle\Phi|\{[(1+\Lambda_1+\Lambda_2)\overline{H}_{2,2\mathrm{B}}]_C + (\Lambda_2\overline{H}_{1,2\mathrm{B}})_C \\ & +(\Lambda_1\overline{H}_{1,2\mathrm{B}})_{DC} + (\Lambda_2\overline{H}_{3,2\mathrm{B}})_C\}|\Phi_{ij}^{ab}\rangle,\end{aligned} \tag{76}$$

$$\begin{aligned}\Xi_a^i(W_N) \;=\; & \langle\Phi|\{[(1+\Lambda_1)\overline{W}_1]_C + [(\Lambda_1+\Lambda_2)\overline{W}_2]_C \\ & +(\Lambda_2\overline{W}_3)_C\}|\Phi_i^a\rangle,\end{aligned} \tag{77}$$

and

$$\begin{aligned}\Xi_{ab}^{ij}(W_N) \;=\; & \langle\Phi|\{[(1+\Lambda_1+\Lambda_2)\overline{W}_2]_C + (\Lambda_2\overline{W}_1)_C \\ & +(\Lambda_1\overline{W}_1)_{DC} + [(\Lambda_1+\Lambda_2)\overline{W}_3]_C \\ & +(\Lambda_2\overline{W}_4)_C\}|\Phi_{ij}^{ab}\rangle,\end{aligned} \tag{78}$$

where C continues to represent the connected operator product and DC stands for the disconnected product expression. The detailed m-scheme-style formulas for the $\Xi_a^i(2\mathrm{B})$, $\Xi_{ab}^{ij}(2\mathrm{B})$, $\Xi_a^i(W_N)$, and $\Xi_{ab}^{ij}(W_N)$ contributions to the ΛCCSD system represented by Eqs. (69) and (70), in terms of the individual matrix elements $\overline{h}_{q_1\ldots q_n}^{p_1\ldots p_n}(2\mathrm{B})$ and $\overline{w}_{q_1\ldots q_n}^{p_1\ldots p_n}$ that define the n-body components of $\overline{H_{N,2\mathrm{B}}}^{(\mathrm{CCSD})}$ and $\overline{W_N}^{(\mathrm{CCSD})}$ are given by

$$\begin{aligned}\Xi_a^i(2\mathrm{B}) \;=\; & \overline{h}_a^i(2\mathrm{B}) + \lambda_c^i\,\overline{h}_a^c(2\mathrm{B}) - \lambda_a^k\,\overline{h}_k^i(2\mathrm{B}) + \lambda_c^k\,\overline{h}_{ka}^{ci}(2\mathrm{B}) \\ & +\tfrac{1}{2}\lambda_{cd}^{ik}\,\overline{h}_{ak}^{cd}(2\mathrm{B}) - \tfrac{1}{2}\lambda_{ac}^{kl}\,\overline{h}_{kl}^{ic}(2\mathrm{B}) \\ & +\tfrac{1}{4}\lambda_{cd}^{kl}\,\overline{h}_{kla}^{cdi}(2\mathrm{B}),\end{aligned} \tag{79}$$

$$\begin{aligned}\Xi_{ab}^{ij}(2\mathrm{B}) \;=\; & \overline{h}_{ab}^{ij}(2\mathrm{B}) + \mathscr{A}_{ab}\mathscr{A}^{ij}\lambda_b^j\,\overline{h}_a^i(2\mathrm{B}) \\ & +\mathscr{A}^{ij}\lambda_c^i\,\overline{h}_{ab}^{cj}(2\mathrm{B}) - \mathscr{A}_{ab}\lambda_a^k\,\overline{h}_{kb}^{ij}(2\mathrm{B}) \\ & +\mathscr{A}_{ab}\lambda_{ac}^{ij}\,\overline{h}_b^c(2\mathrm{B}) - \mathscr{A}^{ij}\lambda_{ab}^{ik}\,\overline{h}_k^j(2\mathrm{B}) \\ & +\mathscr{A}_{ab}\mathscr{A}^{ij}\lambda_{ac}^{ik}\,\overline{h}_{kb}^{cj}(2\mathrm{B}) + \tfrac{1}{2}\lambda_{cd}^{ij}\,\overline{h}_{ab}^{cd}(2\mathrm{B}) \\ & +\tfrac{1}{2}\lambda_{ab}^{kl}\,\overline{h}_{kl}^{ij}(2\mathrm{B}) + \tfrac{1}{2}\mathscr{A}_{ab}\lambda_{ca}^{kl}\,\overline{h}_{kbl}^{ijc}(2\mathrm{B}) \\ & +\tfrac{1}{2}\mathscr{A}^{ij}\lambda_{cd}^{ki}\,\overline{h}_{abk}^{cjd}(2\mathrm{B}),\end{aligned} \tag{80}$$

$$\begin{aligned}\Xi_a^i(W_N) \;=\; & \overline{w}_a^i + \lambda_c^i\,\overline{w}_a^c - \lambda_a^k\,\overline{w}_k^i + \lambda_c^k\,\overline{w}_{ka}^{ci} \\ & +\tfrac{1}{2}\lambda_{cd}^{ik}\,\overline{w}_{ak}^{cd} - \tfrac{1}{2}\lambda_{ac}^{kl}\,\overline{w}_{kl}^{ic} + \tfrac{1}{4}\lambda_{cd}^{kl}\,\overline{w}_{kla}^{cdi},\end{aligned} \tag{81}$$

and

$$\begin{aligned}\Xi_{ab}^{ij}(W_N) \;=\; & \overline{w}_{ab}^{ij} + \mathscr{A}_{ab}\mathscr{A}^{ij}\lambda_b^j\,\overline{w}_a^i + \mathscr{A}^{ij}\lambda_c^i\,\overline{w}_{ab}^{cj} - \mathscr{A}_{ab}\lambda_a^k\,\overline{w}_{kb}^{ij} \\ & +\lambda_c^k\,\overline{w}_{abk}^{ijc} + \mathscr{A}_{ab}\lambda_{ac}^{ij}\,\overline{w}_b^c - \mathscr{A}^{ij}\lambda_{ab}^{ik}\,\overline{w}_k^j \\ & +\mathscr{A}_{ab}\mathscr{A}^{ij}\lambda_{ac}^{ik}\,\overline{w}_{kb}^{cj} + \tfrac{1}{2}\lambda_{cd}^{ij}\,\overline{w}_{ab}^{cd} + \tfrac{1}{2}\lambda_{ab}^{kl}\,\overline{w}_{kl}^{ij} \\ & +\tfrac{1}{2}\mathscr{A}_{ab}\lambda_{ca}^{kl}\,\overline{w}_{kbl}^{ijc} + \tfrac{1}{2}\mathscr{A}^{ij}\lambda_{cd}^{ki}\,\overline{w}_{abk}^{cjd} \\ & +\tfrac{1}{4}\lambda_{cd}^{kl}\overline{w}_{abkl}^{ijcd},\end{aligned} \tag{82}$$

respectively, where

$$\mathscr{A}_{pq} \equiv \mathscr{A}^{pq} = 1 - (pq), \tag{83}$$

with (pq) representing a transposition of p and q, are the usual index antisymmetrizers.

As one can see, the ΛCCSD equations for three-body Hamiltonians, although more complicated than for the case of pairwise interactions, where one would not consider Eqs. (81) and (82), have a relatively simple algebraic structure. In particular, the highest-rank many-body components of the $\overline{H_{N,\mathrm{2B}}}^{\mathrm{(CCSD)}}$ and $\overline{W_N}^{\mathrm{(CCSD)}}$ operators that enter these equations are given by selected types of three-body $\overline{H}_{3,\mathrm{2B}}$ terms and selected types of four-body $\overline{W}_4$ terms. Although, according to the remarks below Eqs. (36)–(39), the $\overline{H_{N,\mathrm{2B}}}^{\mathrm{(CCSD)}}$ and $\overline{W_N}^{\mathrm{(CCSD)}}$ operators contain various higher–than–four-body terms, the right-hand projections on the singly and doubly excited determinants in Eqs. (67) and (68) or (71)–(74) eliminate such complicated expressions. This greatly simplifies the computer implementation effort. Again, in performing the left-eigenstate CCSD calculations for the closed-shell nuclei reported in this work, following the recipe presented in Ref. [78], we convert the m-scheme expressions for the $\Xi^i_a(\mathrm{2B})$, $\Xi^{ij}_{ab}(\mathrm{2B})$, $\Xi^i_a(W_N)$, and $\Xi^{ij}_{ab}(W_N)$ contributions into their angular-momentum-coupled representation. The key quantities for setting up the underlying Eqs. (79)–(82) are the matrix elements $\overline{h}^{q_1\ldots q_n}_{p_1\ldots p_n}(\mathrm{2B})$ and $\overline{w}^{q_1\ldots q_n}_{p_1\ldots p_n}$ of the similarity-transformed $\overline{H_{N,\mathrm{2B}}}^{\mathrm{(CCSD)}}$ and $\overline{W_N}^{\mathrm{(CCSD)}}$ operators. Before discussing the sources of information about the matrix elements of $\overline{H_{N,\mathrm{2B}}}^{\mathrm{(CCSD)}}$ and $\overline{W_N}^{\mathrm{(CCSD)}}$ that enter Eqs. (79)–(82), let us comment on the physical and mathematical content of these equations, including important additional simplifications in the NO2B contributions $\Xi^i_a(\mathrm{2B})$ and $\Xi^{ij}_{ab}(\mathrm{2B})$ that reduce the usage of higher–than–two-body objects in the equations for the λ^i_a and λ^{ij}_{ab} amplitudes even further.

First, we note that the NO2B and residual $3N$ components of the ΛCCSD equations projected on the singly excited $|\Phi^a_i\rangle$ determinants, $\Xi^i_a(\mathrm{2B})$ and $\Xi^i_a(W_N)$, have the identical general form, i.e., they only differ by the details of the Hamiltonian matrix elements that enter them, but not by their overall algebraic structure (cf. Eqs. (75) or (79) and (77) or (81)). However, in the NO2B case, the contribution

$$\langle\Phi|(\Lambda_2\overline{H}_{3,\mathrm{2B}})_C|\Phi^a_i\rangle = \tfrac{1}{4}\lambda^{kl}_{cd}\,\overline{h}^{cdi}_{kla}(\mathrm{2B}), \tag{84}$$

which contains selected three-body components of $\overline{H_{N,\mathrm{2B}}}^{\mathrm{(CCSD)}}$ and which enters Eqs. (75) and (79) for $\Xi^i_a(\mathrm{2B})$, can be refactorized and rewritten in terms of simpler one- and two-body objects, eliminating the need for the explicit use of the three-body $\overline{H}_{3,\mathrm{2B}}$ terms altogether. Indeed, following the quantum-chemistry literature where interactions in the Hamiltonian are always two-body, we can replace Eq. (84) by (cf., e.g., Ref. [97])

$$\tfrac{1}{4}\lambda^{kl}_{cd}\,\overline{h}^{cdi}_{kla}(\mathrm{2B}) = -\overline{h}^{ie}_{ad}(\mathrm{2B})\,\chi^d_e - \overline{h}^{im}_{an}(\mathrm{2B})\,\chi^n_m, \tag{85}$$

where the additional one-body intermediates χ^d_e and χ^n_m are defined as

$$\chi^d_e = -\tfrac{1}{2}t^{df}_{mn}\lambda^{mn}_{ef} \tag{86}$$

and

$$\chi^l_m = \tfrac{1}{2}t^{ef}_{mn}\lambda^{ln}_{ef}, \tag{87}$$

respectively. In other words, all we need to know to construct the NO2B contribution $\Xi^i_a(\mathrm{2B})$ to the ΛCCSD equations are the matrix elements $\overline{h}^p_q(\mathrm{2B})$ and $\overline{h}^{pq}_{rs}(\mathrm{2B})$ of the similarity-transformed Hamiltonian $\overline{H_{N,\mathrm{2B}}}^{\mathrm{(CCSD)}}$, which appear in Eqs. (79) and (85), and the cluster amplitudes t^a_i and t^{ab}_{ij}, plus two auxiliary one-body intermediates, obtained by contracting the t^{ab}_{ij} and λ^{ij}_{ab} amplitudes, defined by Eqs. (86) and (87). The relevant, computationally efficient, expressions for the one- and two-body matrix elements $\overline{h}^p_q(\mathrm{2B})$ and $\overline{h}^{pq}_{rs}(\mathrm{2B})$ can be found in several sources, for example in Refs. [82, 100, 101], remembering to rely on Eqs. (28) and (29) in the determination of f^p_q and v^{pq}_{rs}. Unfortunately, we cannot provide any additional simplifications in the case of the W_N analog of Eq. (84), entering Eqs. (77) and (81),

$$\langle\Phi|(\Lambda_2\overline{W}_3)_C|\Phi^a_i\rangle = \tfrac{1}{4}\lambda^{kl}_{cd}\,\overline{w}^{cdi}_{kla}, \tag{88}$$

where we have to rely on the intrinsically three-body matrix elements of W_N that do not factorize into simpler, lower-rank objects. In this case, in order to construct the residual $3N$ contribution $\Xi^i_a(W_N)$ to the ΛCCSD equations projected on $|\Phi^a_i\rangle$, given by Eq. (81), we must utilize the explicit formulas for the one-, two-, and three-body matrix elements of the similarity-transformed $\overline{W_N}^{\mathrm{(CCSD)}}$ operator in terms of the appropriate matrix elements w^{pqr}_{stu} of W_N and the CCSD amplitudes t^a_i and t^{ab}_{ij} that are listed in Figs. 1 and 2.

