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How to renormalize coupled cluster theory*

Z. H. Sun,[1] C. A. Bell,[2] G. Hagen,[1,2] and T. Papenbrock[2,1]

[1] *Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[2] *Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*

Coupled cluster theory is an attractive tool to solve the quantum many-body problem because its singles and doubles (CCSD) approximation is computationally affordable and yields about 90% of the correlation energy. Capturing the remaining 10%, e.g. via including triples, is numerically expensive. Here we assume that short-range three-body correlations dominate and – following Lepage [1, "How to renormalize the Schrödinger equation," arXiv:nucl-th/9706029] – that their effects can be included within CCSD by renormalizing the three-body contact interaction. We renormalize this contact in ^{16}O and obtain systematically improved CCSD results for ^{24}O, $^{20-34}$Ne, ^{40,48}Ca, ^{78}Ni, ^{90}Zr, and ^{100}Sn.

Introduction.— In the past two decades computations of atomic nuclei based on Hamiltonians from effective field theories of quantum chromodynamics have advanced from the lightest nuclei to ^{208}Pb [2–12]. This progress is based on ideas and insights from effective field theory [13–15] and the renormalization group [16–18], and on computational solutions of the nuclear many-body problem that are systematically improvable and scale polynomially with increasing mass number [19–25].

Let us take coupled-cluster theory [21, 26–37] as an example. Here, one expresses the ground state as $|\psi\rangle = e^T|\phi\rangle$, where the reference $|\phi\rangle$ is an A-fermion product state and $T = T_1 + T_2 + \cdots + T_A$ is a cluster operator consisting of 1-particle-1-hole (1p-1h) up to Ap-Ah excitations. Its workhorse, the CCSD approximation, truncates $T = T_1 + T_2$ and provides us with an attractive compromise between accuracy and computational cost. In the Hartree-Fock basis, CCSD yields about 90% of the correlation energy (i.e. the difference between the exact energy and the expectation value $\langle\phi|H|\phi\rangle$ of the Hamiltonian H in the reference), while costing an effort that scales as A^2u^4 for a single-particle basis consisting of A occupied and u unoccupied orbitals.

The inclusion of triples excitations, i.e. $T = T_1 + T_2 + T_3$, typically yields about 98-99% of the correlation energy, and similar statements apply to quantum chemistry [38, 39]. It is not well understood why triples account for about 10% of the CCSD correlation energy [40], but size extensivity makes this fraction essentially independent of mass number. However, including triples excitations increases the cost to A^3u^5, which is significant because $A = \mathcal{O}(10)$ to $\mathcal{O}(100)$ and $u \gg A$.

To avoid this problem, several triples approximations have been introduced over the years, see, e.g. Refs. [41–48]. These approaches reduce the computing (and sometimes also storage) demands by expressing the triples amplitudes in terms of known quantities or by including only a subset of diagrams in their computation. They all aim at computing the energy gain from triples excitations included in the wavefunction.

Here, we propose a different path that focuses on shifting the effects of triples excitations from the wavefunction to the Hamiltonian. This approach seems particularly attractive in nuclear physics where one deals with Hamiltonians containing two- and three-nucleon interactions. These are resolution-scale dependent [16, 17, 49–52], i.e. they depend on an arbitrarily chosen dividing scale (i.e. the high-momentum cutoff Λ) that separates resolved long-range physics from unresolved (and unknown) short-range stuff. However, low-energy observables are resolution-scale independent and the change of the resolution (or renormalization) scale can be viewed as a similarity transformation [17]. Such transformations shift physics from the Hamiltonian to the wavefunction (and vice versa). We mention several examples. Lepage [1] showed how the removal ("integrating out") of short-range physics involving momenta larger than a given cutoff Λ can be compensated by renormalization using a short-range interaction of physical range $1/\Lambda$ or smaller. This is beautifully demonstrated in similarity renormalization group transformations of light nuclei [50, 53, 54], in the resolution-scale dependent interpretations of electron-nucleon scattering experiments [55–61], and in the computation of the β decay of ^{100}Sn with interactions and two-body currents from chiral effective field theory [62].

This motivates us to think about short-range correlations in the coupled-cluster state $|\psi\rangle$. The CCSD approximation introduces two-body correlations, and this in particular includes short-range two-body correlations. Thus, the CCSD wavefunction is accurate when two particles come close to each other, but still further apart than the distance $1/\Lambda$. (Here, we assume that the single-particle basis is sufficiently large and exhibits an ultraviolet cutoff $\Lambda_{\rm UV} \gtrsim \Lambda$ [63].) However, the CCSD ap-

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proximation becomes inaccurate if three (or more) particles are close. The inclusion of triples excitations would remedy this shortcoming. Lepage [1] taught us that one deals with this problem by adding a short-range three-body interaction with a suitably chosen strength such that it renormalizes CCSD. In other words, the CCSD approximation removes (or excludes) short-range physics in the three-body sector from the wavefunction. This then requires the renormalization of the Hamiltonian via a short-range three-body potential.

To see this, we consider the coupled-cluster energy

$$\begin{aligned} E &= \langle\phi|e^{-T_1-T_2-T_3} H e^{+T_1+T_2+T_3}|\phi\rangle \\ &= \langle\phi|e^{-T_1-T_2} \left(e^{-T_3} H e^{T_3}\right) e^{+T_1+T_2}|\phi\rangle \end{aligned} \tag{1}$$

in the singles, doubles, and triples approximation. Here we shifted the T_3 correlations from the wavefunction to the Hamiltonian. Let us now assume that the main effects of triples T_3 consist of short-ranged three-body correlations. Then, following Ref. [1],

$$e^{-T_3} H e^{T_3} \approx H + V_3 \ . \tag{2}$$

Here, V_3 denotes a three-body contact. The relation (2) is not an operator identity (the right-hand side is Hermitian, while the left-hand side is not) but rather a low-energy (or long wavelength) approximation [1]. Systematic corrections consist of derivatives acting on the contact, see Refs. [1]. These enter as subleading three-nucleon forces in chiral [65] and pion-less effective field theories [66].

We present these arguments in more detail: Bedaque *et al.* [67] presented scattering equations for three bosons[2], where the physics of the two-body subsystem was kept renormalization-group invariant (by employing observables such as the two-body scattering length or the two-body bound-state energy). In those equations, a momentum cutoff for the three-body Jacobi momentum $(2p_3 - p_1 - p_2)/3$ enters, and the variation of this momentum cutoff requires a three-body contact for proper renormalization. Let us assume that coupled-cluster theory is applied in a momentum-space basis, and that one starts to reduce the cutoff in the triples excitations only. Based on Refs. [67, 68] a three-body contact must then be adjusted to keep renormalization group invariance. Removing the triples excitations entirely (i.e. lowering the cutoff to the Fermi momentum) does not change this picture at leading order. Our understanding of effective field theories and the renormalization group also implies that higher precision (e.g. agreement with triples results also for excited states in the nucleus considered for renormalization, or agreement with triples results for ground states of other nuclei) can be obtained by including higher-order three-body contacts [1]. In what follows, we