Similar, albeit not identical, remarks apply to the ΛCCSD equations projected on the doubly excited determinants $|\Phi^{ab}_{ij}\rangle$. Once again, we can refactorize the NO2B contribution

$$\begin{aligned}\langle\Phi|(\Lambda_2\overline{H}_{3,\mathrm{2B}})_C|\Phi^{ab}_{ij}\rangle \;=\; & \tfrac{1}{2}\mathscr{A}_{ab}\lambda^{kl}_{ca}\,\overline{h}^{ijc}_{kbl}(\mathrm{2B}) \\ & +\tfrac{1}{2}\mathscr{A}^{ij}\lambda^{ki}_{cd}\,\overline{h}^{cjd}_{abk}(\mathrm{2B}),\end{aligned} \tag{89}$$

entering Eqs. (76) and (80), which contains selected three-body components of $\overline{H_{N,\mathrm{2B}}}^{\mathrm{(CCSD)}}$, by rewriting it in terms of simpler one- and two-body objects as

$$\begin{aligned}\tfrac{1}{2}\mathscr{A}_{ab}\lambda^{kl}_{ca}\,\overline{h}^{ijc}_{kbl}(\mathrm{2B}) \;+\; & \tfrac{1}{2}\mathscr{A}^{ij}\lambda^{ki}_{cd}\,\overline{h}^{cjd}_{abk}(\mathrm{2B}) \\ =\; & \mathscr{A}_{ab}\overline{h}^{ij}_{ad}(\mathrm{2B})\,\chi^d_b - \mathscr{A}^{ij}\overline{h}^{im}_{ab}(\mathrm{2B})\,\chi^j_m \\ =\; & \mathscr{A}_{ab}v^{ij}_{ad}\chi^d_b - \mathscr{A}^{ij}v^{im}_{ab}\chi^j_m,\end{aligned} \tag{90}$$

using the identity $\overline{h}^{kl}_{cd}(\mathrm{2B}) = v^{kl}_{cd}$ and where χ^d_b and χ^j_m are again given by Eqs. (86) and (87), but we cannot do anything similar for the case of the analogous

$$\langle\Phi|(\Lambda_2\overline{W}_3)_C|\Phi^{ab}_{ij}\rangle = \tfrac{1}{2}\mathscr{A}_{ab}\lambda^{kl}_{ca}\,\overline{w}^{ijc}_{kbl} + \tfrac{1}{2}\mathscr{A}^{ij}\lambda^{ki}_{cd}\,\overline{w}^{cjd}_{abk} \tag{91}$$

expression that appears in Eqs. (78) and (82), where we have to rely on the three-body matrix elements of W_N. As a result, in analogy to the previously examined $\Xi^i_a(\mathrm{2B})$ term, all we need to know to construct the NO2B contribution $\Xi^{ij}_{ab}(\mathrm{2B})$ to the ΛCCSD equations are the matrix elements $\overline{h}^p_q(\mathrm{2B})$ and $\overline{h}^{pq}_{rs}(\mathrm{2B})$ of $\overline{H_{N,\mathrm{2B}}}^{\mathrm{(CCSD)}}$, plus two auxiliary one-body intermediates defined by Eqs. (86) and (87), but one needs additional expressions for the various matrix elements of $\overline{W_N}^{\mathrm{(CCSD)}}$ to construct $\Xi^{ij}_{ab}(W_N)$, Eq. (82). In fact, the situation with the residual W_N contributions to the ΛCCSD equations projected on $|\Phi^{ab}_{ij}\rangle$ is further complicated by the observation that along with the various terms that are analogous to the NO2B case, we also end up with the additional

$$\langle\Phi|(\Lambda_1\overline{W}_3)_C|\Phi^{ab}_{ij}\rangle = \lambda^k_c\,\overline{w}^{ijc}_{abk} \tag{92}$$

and

$$\langle\Phi|(\Lambda_2\overline{W}_4)_C|\Phi^{ab}_{ij}\rangle = \tfrac{1}{4}\lambda^{kl}_{cd}\overline{w}^{ijcd}_{abkl} \tag{93}$$

contributions to $\Xi^{ij}_{ab}(W_N)$, which contain selected three- and four-body components of $\overline{W_N}^{\text{(CCSD)}}$ and which do not have their NO2B equivalents in $\Xi^{ij}_{ab}(2\text{B})$ (cf. Eqs. (76) or (80) and (78) or (82)), since one cannot form such terms from the two-body Hamiltonians. The complete set of expressions for the one-, two-, three-, and four-body matrix elements of $\overline{W_N}^{\text{(CCSD)}}$, in terms of the pertinent w^{pqr}_{stu} matrix elements of W_N and the CCSD amplitudes t^a_i and t^{ab}_{ij} is given in Figs. 1 and 2.

2. *The ΛCCSD(T) correction for three-body Hamiltonians*

We end the present section by deriving the expressions that are used in this work to determine the non-iterative correction $\delta E^{\text{(T)}}$ to the CCSD energy capable of capturing the dominant T_3 effects in the presence of the three-body interactions in the Hamiltonian. As pointed out above, the triples correction $\delta E^{\text{(T)}}$ developed in this work is an extension to $3N$ interactions of the ΛCCSD(T) approach, formulated for two-body Hamiltonians in Refs. [75, 76]. We begin, however, with the more general CR-CC(2,3) methodology, originally introduced in Refs. [79, 80] and examined in the nuclear context in Refs. [38, 61], which contains all kinds of the non-iterative triples corrections to CCSD, including ΛCCSD(T), as approximations. The CR-CC(2,3) expressions provide us with a transparent mechanism for identifying the additional terms in the ΛCCSD(T)-type equations that originate from the explicit inclusion of the $3N$ interactions in the Hamiltonian.

In general, the CR-CC(2,3), CR-CC(2,4), and other approaches in the so-called CR-CC(m,m') hierarchy [79–82, 88], and various closely related approximations, including CCSD[T] [102, 103], CCSD(T) [65], CCSD(TQ$_\text{f}$) [104], ΛCCSD(T) [75, 76], ΛCCSD(TQ$_\text{f}$) [105], CCSD(2)$_\text{T}$ [71–74], CCSD(2) [71–74], CR-CCSD(T) [66–70], CR-CCSD(TQ) [66–70], CR-CC(2,3)+Q [106], LR-CCSD(T) [107], and LR-CCSD(TQ) [107], are based on the idea of adding *a posteriori*, non-iterative corrections due to the higher-order cluster components, such as T_3 or T_3 and T_4, to the energies resulting from the CCSD (or some other lower-level CC) calculations. One of the most convenient approaches for deriving these corrections is by examining the CC energy functional, which is defined as (see, e.g., Refs. [96, 98, 108–112] and Eqs. (1) and (12); cf., also, Refs. [88, 91, 94, 99, 113] for reviews)

$$\Delta E = \langle\tilde{\Psi}|H_N|\Psi\rangle = \langle\Phi|(1+\Lambda)\overline{H_N}|\Phi\rangle, \tag{94}$$

$$\begin{aligned}
\overline{w}^{i}_{a} &= \tfrac{1}{4}w^{ikl}_{acd}t^{cd}_{kl} + \tfrac{1}{2}w^{ikl}_{acd}t^{c}_{k}t^{d}_{l}\\
\overline{w}^{a}_{b} &= \tfrac{1}{4}w^{akl}_{bcd}t^{cd}_{kl} - \tfrac{1}{4}w^{klm}_{bcd}t^{cd}_{kl}t^{a}_{m} + \tfrac{1}{2}w^{klm}_{bcd}t^{c}_{k}t^{ad}_{lm} + \tfrac{1}{2}w^{akl}_{bcd}t^{c}_{k}t^{d}_{l}\\
&\quad -\tfrac{1}{2}w^{klm}_{bcd}t^{c}_{k}t^{d}_{l}t^{a}_{m}\\
\overline{w}^{i}_{j} &= \tfrac{1}{4}w^{ikl}_{cdj}t^{cd}_{kl} + \tfrac{1}{4}w^{ikl}_{cde}t^{cd}_{kl}t^{e}_{j} - \tfrac{1}{2}w^{ikl}_{cde}t^{cd}_{kj}t^{e}_{l} + \tfrac{1}{2}w^{ikl}_{cdj}t^{c}_{k}t^{d}_{l}\\
&\quad +\tfrac{1}{2}w^{ikl}_{cde}t^{c}_{k}t^{d}_{l}t^{e}_{j}\\
\overline{w}^{ij}_{ab} &= w^{ijk}_{abc}t^{c}_{k}\\
\overline{w}^{ai}_{bc} &= \tfrac{1}{2}w^{ikl}_{bcd}t^{ad}_{kl} + w^{ail}_{bcd}t^{d}_{l} + w^{ikl}_{bcd}t^{a}_{k}t^{d}_{l}\\
\overline{w}^{ik}_{ja} &= -\tfrac{1}{2}w^{ikl}_{acd}t^{cd}_{jl} + w^{ikl}_{jac}t^{c}_{l} - w^{ikl}_{acd}t^{c}_{j}t^{d}_{l}\\
\overline{w}^{ab}_{cd} &= -\tfrac{1}{2}\mathscr{A}^{ab}w^{akl}_{cde}t^{be}_{kl} + w^{abk}_{cde}t^{e}_{k} + \tfrac{1}{2}w^{klm}_{cde}t^{ab}_{lm}t^{e}_{k} + \tfrac{1}{2}\mathscr{A}^{ab}w^{klm}_{cde}t^{a}_{k}t^{be}_{lm}\\
&\quad -w^{bkl}_{cde}t^{a}_{k}t^{e}_{l} + w^{klm}_{cde}t^{a}_{l}t^{b}_{m}t^{e}_{k}\\
\overline{w}^{ij}_{kl} &= -\tfrac{1}{2}\mathscr{A}_{kl}w^{ijm}_{kcd}t^{cd}_{ml} + w^{ijm}_{klc}t^{c}_{m} + \tfrac{1}{2}w^{ijm}_{cde}t^{de}_{kl}t^{c}_{m} + \tfrac{1}{2}\mathscr{A}_{kl}w^{ijm}_{cde}t^{cd}_{lm}t^{e}_{k}\\
&\quad +w^{ijm}_{cdl}t^{c}_{k}t^{d}_{m} + w^{ijm}_{cde}t^{d}_{k}t^{e}_{l}t^{c}_{m}\\
\overline{w}^{aj}_{ib} &= -\tfrac{1}{2}w^{ajk}_{bcd}t^{cd}_{ik} + \tfrac{1}{2}w^{jkl}_{bci}t^{ac}_{kl} + w^{ajk}_{bci}t^{c}_{k} - \tfrac{1}{2}w^{jkl}_{bcd}t^{cd}_{il}t^{a}_{k} - \tfrac{1}{2}w^{jkl}_{bcd}t^{ad}_{kl}t^{c}_{i}\\
&\quad +w^{jkl}_{bcd}t^{ac}_{ik}t^{d}_{l} + w^{ajk}_{bcd}t^{c}_{k}t^{d}_{i} - w^{jkl}_{bci}t^{c}_{k}t^{a}_{l} - w^{jkl}_{bcd}t^{a}_{l}t^{c}_{k}t^{d}_{i}\\
\overline{w}^{ab}_{ci} &= -w^{abk}_{cdi}t^{d}_{k} + \tfrac{1}{2}\mathscr{A}^{ab}w^{akl}_{cde}t^{de}_{ik}t^{b}_{l} + \tfrac{1}{2}\mathscr{A}^{ab}w^{akl}_{cde}t^{bd}_{kl}t^{e}_{i} + \mathscr{A}^{ab}w^{akl}_{cde}t^{be}_{il}t^{d}_{k}\\
&\quad -\tfrac{1}{2}w^{klm}_{cdi}t^{ab}_{lm}t^{d}_{k} - \tfrac{1}{2}\mathscr{A}^{ab}w^{klm}_{cdi}t^{bd}_{kl}t^{a}_{m} - w^{abk}_{cde}t^{d}_{k}t^{e}_{i} + \mathscr{A}^{ab}w^{bkl}_{cdi}t^{d}_{k}t^{a}_{l}\\
&\quad +\tfrac{1}{2}w^{klm}_{cde}t^{ab}_{im}t^{d}_{k}t^{e}_{l} - \mathscr{A}^{ab}w^{klm}_{cde}t^{be}_{il}t^{d}_{k}t^{a}_{m} + \tfrac{1}{2}w^{klm}_{cde}t^{de}_{il}t^{b}_{k}t^{a}_{m}\\
&\quad -\tfrac{1}{2}\mathscr{A}^{ab}w^{klm}_{cde}t^{ae}_{lm}t^{b}_{k}t^{d}_{i} - \tfrac{1}{2}w^{klm}_{cde}t^{ab}_{lm}t^{d}_{k}t^{e}_{i} - \mathscr{A}^{ab}w^{akl}_{cde}t^{d}_{k}t^{b}_{l}t^{e}_{i}\\
&\quad +w^{klm}_{cdi}t^{a}_{m}t^{b}_{l}t^{d}_{k} + w^{klm}_{cde}t^{a}_{m}t^{b}_{l}t^{d}_{k}t^{e}_{i} - \tfrac{1}{4}w^{klm}_{cde}t^{ab}_{ki}t^{de}_{lm} + \tfrac{1}{4}w^{klm}_{cde}t^{ab}_{kl}t^{de}_{im}\\
&\quad -\tfrac{1}{2}\mathscr{A}^{ab}w^{klm}_{cde}t^{ad}_{kl}t^{eb}_{mi}\\
\overline{w}^{ia}_{jk} &= w^{ial}_{jkc}t^{c}_{l} + \tfrac{1}{2}\mathscr{A}_{jk}w^{ilm}_{jcd}t^{ac}_{lm}t^{d}_{k} + \tfrac{1}{2}\mathscr{A}_{jk}w^{ilm}_{jcd}t^{cd}_{kl}t^{a}_{m} + \mathscr{A}_{jk}w^{ilm}_{jcd}t^{ad}_{km}t^{c}_{l}\\
&\quad -\tfrac{1}{2}w^{ail}_{cde}t^{de}_{jk}t^{c}_{l} + \tfrac{1}{2}\mathscr{A}_{jk}w^{ail}_{cde}t^{cd}_{lk}t^{e}_{j} - w^{ilm}_{jck}t^{c}_{l}t^{a}_{m} - \mathscr{A}_{jk}w^{ail}_{cdk}t^{c}_{l}t^{d}_{j}\\
&\quad +\tfrac{1}{2}w^{ilm}_{cde}t^{ae}_{kj}t^{c}_{l}t^{d}_{m} + \mathscr{A}_{jk}w^{ilm}_{cde}t^{ad}_{km}t^{c}_{l}t^{e}_{j} - w^{ilm}_{cde}t^{ad}_{lm}t^{c}_{k}t^{e}_{j}\\
&\quad -\tfrac{1}{2}\mathscr{A}_{jk}w^{ilm}_{cde}t^{de}_{mj}t^{c}_{k}t^{a}_{l} + \mathscr{A}_{jk}w^{ilm}_{cde}t^{ae}_{jm}t^{c}_{l}t^{d}_{k} - \mathscr{A}_{jk}w^{ilm}_{jcd}t^{a}_{m}t^{c}_{l}t^{d}_{k}\\
&\quad +w^{ail}_{cde}t^{c}_{l}t^{d}_{k}t^{e}_{j} - w^{ilm}_{cde}t^{a}_{m}t^{c}_{l}t^{d}_{k}t^{e}_{j} + \tfrac{1}{4}w^{ilm}_{cde}t^{ca}_{jk}t^{de}_{lm} - \tfrac{1}{4}w^{ilm}_{cde}t^{cd}_{jk}t^{ae}_{lm}\\
&\quad +\tfrac{1}{2}\mathscr{A}_{jk}w^{ilm}_{cde}t^{cd}_{jl}t^{ea}_{mk}
\end{aligned}$$

FIG. 1: Explicit expressions for the one- and two-body matrix elements of the similarity-transformed form of the the residual three-body interaction term W_N, designated by $\overline{W_N}^{\text{(CCSD)}}$ and defined by Eq. (56), which are needed to construct the $\Xi^{i}_{a}(W_N)$ and $\Xi^{ij}_{ab}(W_N)$ contributions to the ΛCCSD equations, Eqs. (81) and (82), respectively.

or, more precisely, its asymmetric analog, which in the case of correcting the CCSD energy can be written as [79, 80, 88]

$$\Delta E = \langle\Phi|\mathscr{L}\,\overline{H_N}^{\text{(CCSD)}}|\Phi\rangle, \tag{95}$$

where $\overline{H_N}^{\text{(CCSD)}}$ is the similarity-transformed Hamiltonian of CCSD, Eq. (50). The usefulness of the above expression in the context of correcting the CCSD results for the effects of higher–than–doubly excited clusters stems from the fact that Eq. (95) is equivalent to the exact (i.e., full CI) correlation energy when $\langle\Phi|\mathscr{L}$ represents the lowest-energy left eigenstate of $\overline{H_N}^{\text{(CCSD)}}$ obtained by diagonalizing the latter operator in the entire A-particle Hilbert space. Indeed, when the hole-particle deexcitation operator $\mathscr{L}$ entering Eq. (95) originates from parametrizing the full CI bra state through the

$$\begin{aligned}
\overline{w}^{ija}_{kbl} &= w^{ija}_{kbl} + \mathscr{A}_{kl} w^{ijm}_{kbc} t^{ac}_{lm} + \tfrac{1}{2} w^{ija}_{cbd} t^{cd}_{kl} - \mathscr{A}_{kl} w^{ija}_{bcl} t^{c}_{k} + w^{ijm}_{bkl} t^{a}_{m} \\
&\quad - w^{ijm}_{bcd} t^{ad}_{kl} t^{c}_{m} - \mathscr{A}_{kl} w^{ijm}_{bcd} t^{ad}_{lm} t^{c}_{k} + \tfrac{1}{2} w^{ijm}_{bcd} t^{cd}_{kl} t^{a}_{m} \\
&\quad + \mathscr{A}_{kl} w^{ijm}_{bcl} t^{c}_{k} t^{a}_{m} + w^{ija}_{cbd} t^{c}_{k} t^{d}_{l} + w^{ijm}_{bcd} t^{c}_{k} t^{d}_{l} t^{a}_{m} \\
\overline{w}^{ajb}_{cdi} &= w^{ajb}_{cdi} + \mathscr{A}^{ab} w^{ajk}_{cde} t^{be}_{ik} + \tfrac{1}{2} w^{kjl}_{cdi} t^{ab}_{kl} - \mathscr{A}^{ab} w^{bkj}_{cdi} t^{a}_{k} \\
&\quad - w^{abj}_{cde} t^{e}_{i} + w^{jkl}_{cde} t^{ab}_{il} t^{e}_{k} + \mathscr{A}^{ab} w^{jkl}_{cde} t^{be}_{il} t^{a}_{k} - \tfrac{1}{2} w^{jkl}_{cde} t^{ab}_{kl} t^{e}_{i} \\
&\quad - \mathscr{A}^{ab} w^{ajk}_{cde} t^{b}_{k} t^{e}_{i} + w^{kjl}_{cdi} t^{a}_{k} t^{b}_{l} - w^{jkl}_{cde} t^{a}_{k} t^{b}_{l} t^{e}_{i} \\
\overline{w}^{abk}_{ijc} &= w^{abk}_{ijc} + \tfrac{1}{2} w^{abk}_{cde} t^{de}_{ij} + \mathscr{A}^{ab} \mathscr{A}_{ij} w^{bkl}_{jcd} t^{ad}_{il} + \tfrac{1}{2} w^{klm}_{ijc} t^{ab}_{lm} \\
&\quad - \tfrac{1}{2} \mathscr{A}^{ab} w^{klm}_{cde} t^{ad}_{ij} t^{be}_{lm} + \tfrac{1}{2} \mathscr{A}^{ab} \mathscr{A}_{ij} w^{klm}_{cde} t^{ad}_{il} t^{be}_{jm} + \tfrac{1}{4} w^{klm}_{cde} t^{ab}_{lm} t^{de}_{ij} \\
&\quad - \tfrac{1}{2} \mathscr{A}_{ij} w^{klm}_{cde} t^{ab}_{il} t^{de}_{jm} + \mathscr{A}_{ij} w^{abk}_{cdj} t^{d}_{i} - \mathscr{A}^{ab} w^{klb}_{ijc} t^{a}_{l} - \tfrac{1}{2} \mathscr{A}^{ab} w^{klb}_{cde} t^{de}_{ij} t^{a}_{l} \\
&\quad - \mathscr{A}^{ab} \mathscr{A}_{ij} w^{akl}_{cde} t^{be}_{jl} t^{d}_{i} + \tfrac{1}{2} \mathscr{A}_{ij} w^{klm}_{cdj} t^{ab}_{lm} t^{d}_{i} + \mathscr{A}^{ab} \mathscr{A}_{ij} w^{klm}_{cdi} t^{bd}_{jm} t^{a}_{l} \\
&\quad - \mathscr{A}^{ab} w^{akl}_{cde} t^{be}_{ij} t^{d}_{l} + \mathscr{A}_{ij} w^{klm}_{cdi} t^{ab}_{jm} t^{d}_{l} + w^{abk}_{cde} t^{d}_{i} t^{e}_{j} - \mathscr{A}^{ab} \mathscr{A}_{ij} w^{bkl}_{cdj} t^{a}_{l} t^{d}_{i} \\
&\quad + w^{klm}_{ijc} t^{a}_{l} t^{b}_{m} + \tfrac{1}{2} w^{klm}_{cde} t^{de}_{ij} t^{a}_{l} t^{b}_{m} - \mathscr{A}^{ab} \mathscr{A}_{ij} w^{klm}_{cde} t^{be}_{jm} t^{a}_{l} t^{d}_{i} + \tfrac{1}{2} w^{klm}_{cde} t^{ab}_{lm} t^{d}_{i} t^{e}_{j} \\
&\quad - \mathscr{A}^{ab} w^{klm}_{cde} t^{eb}_{ij} t^{a}_{m} t^{d}_{l} - \mathscr{A}_{ij} w^{klm}_{cde} t^{ab}_{mj} t^{d}_{l} t^{e}_{i} - \mathscr{A}^{ab} w^{bkl}_{cde} t^{a}_{l} t^{d}_{i} t^{e}_{j} \\
&\quad + \mathscr{A}_{ij} w^{klm}_{cdj} t^{a}_{l} t^{b}_{m} t^{d}_{i} + w^{klm}_{cde} t^{a}_{l} t^{b}_{m} t^{d}_{i} t^{e}_{j} \\
\overline{w}^{ijc}_{abk} &= w^{ijc}_{abk} + w^{ijc}_{abd} t^{d}_{k} - w^{ijl}_{abk} t^{c}_{l} - w^{ijl}_{abd} t^{c}_{l} t^{d}_{k} + w^{ijl}_{abd} t^{cd}_{kl} \\
\overline{w}^{ijcd}_{abkl} &= \mathscr{A}^{cd} w^{ijc}_{abe} t^{ed}_{kl} - \mathscr{A}_{kl} w^{ijm}_{abk} t^{cd}_{ml} - \mathscr{A}^{cd} w^{ijm}_{abe} t^{ed}_{kl} t^{c}_{m} - \mathscr{A}_{kl} w^{ijm}_{abe} t^{cd}_{ml} t^{e}_{k}
\end{aligned}$$

FIG. 2: Explicit expressions for the selected three- and four-body matrix elements of the similarity-transformed form of the the residual three-body interaction term W_N, designated by $\overline{W_N}^{(\mathrm{CCSD})}$ and defined by Eq. (56), which are needed to construct the $\Xi^{i}_{a}(W_N)$ and $\Xi^{ij}_{ab}(W_N)$ contributions to the ΛCCSD equations, Eqs. (81) and (82), respectively.

ansatz $\langle\Psi| \sim \langle\Phi|\mathscr{L} e^{-T^{(\mathrm{CCSD})}}$, where we assume the normalization condition $\langle\Phi|\mathscr{L}|\Phi\rangle = 1$, the asymmetric energy expression given by Eq. (95) produces the exact correlation energy. At the same time, since the matrix elements $\langle\Phi^{a}_{i}|\overline{H_N}^{(\mathrm{CCSD})}|\Phi\rangle$ and $\langle\Phi^{ab}_{ij}|\overline{H_N}^{(\mathrm{CCSD})}|\Phi\rangle$ vanish in the CCSD case as required by Eqs. (48) and (49), it is easy to demonstrate that the lowest-energy eigenvalue of $\overline{H_N}^{(\mathrm{CCSD})}$ in the subspace of the Hilbert space spanned by the reference determinant $|\Phi\rangle$ and the singly and doubly excited determinants $|\Phi^{a}_{i}\rangle$ and $|\Phi^{ab}_{ij}\rangle$ is the CCSD correlation energy $\Delta E^{(\mathrm{CCSD})}$. Thus, as shown for example in Refs. [71–73, 79, 80] (cf. Ref. [88] for a review), we can formally split the exact correlation energy ΔE into the CCSD part $\Delta E^{(\mathrm{CCSD})}$ and the non-iterative correction δE that describes all of the remaining correlations missing in CCSD by inserting the resolution of the identity in the A-particle Hilbert space, written as

$$|\Phi\rangle\langle\Phi| + P + Q = 1, \tag{96}$$

where

$$P = P_1 + P_2, \tag{97}$$

$$Q = P_3 + \cdots + P_A, \tag{98}$$

and

$$P_n = \sum_{\substack{i_1<\cdots<i_n \\ a_1<\cdots<a_n}} |\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}\rangle\langle\Phi^{a_1\ldots a_n}_{i_1\ldots i_n}|, \tag{99}$$

into Eq. (95), and perform some additional manipulations, that lead to

$$\Delta E = \Delta E^{(\mathrm{CCSD})} + \langle\Phi|\mathscr{L} Q\, \overline{H_N}^{(\mathrm{CCSD})}|\Phi\rangle. \tag{100}$$

The resulting biorthogonal moment expansions of δE, which result in the aforementioned CR-CC(m,m') hierarchy [79–82, 88], or the perturbative expansions of δE employing Löwdin's partitioning technique [114], as in Refs. [71–76] (cf., also, Ref. [115]), which lead to methods such as ΛCCSD(T), ΛCCSD(TQ$_\mathrm{f}$) or CCSD(2), provide us with the desired mathematical expressions for the non-iterative corrections due to T_3, T_4, and other higher-order clusters.

In particular, the leading post-CCSD term in the difference δE between the exact and CCSD energies, which emerges from the above considerations and which captures the correlation effects due to the connected T_3 clusters can be represented by the following generic form [79, 80, 88]

$$\delta E^{(\mathrm{T})} = \langle\Phi|\mathscr{L}_3\, \overline{H_N}^{(\mathrm{CCSD})}|\Phi\rangle = \tfrac{1}{36}\, \ell^{ijk}_{abc}\, \mathfrak{M}^{abc}_{ijk}, \tag{101}$$

where

$$\mathscr{L}_3 = \frac{1}{36} \sum_{i,j,k,a,b,c} \ell^{ijk}_{abc}\, a^{\dagger}_{a} a^{\dagger}_{b} a^{\dagger}_{c} a_k a_j a_i \tag{102}$$

is the three-body component of the $\mathscr{L}$ operator entering Eq. (95) and (100), with ℓ^{ijk}_{abc} representing the corresponding matrix elements, and

$$\mathfrak{M}^{abc}_{ijk} = \langle\Phi^{abc}_{ijk}|\overline{H_N}^{(\mathrm{CCSD})}|\Phi\rangle = \langle\Phi^{abc}_{ijk}|(\overline{H_N}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi\rangle \tag{103}$$

are the so-called generalized moments of the CCSD equations [66–70, 116] corresponding to projections of these equations on the triply excited determinants. At this point, the above expressions are still exact, i.e., one would have to diagonalize $\overline{H_N}^{(\mathrm{CCSD})}$ in the entire A-particle Hilbert space to extract the $\mathscr{L}_3$ component of $\mathscr{L}$ that enters Eq. (101). Thus, in order to apply Eq. (101) in practice, we have to develop practical recipes for determining $\mathscr{L}_3$ or ℓ^{ijk}_{abc} that rely on the information that one can extract from CCSD-level calculations. The CR-CC(2,3) approach of Refs. [79, 80] and the ΛCCSD(T) method of Refs. [75, 76], in which some higher-order terms in the CR-CC(2,3) expressions for the $\delta E^{(\mathrm{T})}$ correction are neglected, provide such recipes.

In the CR-CC(2,3) theory of Refs. [79, 80], presented here in the general, orbital-rotation invariant form, where in analogy to the CCSD energy, the resulting triples correction $\delta E^{(\mathrm{T})}$ is invariant with respect to rotations among the occupied and unoccupied single-particle states, we determine the desired $\mathscr{L}_3$ operator or the corresponding amplitudes ℓ^{ijk}_{abc}, which enter Eq. (101), in a quasi-perturbative manner, using the expression (see [79, 80, 88])

$$\langle\Phi|\mathscr{L}_3 = \langle\Phi|(1 + \Lambda^{(\mathrm{CCSD})})\, \overline{H_N}^{(\mathrm{CCSD})} \mathscr{R}^{(\mathrm{CCSD})}_3, \tag{104}$$

where

$$\mathscr{R}_3^{(\mathrm{CCSD})} = \frac{P_3}{\Delta E^{(\mathrm{CCSD})} - \overline{H_N}^{(\mathrm{CCSD})}}, \tag{105}$$

with

$$P_3 = \sum_{\substack{i<j<k \\ a<b<c}} |\Phi_{ijk}^{abc}\rangle\langle\Phi_{ijk}^{abc}|, \tag{106}$$

is the appropriate reduced resolvent of $\overline{H_N}^{(\mathrm{CCSD})}$ in the subspace spanned by the triply excited determinants $|\Phi_{ijk}^{abc}\rangle$ and $\Lambda^{(\mathrm{CCSD})}$ is the familiar Λ operator obtained by solving the left-eigenstate CCSD equations, Eqs. (67) and (68). As a result, the CR-CC(2,3) correction $\delta E^{(\mathrm{T})}$, which offers an accurate representation of the T_3 effects on the correlation energy without forcing one to solve for T_3 using the full CCSDT approach, assumes the following compact form:

$$\delta E^{(\mathrm{T})} = \langle\Phi|(1 + \Lambda^{(\mathrm{CCSD})})\, \overline{H_N}^{(\mathrm{CCSD})} \mathscr{R}_3^{(\mathrm{CCSD})}\, \overline{H_N}^{(\mathrm{CCSD})}|\Phi\rangle. \tag{107}$$

Alternatively, to avoid the explicit construction of the reduced resolvent $\mathscr{R}_3^{(\mathrm{CCSD})}$, Eq. (105), in the above expression for $\delta E^{(\mathrm{T})}$, we can determine the ℓ_{abc}^{ijk} amplitudes by solving the linear system

$$\begin{aligned} \sum_{\substack{l<m<n \\ d<e<f}} & \langle\Phi_{lmn}^{def}|(\Delta E^{(\mathrm{CCSD})} - \overline{H_N}^{(\mathrm{CCSD})})|\Phi_{ijk}^{abc}\rangle\, \ell_{def}^{lmn} \\ & = \langle\Phi|(1 + \Lambda^{(\mathrm{CCSD})})\, \overline{H_N}^{(\mathrm{CCSD})}|\Phi_{ijk}^{abc}\rangle, \end{aligned} \tag{108}$$

which can be further simplified to

$$\begin{aligned} - \sum_{\substack{l<m<n \\ d<e<f}} & \langle\Phi_{lmn}^{def}|(\overline{H_N}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi_{ijk}^{abc}\rangle\, \ell_{def}^{lmn} \\ & = \langle\Phi|(1 + \Lambda^{(\mathrm{CCSD})})\, (\overline{H_N}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi_{ijk}^{abc}\rangle, \end{aligned} \tag{109}$$

and use the resulting values of ℓ_{abc}^{ijk}, along with the generalized moments $\mathfrak{M}_{ijk}^{abc}$, Eq. (103), to calculate $\delta E^{(\mathrm{T})}$. As explained in Refs. [79, 80, 88], we obtain Eq. (104), or the equivalent linear system given by Eq. (108), by approximating the exact $\mathscr{L}$ operator in the left eigenvalue problem $\langle\Phi|\mathscr{L}\, \overline{H_N}^{(\mathrm{CCSD})} = \Delta E\, \langle\Phi|\mathscr{L}$, which this operator has to satisfy and which we right-project on the triply excited determinants $|\Phi_{ijk}^{abc}\rangle$, by the sum of $(1 + \Lambda^{(\mathrm{CCSD})})$, obtained by solving the left-eigenstate CCSD equations, Eqs. (67) and (68), and the unknown $\mathscr{L}_3$ component, and by replacing the exact correlation energy ΔE in the resulting equations by its CCSD counterpart $\Delta E^{(\mathrm{CCSD})}$.

The above is the most general form of the CR-CC(2,3) theory, which encompasses other forms of non-iterative triples corrections available in the literature, such as ΛCCSD(T), and which satisfies a number of important properties, including the aforementioned rotational invariance (mischaracterized in Ref. [76], but correctly described here) and the strict size extensivity characterizing all of the commonly used CC approaches, such as CCSD or CCSDT. If we are willing to lift the requirement of the strict invariance of the $\delta E^{(\mathrm{T})}$ correction with respect to arbitrary rotations among the occupied and unoccupied orbitals, which can be justified by the fact that typical calculations of such corrections, including those presented in this work, utilize the Hartree-Fock (i.e., fixed) orbitals, we can eliminate the iterative steps associated with the need for solving the linear system for the ℓ_{abc}^{ijk} amplitudes, Eq. (108) or (109), and replace those steps by non-iterative expressions, such as [79–82, 88]

$$\ell_{abc}^{ijk} = \langle\Phi|(1 + \Lambda^{(\mathrm{CCSD})})\, (\overline{H_N}^{(\mathrm{CCSD})})_{\mathrm{open}}|\Phi_{ijk}^{abc}\rangle / D_{ijk}^{abc}, \tag{110}$$

where

$$\begin{aligned} D_{ijk}^{abc} &= \Delta E^{(\mathrm{CCSD})} - \langle\Phi_{ijk}^{abc}|\overline{H_N}^{(\mathrm{CCSD})})|\Phi_{ijk}^{abc}\rangle \\ &= -\sum_{n=1}^{3} \langle\Phi_{ijk}^{abc}|\overline{H}_n|\Phi_{ijk}^{abc}\rangle, \end{aligned} \tag{111}$$

if there are no degeneracies among orbitals i, j, k or a, b, c, with $\overline{H}_n$ representing the n-body component of $\overline{H_N}^{(\mathrm{CCSD})}$ (we still have to solve small linear subsystems of the type of Eqs. (108) or (109) for the subsets of the ℓ_{abc}^{ijk} amplitudes involving orbital degeneracies to retain the invariance of $\delta E^{(\mathrm{T})}$ with respect to the rotations among degenerate orbitals, but this is much less expensive than dealing with the complete (108) or (109) system). We refer the reader to Refs. [79–82, 88] for a thorough discussion of such expressions. Encouraged by the superb performance of the CR-CC(2,3) approach in the nuclear applications involving two-body Hamiltonians, which we reported in Refs. [38, 61], one of our future objectives is to implement the complete CR-CC(2,3) theory, as summarized above, for Hamiltonians including $3N$ interactions, but in this study we focus on the simplifications in the CR-CC(2,3) expressions for the $\delta E^{(\mathrm{T})}$ corrections offered by the ΛCCSD(T) approach of Refs. [75, 76], which facilitate the derivations of the programmable expressions for the triples correction $\delta E^{(\mathrm{T})}$. Considering, however, the fact that the original publications on the ΛCCSD(T) method [75, 76] make explicit use of the assumption that the underlying interactions in the Hamiltonian are two-body, we use the more general CR-CC(2,3) formulas, Eqs. (101)–(111), to identify terms in the ΛCCSD(T) equations for $\delta E^{(\mathrm{T})}$ that result from adding the $3N$ interactions to the Hamiltonian.

The ΛCCSD(T) approach is formally obtained by keeping only the lowest-order terms in the definitions of the moments $\mathfrak{M}_{ijk}^{abc}$, Eq. (103), and amplitudes ℓ_{abc}^{ijk}, Eqs. (108), (109), or (110), that define the CR-CC(2,3) correction $\delta E^{(\mathrm{T})}$. Thus, assuming that the Hamiltonian contains up to three-body interactions, we approximate the moments $\mathfrak{M}_{ijk}^{abc}$, Eq. (103), by retaining terms in $(\overline{H_N}^{(\mathrm{CCSD})})_{\mathrm{open}}$ that are at most linear in T, i.e.,

$$\begin{aligned} \mathfrak{M}_{ijk}^{abc} &\approx \langle\Phi_{ijk}^{abc}|[H_N(1 + T_1 + T_2)]_C|\Phi\rangle \\ &= \mathfrak{M}_{ijk}^{abc}(2\mathrm{B}) + \mathfrak{M}_{ijk}^{abc}(W_N), \end{aligned} \tag{112}$$

where the NO2B contribution to $\mathfrak{M}^{abc}_{ijk}$ is given by

$$\begin{aligned}\mathfrak{M}^{abc}_{ijk}(2\text{B}) &= \langle\Phi^{abc}_{ijk}|[H_{N,2\text{B}}(1+T_1+T_2)]_C|\Phi\rangle \\ &= \langle\Phi^{abc}_{ijk}|(V_N T_2)_C|\Phi\rangle \qquad (113)\end{aligned}$$

and the contribution due to the residual $3N$ interactions has the form

$$\mathfrak{M}^{abc}_{ijk}(W_N) = \langle\Phi^{abc}_{ijk}|[W_N(1+T_1+T_2)]_C|\Phi\rangle. \qquad (114)$$

In order to derive the analogous expressions for the amplitudes ℓ^{ijk}_{abc}, which would be consistent with the approximations that lead to the non-iterative ΛCCSD(T) approach of Refs. [75, 76], where one makes an assumption that the Fock operator is diagonal in the occupied and unoccupied single-particle spaces, so that $f^i_j = \epsilon_i\delta_{ij}$ and $f^a_b = \epsilon_a\delta_{ab}$, where ϵ_p represents the diagonal matrix element f^p_p, which is automatically satisfied by the calculations reported in this study since they rely on the canonical Hartree-Fock orbitals, we replace the reduced resolvent $\mathscr{R}^{(\text{CCSD})}_3$ entering the CR-CC(2,3) correction $\delta E^{(\text{T})}$, Eq. (107), by its simplified Møller-Plesset form adopted in the ΛCCSD(T) considerations [75, 76], i.e.,

$$\begin{aligned}\mathscr{R}^{(\text{CCSD})}_3 &= -\frac{P_3}{(\overline{H_N}^{(\text{CCSD})})_{\text{open}}} \approx -\frac{P_3}{F_N} \\ &= \sum_{\substack{i<j<k\\ a<b<c}} (\epsilon^{abc}_{ijk})^{-1}|\Phi^{abc}_{ijk}\rangle\langle\Phi^{abc}_{ijk}|, \qquad (115)\end{aligned}$$

where

$$\epsilon^{abc}_{ijk} = \epsilon_i + \epsilon_j + \epsilon_k - \epsilon_a - \epsilon_b - \epsilon_c \qquad (116)$$

is the orbital energy difference for triples. The latter approximation is equivalent to replacing $(\overline{H_N}^{(\text{CCSD})})_{\text{open}}$ in the left-hand side of the linear system given by Eq. (109), which corresponds to the more elaborate CR-CC(2,3) treatment, by the F_N operator. If we further approximate $\overline{H_N}^{(\text{CCSD})}$ in the right-hand side of Eq. (109) by the leading contribution to $\overline{H_N}^{(\text{CCSD})}$, which is the normal-ordered Hamiltonian H_N itself, we can replace the linear system given by Eq. (109) by its simplified form

$$\begin{aligned}&-\sum_{\substack{l<m<n\\ d<e<f}} \langle\Phi^{def}_{lmn}|F_N|\Phi^{abc}_{ijk}\rangle\, \ell^{lmn}_{def} \\ &\quad = \langle\Phi|(1+\Lambda^{(\text{CCSD})})\, H_N|\Phi^{abc}_{ijk}\rangle \qquad (117)\end{aligned}$$

form, which immediately allows us to write

$$\ell^{ijk}_{abc} = (\epsilon^{abc}_{ijk})^{-1}\langle\Phi|(1+\Lambda^{(\text{CCSD})})\, H_N|\Phi^{abc}_{ijk}\rangle. \qquad (118)$$

After splitting the above expression into the NO2B and residual $3N$ contributions and identifying the non-vanishing terms, we obtain

$$\ell^{ijk}_{abc} = \ell^{ijk}_{abc}(2\text{B}) + \ell^{ijk}_{abc}(W_N), \qquad (119)$$

where

$$\begin{aligned}\ell^{ijk}_{abc}(2\text{B}) &= \langle\Phi|[(\Lambda_1 V_N)_{DC} + (\Lambda_2 F_N)_{DC} \\ &\quad +(\Lambda_2 V_N)_C]|\Phi^{abc}_{ijk}\rangle/\epsilon^{abc}_{ijk} \qquad (120)\end{aligned}$$

and

$$\begin{aligned}\ell^{ijk}_{abc}(W_N) &= \langle\Phi|[W_N + (\Lambda_1 W_N)_C \\ &\quad +(\Lambda_2 W_N)_C]|\Phi^{abc}_{ijk}\rangle/\epsilon^{abc}_{ijk}. \qquad (121)\end{aligned}$$

Equation (101), with moments $\mathfrak{M}^{abc}_{ijk}$ approximated by Eqs. (112)–(114) and amplitudes ℓ^{ijk}_{abc} by Eqs. (119)–(121), is the desired extension of the ΛCCSD(T) correction due to the connected T_3 clusters to the $3N$ interaction case. By comparing the expressions for the NO2B contributions to $\mathfrak{M}^{abc}_{ijk}$ and ℓ^{ijk}_{abc} given by Eqs. (113) and (120), respectively, with the analogous formulas for the two-body Hamiltonians reported in Ref. [76], we can immediately see that the ΛCCSD(T) approach presented here, which we derived by simplifying the CR-CC(2,3) equations, reduces to the ΛCCSD(T) theory of Refs. [75, 76], when the Hamiltonian of interest contains pairwise interactions only.

Based on the above considerations, we can give the triples correction formula for the three-body Hamiltonians, within the ΛCCSD(T) approximation scheme discussed in this work, the physically meaningful form

$$\delta E^{(\text{T})} = \delta E^{(\text{T})}_{2\text{B}} + \delta E^{(\text{T})}_{3\text{B}}, \qquad (122)$$

where the pure NO2B contribution $\delta E^{(\text{T})}_{2\text{B}}$ is defined as

$$\delta E^{(\text{T})}_{2\text{B}} = \tfrac{1}{36}\, \ell^{ijk}_{abc}(2\text{B})\, \mathfrak{M}^{abc}_{ijk}(2\text{B}), \qquad (123)$$

whereas the $\delta E^{(\text{T})}_{3\text{B}}$ component of $\delta E^{(\text{T})}$, which is present only when the residual $3N$ interactions are taken into account, is given by

$$\begin{aligned}\delta E^{(\text{T})}_{3\text{B}} &= \tfrac{1}{36}\,[\ell^{ijk}_{abc}(2\text{B})\, \mathfrak{M}^{abc}_{ijk}(W_N) + \ell^{ijk}_{abc}(W_N)\, \mathfrak{M}^{abc}_{ijk}(2\text{B}) \\ &\quad +\ell^{ijk}_{abc}(W_N)\, \mathfrak{M}^{abc}_{ijk}(W_N)]. \qquad (124)\end{aligned}$$

The explicit m-scheme-type expressions for the NO2B contributions to moments $\mathfrak{M}^{abc}_{ijk}$ and amplitudes ℓ^{ijk}_{abc}, within the ΛCCSD(T) approximation defined by Eqs. (113), (114), (120) and (121), are

$$\mathfrak{M}^{abc}_{ijk}(2\text{B}) = \mathscr{A}^{ab/c}\mathscr{A}_{ij/k}(v^{ab}_{kd}t^{dc}_{ij} - v^{cl}_{ij}t^{ab}_{lk}) \qquad (125)$$

and

$$\begin{aligned}\ell^{ijk}_{abc}(2\text{B}) &= \mathscr{A}_{ab/c}\mathscr{A}^{ij/k}(f^k_c\lambda^{ij}_{ab} + v^{ij}_{ab}\lambda^k_c + v^{kd}_{ab}\lambda^{ij}_{dc} \\ &\quad -v^{ij}_{cl}\lambda^{lk}_{ab})/\epsilon^{abc}_{ijk}, \qquad (126)\end{aligned}$$

respectively (the analogous equations can also be found in Ref. [76], although the equation in Ref. [76], which would be equivalent to our Eq. (126), is applicable to real orbitals only). For the residual $3N$ contributions to $\mathfrak{M}^{abc}_{ijk}$ and amplitudes ℓ^{ijk}_{abc}, we can write

$$\begin{aligned}\mathfrak{M}^{abc}_{ijk}(W_N) &= w^{abc}_{ijk} - \mathscr{A}^{ab/c}w^{abl}_{ijk}t^c_l + \mathscr{A}_{ij/k}w^{abc}_{ijd}t^d_k \\ &\quad +\tfrac{1}{2}\mathscr{A}_{ij/k}w^{abc}_{dek}t^{de}_{ij} + \tfrac{1}{2}\mathscr{A}^{ab/c}w^{lmc}_{ijk}t^{ab}_{lm} \\ &\quad +\mathscr{A}^{ab/c}\mathscr{A}_{ij/k}w^{abl}_{ijd}t^{cd}_{kl} \qquad (127)\end{aligned}$$

and

$$\begin{aligned}\ell^{ijk}_{abc}(W_N) &= (w^{ijk}_{abc} - \mathscr{A}_{ab/c} w^{ijk}_{abl}\lambda^{l}_{c} + \mathscr{A}^{ij/k} w^{ijd}_{abc}\lambda^{k}_{d} \\ &\quad + \tfrac{1}{2}\mathscr{A}^{ij/k} w^{dek}_{abc}\lambda^{ij}_{de} + \tfrac{1}{2}\mathscr{A}_{ab/c} w^{ijk}_{lmc}\lambda^{lm}_{ab} \\ &\quad + \mathscr{A}_{ab/c}\mathscr{A}^{ij/k} w^{ijd}_{abl}\lambda^{kl}_{cd})/\epsilon^{abc}_{ijk}, \end{aligned} \tag{128}$$

respectively. The three-index antisymmetrizers $\mathscr{A}_{pq/r} = \mathscr{A}^{pq/r}$, which enter the above formulas along with the previously defined two-index antisymmetrizers $\mathscr{A}_{pq} = \mathscr{A}^{pq}$, Eq. (83), are defined in a usual way, *viz.*,

$$\mathscr{A}_{pq/r} \equiv \mathscr{A}^{pq/r} = 1 - (pr) - (qr), \tag{129}$$

where we use the (pq) symbol once again to represent a transposition of two indices. As in the case of the CCSD and ΛCCSD equations discussed in Sec. II C 1, the m-scheme-style expressions Eqs. (125)–(128) can again be convert into an angular-momentum-coupled form which greatly facilitates the computations.

We finalize our formal presentation of the ΛCCSD(T) theory for three-body Hamiltonians by emphasizing the differences between ΛCCSD(T) in the NO2B approximation and the complete ΛCCSD(T) treatment including the residual $3N$ interactions W_N. According to the above analysis, in the full treatment of three-body interactions within the ΛCCSD(T) description, one determines the total energy E, designated as $E^{(\Lambda\text{CCSD(T)})}$, as follows:

$$\begin{aligned}&E^{(\Lambda\text{CCSD(T)})} = \\ &\quad E_{\text{ref}} + \Delta E^{(\text{CCSD})}_{2\text{B}} + \delta E^{(\text{T})}_{2\text{B}} + \Delta E^{(\text{CCSD})}_{3\text{B}} + \delta E^{(\text{T})}_{3\text{B}},\end{aligned} \tag{130}$$

where we calculate the NO2B-type correlation energy contributions $\Delta E^{(\text{CCSD})}_{2\text{B}}$ and $\delta E^{(\text{T})}_{2\text{B}}$ using Eqs. (65) and (123), respectively, and the contributions associated with the presence of the residual $3N$ interactions, $\Delta E^{(\text{CCSD})}_{3\text{B}}$ and $\delta E^{(\text{T})}_{3\text{B}}$, using Eqs. (66) and (124), respectively. The reference energy E_{ref}, which obviously does not contain any information about the residual $3N$ effects represented by the normal-ordered operator W_N, is calculated using Eq. (31). In the case of ΛCCSD(T) calculations in the NO2B approximation, we replace the complete energy expression given by Eq. (130) by its simplified form, in which the W_N-containing terms, $\Delta E^{(\text{CCSD})}_{3\text{B}}$ and $\delta E^{(\text{T})}_{3\text{B}}$, are neglected, i.e.,

$$E^{(\Lambda\text{CCSD(T)})}_{2\text{B}} = E_{\text{ref}} + \Delta E^{(\text{CCSD})}_{2\text{B}} + \delta E^{(\text{T})}_{2\text{B}}. \tag{131}$$

We stress, however, that the differences between the complete and NO2B treatments of the $3N$ interactions in the ΛCCSD(T) calculations are not limited to the final energy expressions. In the most complete ΛCCSD(T) calculations, in which the three-body interactions in the Hamiltonian are treated fully, the singly and doubly excited cluster amplitudes, t^{a}_{i} and t^{ab}_{ij}, and their singly and doubly deexcited λ^{i}_{a} and λ^{ij}_{ab} counterparts are determined from CCSD and left-eigenstate CCSD calculations with all terms in the normal-ordered three-body Hamiltonian H_N, Eq. (24), including those that contain W_N, properly accounted for, as in Eqs. (48) and (49) for CCSD and (69) and (70) for ΛCCSD. This should be contrasted with the NO2B approximation to the ΛCCSD(T) approach, in which the t^{a}_{i}, t^{ab}_{ij}, λ^{i}_{a}, and λ^{ij}_{ab} amplitudes, which are needed to construct the $\Delta E^{(\text{CCSD})}_{2\text{B}}$ and $\delta E^{(\text{T})}_{2\text{B}}$ energy components in Eq. (131), are obtained by solving the CCSD and left-eigenstate CCSD equations, where the W_N-containing $\Theta^{a}_{i}(W_N)$ and $\Theta^{ab}_{ij}(W_N)$ terms in the CCSD system, Eqs. (48) and (49), and the $\Xi^{i}_{a}(W_N)$ and $\Xi^{ij}_{ab}(W_N)$ terms in the ΛCCSD system, Eqs. (69) and (70), are neglected. Clearly, very similar remarks apply to a comparison of the complete and NO2B treatments of the $3N$ interactions in the underlying CCSD calculations, where the corresponding total energies are defined as

$$\begin{aligned}E^{(\text{CCSD})} &= E_{\text{ref}} + \Delta E^{(\text{CCSD})}_{2\text{B}} + \Delta E^{(\text{CCSD})}_{3\text{B}} && (132)\\ &\equiv E_{\text{ref}} + \Delta E^{(\text{CCSD})} && (133)\end{aligned}$$

in the former case, and

$$E^{(\text{CCSD})}_{2\text{B}} = E_{\text{ref}} + \Delta E^{(\text{CCSD})}_{2\text{B}}, \tag{134}$$

in the latter case. One of the interesting questions that our calculations discussed in Section III try to address is if it is beneficial to consider an intermediate ΛCCSD(T) approximation, where the $3N$ forces are treated fully at the CCSD level, while using the NO2B approximation in the determination of the $\delta E^{(\text{T})}$ triples correction, so that the full ΛCCSD(T) energy expression, Eq. (130), is replaced by the somewhat simpler formula

$$\tilde{E}^{(\Lambda\text{CCSD(T)})} = E_{\text{ref}} + \Delta E^{(\text{CCSD})} + \delta E^{(\text{T})}_{2\text{B}}. \tag{135}$$

Finally, it is worth pointing out that one of the most interesting differences between the ΛCCSD(T) calculations with the NO2B and full treatments of the $3N$ interactions in the Hamiltonian is the significance of the T_3 contributions induced by the residual W_N component. As in conventional many-body theory based on pairwise interactions, the NO2B approximation shifts the T_3 contribution to the second and higher orders of the many-body perturbation theory (MBPT) in the wave function and the fourth and higher MBPT orders in the energy, since in the absence of the W_N component in the Hamiltonian, the lowest-order approximation to T_3 originates from the formula (cf., e.g., Ref. [103], and references therein) $T^{(2)}_{3}|\Phi\rangle = (\mathscr{R}_3 V_N \mathscr{R}_2 V_N)_C|\Phi\rangle$, where $\mathscr{R}_n = -(F_N)^{-1}P_n$ is the n-body component of the MBPT reduced resolvent (assuming, for simplicity, Hartree-Fock orbitals). The fourth- and higher-order MBPT contributions to the energy due to the T_3 clusters originating from the pairwise interaction term V_N in H_N are captured by the $\delta E^{(\text{T})}_{2\text{B}}$ correction, Eq. (123), which is present in any form of the ΛCCSD(T) (or even CCSD(T) or CCSD[T]) calculations, including those in which the $3N$ interactions are completely neglected. The situation changes when we include the residual $3N$ interaction term W_N in the calculations. In this case, the T_3 cluster component due to W_N shows up already in the first MBPT order in the wave function and the second MBPT order in the energy, since one can form the connected wave function diagram with six external lines representing T_3 using the formula $T^{(1)}_{3}|\Phi\rangle =$

$(\mathscr{R}_3 W_N)_C|\Phi\rangle$. The corresponding second-order MBPT contribution due to the T_3 cluster component originating from the presence of W_N in the Hamiltonian is captured by the $\delta E_{3\mathrm{B}}^{(\mathrm{T})}$ correction, through the last $\frac{1}{36}\,\ell_{abc}^{ijk}(W_N)\,\mathfrak{M}_{ijk}^{abc}(W_N)$ term in Eq. (124), which, based on Eqs. (127) and (128), contains the second-order $\frac{1}{36}\sum_{i,j,k,a,b,c} w_{ijk}^{abc} w_{abc}^{ijk}/\epsilon_{ijk}^{abc}$ expression as the leading component. It is trivial to show that the latter expression is equivalent to the vacuum diagram representing $\langle\Phi|(W_N T_3^{(1)})_C|\Phi\rangle$. Clearly, such a term cannot be captured by CCSD, even when the W_N interactions are included in the calculations, since CCSD ignores the T_3 contributions altogether and the CCSD correlation energy can only directly engage the T_1T_2 and $\frac{1}{6}T_1^3$ clusters, as in $\Delta E_{3\mathrm{B}}^{(\mathrm{CCSD})}$, Eq. (66). We would have the $\langle\Phi|(W_N T_3)_C|\Phi\rangle$ component in the correlation energy if we used the full CCSDT approach with the residual W_N interactions. It is, therefore, very encouraging to observe that the extension of the ΛCCSD(T) approach to three-body Hamiltonians developed in this work captures the sophisticated T_3-cluster physics originating from the residual $3N$ forces represented by the W_N operator, which normally requires the full CCSDT treatment, via the $\delta E_{3\mathrm{B}}^{(\mathrm{T})}$ energy component defined by Eq. (124).

III. APPLICATION TO MEDIUM-MASS NUCLEI

A. Hamiltonian and basis

We use the chiral NN interaction at N^{3}LO [117] and a local form of the chiral $3N$ interaction at N^{2}LO [118]. The initial Hamiltonian is transformed through a similarity renormalization group (SRG) evolution at the two- and three-body level to enhance the convergence behavior of the many-body calculation. The SRG transformation represents a continuous unitary transformation parametrized by a flow parameter α, with the initial Hamiltonian corresponding to $\alpha = 0$ [13, 119, 120]. We use the 400 MeV reduced-cutoff version of the chiral $3N$ interaction as described in [13, 14, 16, 121]. This cutoff reduction is motivated by the observation that SRG-induced $4N$ interactions have a sizable impact on ground-state energies of medium-mass nuclei, which can be reduced efficiently by lowering the cutoff.

We will employ two types of SRG-evolved Hamiltonians: The NN+$3N$-full Hamiltonian starts with the initial chiral NN+$3N$ Hamiltonian and retains all terms up to the three-body level in the SRG evolution; the NN+$3N$-induced Hamiltonian omits the chiral $3N$ interaction from the initial Hamiltonian, but keeps all induced three-body terms throughout the evolution. The three-body SRG evolution is performed in an harmonic-oscillator (HO) model space with up to 40 oscillator quanta [13, 121]. To ensure the sufficiency of this model space for smaller HO frequencies we apply a frequency conversion technique [121]: We evolve the Hamiltonian at an adequate HO frequency, here $\hbar\Omega = 28\,\mathrm{MeV}$, and convert the Hamiltonian matrix elements to the HO basis with the desired frequency for the many-body calculation, afterwards. Furthermore, we consider a range of flow parameters α in order to observe how the individual contributions in the CC calculations evolve with the SRG flow.

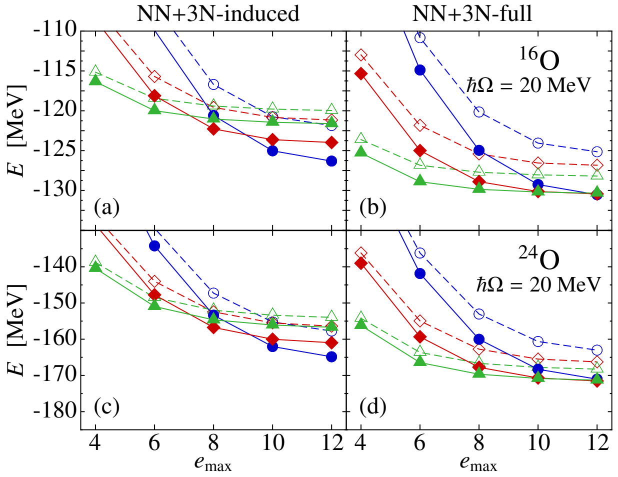

FIG. 3: (color online) CCSD (dashed lines) and ΛCCSD(T) (solid lines) ground-state energies for ^{16}O and ^{24}O as function of $e_{\max}$ for the two types of Hamiltonians (see column headings) for SRG flow parameters: $\alpha = 0.02\,\mathrm{fm}^4$ (●), $0.04\,\mathrm{fm}^4$ (◆), $0.08\,\mathrm{fm}^4$ (▲).

For our coupled-cluster calculations, the underlying single-particle basis is a HO basis truncated in the principal oscillator quantum number $2n + l = e \leq e_{\max}$ and we go up to $e_{\max} = 12$. We perform Hartree-Fock calculations including explicitly the $3N$ interaction for each set of basis parameters to obtain an optimized single-particle basis and stabilize the convergence of the CC iterations. Due to their enormous number it is not possible to include all $3N$ matrix elements that would appear in the larger bases. Therefore, regarding computing time, we restrict our calculations to three-body matrix elements with $e_1 + e_2 + e_3 \leq E_{3\,\max} = 12$. For this particular value of $E_{3\,\max}$ we capture a significant part of the $3N$ interaction, but, mostly for the harder interactions, we are not yet fully converged with respect to $E_{3\,\max}$ [64]. However, this is not expected to impact the discussion in this article.

For closed-shell nuclei we use an angular-momentum coupled formulation of coupled-cluster theory [78] which enables us to operate with reduced matrix elements for all operators involved, in particular the Hamiltonian. This leads to a drastic reduction of the number of matrix elements to be processed compared to an m-scheme description and hence greatly extends the range of the method to medium-mass nuclei and beyond.

B. Results

To assess the overall importance of triply excited clusters in nuclear-structure calculations, in Fig. 3 we compare the CCSD and ΛCCSD(T) ground-state energies $E^{(\mathrm{CCSD})}$ and $E^{(\Lambda\mathrm{CCSD(T)})}$ using the complete $3N$ information, as function of $e_{\max}$ for ^{16}O, ^{24}O and for the two $3N$ Hamiltonians discussed in the previous section. First, we notice that we are reasonably converged within the model spaces we operate in and we observe the expected faster convergence with respect to model space-size for the softer, further evolved, interactions. Furthermore, the triples correction $\delta E^{(\mathrm{T})}$ provides about 2–5 % of the binding energy for all nuclei considered, where, as expected, the contribution of the triply excited clusters decreases with the SRG flow parameter. Therefore, if one eventually targets at an accuracy in ground-state calculations of about 1 %, the cluster truncation is identified as one of the larger sources of uncertainty and it is not sufficiently converged at the level of CCSD for triple excitation effects to be negligible, even for the softest interaction considered.

Next we address the importance of the residual $3N$ interaction in CCSD and ΛCCSD(T) calculations. This discussion is complicated by the fact that energy values are not only determined by their expressions in terms of the T and Λ amplitudes t_i^a, t_{ij}^{ab} and λ_a^i, λ_{ab}^{ij}, but also by the type of equations – with or without inclusion of the W_N terms – used to determine the amplitudes in the first place. This leads to various possible and reasonable combinations to consider.

In Fig. 4, where for ^{16,24}O, ^{40}Ca and both, the $NN + 3N$-induced and $NN + 3N$-full Hamiltonian we show results for a series of increasingly complete calculations of the energy. The energy $E_{2B}^{(\mathrm{CCSD})}$ is calculated in NO2B approximation, i.e., the W_N terms are neglected in the equations determining the T amplitudes. For the calculation of all other energies we use T and Λ amplitudes determined from their respective amplitude equations including the W_N terms. By comparing $E_{2B}^{(\mathrm{CCSD})}$ with $E^{(\mathrm{CCSD})}$, we obtain a direct quantification of the combined effect of the additional W_N terms in the CCSD amplitude equations and energy expression. Note that $E^{(\mathrm{CCSD})} - E_{2B}^{(\mathrm{CCSD})} \neq \Delta E_{3B}^{(\mathrm{CCSD})}$ here, due to the use of different amplitudes. The interesting question of whether the W_N terms are more important in the determination of the amplitudes or in the energy expression will be adressed further below. Contrary to the previous situation, the same amplitudes are used in the calculation of $\delta E_{2B}^{(\mathrm{T})}$ and $\delta E_{3B}^{(\mathrm{T})}$. Therefore, using these numbers we can only quantify how important the W_N contributions, simply given by $\delta E_{3B}^{(\mathrm{T})}$, are in the calculation of the total triples correction $\delta E^{(\mathrm{T})}$, i.e., we can compare the approximate energy expression $\tilde{E}^{(\Lambda\mathrm{CCSD(T)})}$, Eq. (135), to the full form $E^{(\Lambda\mathrm{CCSD(T)})}$, Eq. (130), but we cannot at the same time assess the relevance of W_N terms in the respective equations determining the T and Λ amplitudes. Particularly for $\delta E_{2B}^{(\mathrm{T})}$, other choices of where to include W_N terms in the amplitude equations seem reasonable. We come back to this issue below but already mention here that for $\delta E_{2B}^{(\mathrm{T})}$ other choices of amplitude equations lead to practically the same results.

All data shown in Fig. 4 is compiled in Tab. I, and in the following we consider ^{16}O with the NN+$3N$-full Hamiltonian [Fig. 4(b)] at flow parameter values $\alpha = 0.02\,\mathrm{fm}^4$ and $0.08\,\mathrm{fm}^4$ as an example. For increasing α, more and more of the binding energy is shifted to lower orders of the cluster expansion and the contributions from the higher orders consequently get smaller with the SRG flow: The size of the reference energy E_{ref} grows from –56.11 MeV to –101.67 MeV, while the CCSD correlation energy $\Delta E^{(\mathrm{CCSD})}$ decreases from –69.03 MeV to –26.52 MeV as we go from $\alpha = 0.02\,\mathrm{fm}^4$ to

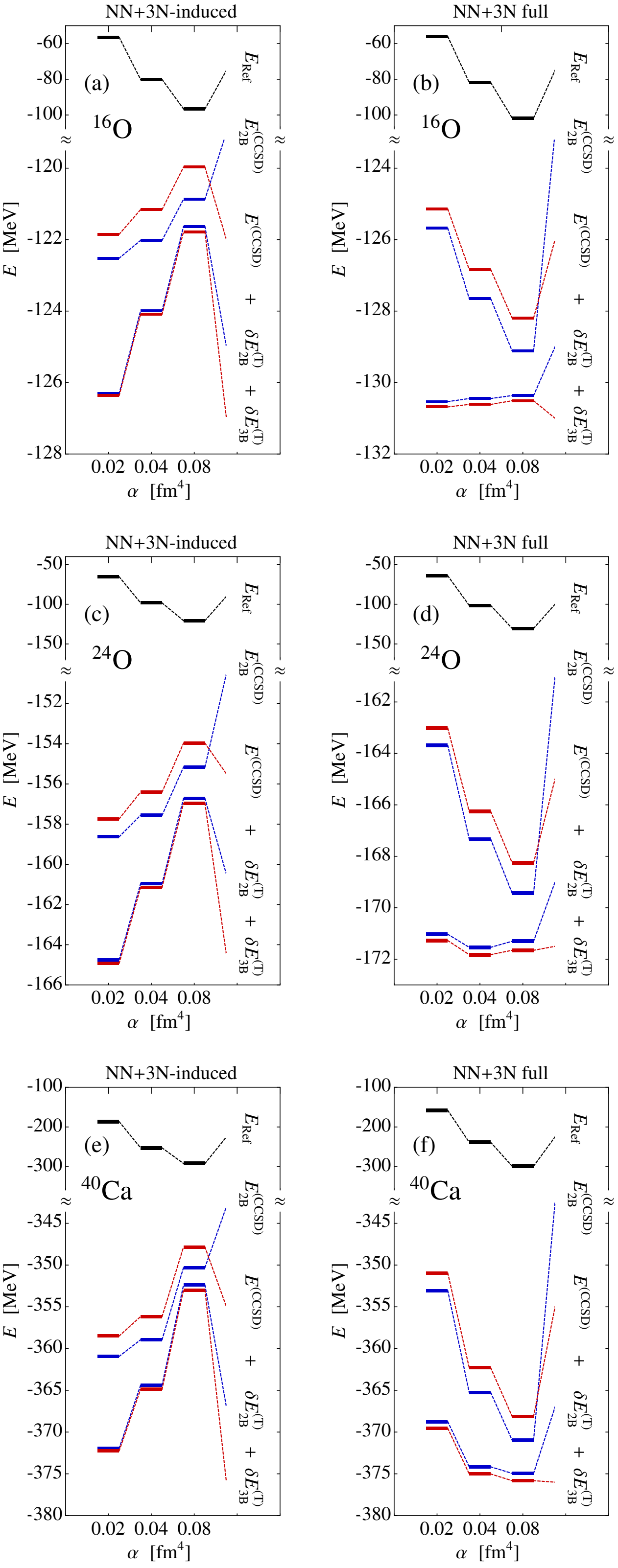

FIG. 4: (color online) Anatomy of individual contributions from CCSD and ΛCCSD(T) to the total binding energy of ^{16,24}O and ^{40}Ca for the two types of Hamiltonians and SRG flow parameters $\alpha = 0.02, 0.04, 0.08\,\mathrm{fm}^4$. For ^{16,24}O, an $e_{\max} = 12$ model space and oscillator frequency $\hbar\Omega = 20\,\mathrm{MeV}$ was used, whereas for ^{40}Ca we work in an $e_{\max} = 10$ model space with $\hbar\Omega = 24\,\mathrm{MeV}$.

$0.08\,\mathrm{fm}^4$ and the ΛCCSD(T) energy correction $\delta E^{(\mathrm{T})}$, which we also consider as a measure for the contributions of the omitted cluster operators beyond the three-body level [64], decreases from $-5.54\,\mathrm{MeV}$ to $-2.34\,\mathrm{MeV}$, corresponding to 4.2 % and 1.8 % of the total binding energy. In the medium-mass regime, these uncertainties related to the cluster truncation are typically the largest in our calculations for a given Hamiltonian, and therefore they set the overall level of accuracy we target at [64].

Examining the contributions from the residual $3N$ interaction to $\Delta E^{(\mathrm{CCSD})}$ we find that, while the absolute value of $\Delta E^{(\mathrm{CCSD})}$ decreases by about 30 MeV when we evolve the Hamiltonian from $\alpha = 0.02\,\mathrm{fm}^4$ further to $0.08\,\mathrm{fm}^4$, $\Delta E^{(\mathrm{CCSD})} - \Delta E^{(\mathrm{CCSD})}_{2\mathrm{B}}$ is only subject to a slight increase from 0.54 MeV to 0.92 MeV, corresponding to 0.4 % and 0.7 % of the total binding energy. Consequently, the relative as well as the absolute importance of the residual $3N$ interaction to the CCSD correlation energy grows with the SRG flow.

Furthermore, while for the harder Hamiltonian at $\alpha = 0.02\,\mathrm{fm}^4$ the W_N contributions to $\Delta E^{(\mathrm{CCSD})}$ are about an order of magnitude smaller than the accuracy level set by $\delta E^{(\mathrm{T})}$, for the softer $\alpha = 0.08\,\mathrm{fm}^4$ Hamiltonian the W_N contributions have an comparable size of about 39 % of the triples correction. Therefore, in order to keep different errors at a consistent level, for soft interactions the residual $3N$ contributions should be included in CCSD if the triples correction is considered as well.

For the ΛCCSD(T) triples correction $\delta E^{(\mathrm{T})}$ itself, the W_N contributions $\delta E^{(\mathrm{T})}_{3\mathrm{B}}$, despite containing second-order MBPT contributions, have very small values of about $-15\,\mathrm{keV}$. This effect is about one order of magnitude smaller than the targeted accuracy given by the size of $\delta E^{(\mathrm{T})}$, and may therefore be neglected. From another perspective, the W_N contributions to $\delta E^{(\mathrm{T})}$ constitutes about 0.1 % of the total binding energy, which clearly is beyond the level of accuracy of any many-body method operating in the medium-mass regime today.

As is apparent from Fig. 4, the discussion for the $NN+3N$-induced Hamiltonian and the heavier nuclei ^{24}O, ^{40}Ca is similar. In the case of ^{40}Ca we work in the smaller $e_{\max} = 10$ model space in order to keep the computational cost reasonable. In this model space the results are not fully converged with respect to $e_{\max}$, but since the quality of NO2B is largely independent of $e_{\max}$ [64] this does not affect the present discussion. For the $NN+3N$-induced Hamiltonian, for example, the relative contribution of W_N to the CCSD correlation energy grows from 1.3 % for $\alpha = 0.02\,\mathrm{fm}^4$ to 4.2 % for $\alpha = 0.08\,\mathrm{fm}^4$, in both cases constituting about 0.6 % of the total binding energy. Again, as the SRG flow parameter increases, the contributions of W_N to the CCSD correlation energy on the one hand, and the triples correction on the other hand, become comparable, where $\Delta E^{(\mathrm{CCSD})} - \Delta E^{(\mathrm{CCSD})}_{2\mathrm{B}}$ is about 18 % of the size of the triples correction at $\alpha = 0.02\,\mathrm{fm}^4$ and already about 48 % at $\alpha = 0.08\,\mathrm{fm}^4$. The W_N effect to the triples correction is again negligible, about one order of magnitude smaller than the triples correction itself, namely about 2 % of $\delta E^{(\mathrm{T})}$ for $\alpha = 0.02\,\mathrm{fm}^4$ and about 11 % for $\alpha = 0.08\,\mathrm{fm}^4$, or 0.1 % and 0.2 % of the total binding energy $E^{(\Lambda\mathrm{CCSD(T)})}$.

In summary, for hard interactions, the residual $3N$ effects to the CCSD correlation energy $E^{(\mathrm{CCSD})}$ are rather small compared to the triples correction $\delta E^{(\mathrm{T})}$, but they become comparable for soft interactions. Therefore, when using soft interactions, the residual $3N$ interaction should be included in CCSD if the desired accuracy level also demands inclusion of triples excitation effects. For the triples correction, on the other hand, the residual $3N$ interaction only plays an insignificant role, providing contributions that are shadowed by the considerably larger uncertainties stemming, e.g., from the cluster truncation. This motivates the use of the truncated energy expression $\tilde{E}^{(\Lambda\mathrm{CCSD(T)})}$, Eq. (135), instead of the full form $E^{(\Lambda\mathrm{CCSD(T)})}$, Eq. (130), resulting in only negligible losses in accuracy.

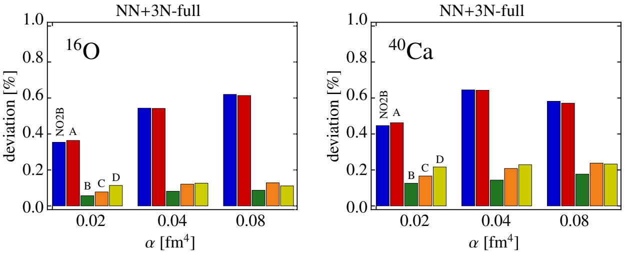

FIG. 5: (color online) Comparison of the deviations introduced by the different approximation schemes Eqs. (136)–(140) described in the text to the full inclusion of the residual $3N$ interaction in all steps involving a CCSD and ΛCCSD(T) calculation.

The above considerations indicate that the residual $3N$ interaction may be neglected in calculating the ΛCCSD(T) energy correction $\delta E^{(\mathrm{T})}$ without significantly affecting the overall accuracy, leading to Eq. (135) as an approximate form for $E^{(\Lambda\mathrm{CCSD(T)})}$. From a practitioner's point of view, discarding the W_N contributions to $\delta E^{(\mathrm{T})}$, Eqs. (127)–(128), already leads to significant savings in the implementational effort and computing time, but one still has to solve the CCSD equations determining the T amplitudes t_i^a and t_{ij}^{ab} as well as the ΛCCSD equations determining the Λ amplitudes λ_a^i and λ_{ab}^{ij} with full incorporation of W_N. Particularly solving the ΛCCSD equations, for which the effective Hamiltonian contributions given in Fig. 1 and 2 have to be evaluated, consumes most of the computing time in our calculations. Therefore, it is also worthwhile to investigate how much of the residual $3N$ information has to be incluced in solving for the amplitudes of the T and Λ operators that enter the energy expressions, in order to obtain accurate results at the lowest possible computational cost.

In order to distinguish different approximation schemes we introduce the following notation in which for energy quantities that only depend on T amplitudes the label in brackets denote if the T amplitudes were determined from the amplitude equations with (3B) or without residual $3N$ interaction (2B). Similarly, for quantities that depend on both, T and Λ amplitudes, the first label denotes the type of equation used to determine the T amplitudes and the second corresponds to the ΛCCSD equations. For example, $\tilde{E}^{(\Lambda\mathrm{CCSD(T)})}(3\mathrm{B}, 2\mathrm{B})$ refers to the energy expression (135), calculated using T amplitudes determined from Eqs. (58), (59), (60) and (61) while the Λ amplitudes are determined from Eqs. (79) and (80) only.

TABLE I: Summary of the individual contributions to the ΛCCSD(T) ground-state energies in MeV for ^{16,24}O and ^{40}Ca and for the $NN + 3N$-induced and $NN + 3N$-full Hamiltonian, obtained for ^{16,24}O from an $e_{\max} = 12$ model space with oscillator frequency $\hbar\Omega = 20$ MeV and for ^{40}Ca from an $e_{\max} = 10$ model space with $\hbar\Omega = 24$ MeV. For the calculation of $\Delta E_{2B}^{(CCSD)}$, amplitudes from the NO2B approximation have been used, while for the calculation of all other quantities amplitudes have been determined from equations including the residual $3N$ interaction.

NN+3N-induced	α [fm^4]	$E^{(\Lambda CCSD(T))}$	E_{ref}	$\Delta E_{2B}^{(CCSD)}$	$\Delta E^{(CCSD)} - \Delta E_{2B}^{(CCSD)}$	$\delta E_{2B}^{(T)}$	$\delta E_{3B}^{(T)}$
^{16}O	0.02	–126.37	–56.47	–66.05	0.67	–4.46	–0.06
	0.04	–124.09	–80.09	–41.93	0.86	–2.83	–0.10
	0.08	–121.78	–96.59	–24.28	0.90	–1.66	–0.15
^{24}O	0.02	–164.92	–65.41	–93.22	0.89	–7.01	–0.18
	0.04	–161.14	–98.32	–59.23	1.15	–4.56	–0.18
	0.08	–156.97	–120.64	–34.52	1.19	–2.75	–0.24
^{40}Ca	0.02	–372.25	–186.58	–174.35	2.44	–13.44	–0.31
	0.04	–364.87	–252.67	–106.28	2.78	–8.22	–0.49
	0.08	–353.00	–291.98	–58.32	2.46	–4.56	–0.59
NN+3N-full	α[fm^4]	$E^{(\Lambda CCSD(T))}$	E_{ref}	$\Delta E_{2B}^{(CCSD)}$	$\Delta E^{(CCSD)} - \Delta E_{2B}^{(CCSD)}$	$\delta E_{2B}^{(T)}$	$\delta E_{3B}^{(T)}$
^{16}O	0.02	–130.68	–56.11	–69.57	0.54	–5.39	–0.15
	0.04	–130.61	–81.79	–45.87	0.82	–3.61	–0.16
	0.08	–130.51	–101.67	–27.44	0.92	–2.17	–0.17
^{24}O	0.02	–171.28	–64.16	–99.53	0.67	–8.01	–0.25
	0.04	–171.82	–101.52	–65.81	1.07	–5.28	–0.28
	0.08	–171.65	–130.43	–39.01	1.18	–3.05	–0.35
^{40}Ca	0.02	–369.56	–158.28	–194.80	2.12	–17.80	–0.80
	0.04	–375.02	–238.62	–126.64	2.96	–11.86	–0.86
	0.08	–375.82	–298.75	–72.23	2.85	–6.82	–0.87

We consider the following approximation schemes, in which the W_N contributions $\delta E_{3B}^{(T)}$ to the triples correction are always neglected: For the "NO2B" scheme, all W_N terms are discarded in both, the determination of the T and Λ amplitudes and the energy $E_{2B}^{(\Lambda CCSD(T))}$, Eq. (131),

$$E^{(NO2B)} = E_{2B}^{(\Lambda CCSD(T))}(2B, 2B)\,. \tag{136}$$

This of course corresponds to an ordinary ΛCCSD(T) calculation in NO2B approximation. For scheme "A", we compute $E_{2B}^{(\Lambda CCSD(T))}$ as in the NO2B case and also add $\Delta E_{3B}^{(CCSD)}$ with T amplitudes obtained from the NO2B CCSD calculation,

$$E^{(A)} = E_{2B}^{(\Lambda CCSD(T))}(2B, 2B) + \Delta E_{3B}^{(CCSD)}(2B)\,. \tag{137}$$

This represents the simplest and most economic way to include W_N information, where it only enters in the expression for the energy contribution $\Delta E_{3B}^{(CCSD)}$, Eq. (66), but not in the considerably more complex equations that determinate the amplitudes. In scheme "B", we include full W_N information in the calculation of the CCSD correlation energy, keeping the W_N terms in the amplitude equations as well as in the energy expression. The triples correction, however, is calculated without any W_N information,

$$E^{(B)} = E^{(CCSD)}(3B) + \delta E_{2B}^{(T)}(2B, 2B)\,. \tag{138}$$

This way we keep consistency between the T and Λ amplitudes that enter the triples correction, while capturing all residual $3N$ effects in the CCSD energy $\Delta E^{(CCSD)}$. In scheme "C", we introduce an inconsistency between the T and Λ amplitudes by solving for T with the W_N terms present, while we solve for Λ without W_N terms and the energy expression is given by $\tilde{E}^{(\Lambda CCSD(T))}$, Eq. (135),

$$E^{(C)} = \tilde{E}^{(\Lambda CCSD(T))}(3B, 2B)\,. \tag{139}$$

This variant is reasonable since one typically has to solve for the T amplitude equations with W_N terms anyway in order to obtain the comparatively large $\Delta E_{3B}^{(CCSD)}$ contribution to the energy while one would like to avoid to solve for the Λ amplitudes in this manner. Finally, in scheme "D", in which we only neglect the residual $3N$ interaction terms in the expression for $\delta E^{(T)}$, we use the full, W_N-containing equations to solve for the T and Λ amplitudes and determine the energy via Eq. (135),

$$E^{(D)} = \tilde{E}^{(\Lambda CCSD(T))}(3B, 3B)\,. \tag{140}$$

As in the discussion of Fig. 4, this variant allows to estimate the importance of W_N for the Λ amplitudes.

In Fig. 5, for the case of ^{16}O, ^{40}Ca and the $NN + 3N$-full Hamiltonian, we compare the deviations of all the aforementioned approximation schemes to the complete $3N$ calculations. For ^{24}O and the $NN + 3N$-induced Hamiltonian we obtain very similar results. As expected, the "NO2B" scheme shows the largest deviations because the contributions of W_N to CCSD are completely missing. Including the W_N terms in the energy expression for the CCSD correlation energy but evaluating it using T amplitudes without W_N information in scheme "A" virtually does not change the result. Therefore, we can conclude that it is the W_N effect on the T amplitudes that is most important for CCSD, rather than the additional terms $\Delta E_{3B}^{(CCSD)}$. In our calculations, the best approximation to the complete calculations provides scheme "B", where we use full W_N information to determine the CCSD correlation energy, but otherwise no W_N information enters at all in the calculation of the triples correction. However, approximation schemes "B","C" and "D" give very similar results, again hinting at the W_N effect on the T amplitudes to be the most important ingredient in the inclusion of residual $3N$ interactions in CCSD and ΛCCSD(T) calculations.

IV. CONCLUSIONS

In this article we considered the extension of CC theory with full treatment of singly and doubly excited clusters and a non-iterative treatment of triply excited clusters to three-body Hamiltonians. The incorporation of $3N$ interactions into CCSD was previously discussed in detail in Ref. [63], so in this article we focused on the corresponding generalization of the non-iterative treatment of triply excited clusters. Among various triples corrections, for this first study we chose the ΛCCSD(T) approach due to its relatively simple structure.

The ΛCCSD(T) approach requires to solve the ΛCCSD equations prior to the computation of the actual energy correction and therefore we provided a detailed discussion of the inclusion of $3N$ interactions into these equations, where we list complete and explicit programmable expressions. The effective Hamiltonian is a central quantity of coupled-cluster theory and in this article we give explicit expressions for the contributions of the residual $3N$ interactions to all one- and two-body parts as well as selected three- and four-body parts of the effective Hamiltonian. We derived the ΛCCSD(T) method as an approximation from the more complete CR-CC(2,3) approach which allows for an easy identification of new terms arising due to the presence of residual $3N$ interactions, and we provide complete and explicit expressions required for the calculation of the ΛCCSD(T) energy correction.

An important outcome of our study is the realization that through the use of explicit $3N$ interactions in ΛCCSD(T), compared to the approximate NO2B treatment, contributions of the triply excited clusters are moved from second to first order in MBPT for the wave function, and from fourth to second order for the energy.

The method was applied to the medium-mass closed-shell nuclei ^{16}O, ^{24}O and ^{40}Ca using NN + $3N$ Hamiltonians obtained from chiral EFT. For the total binding energies, the effect of the residual three-body interactions at level of CCSD can become comparable to the ΛCCSD(T) correction, particularly for soft interactions, while for the ΛCCSD(T) correction itself, contributions of the residual $3N$ interactions were shown to be negligible. Therefore, for CCSD and ΛCCSD(T) calculations, by only including explicit $3N$ interactions at the CCSD level, we can practically eliminate the error introduced by the normal-ordering approximation. We further discussed various combinations of where to include the residual $3N$ interactions in the determination of the amplitudes from which energies are calculated, and found that the residual $3N$ interactions have their most significant effect on the cluster amplitudes.

V. ACKNOWLEDGMENTS

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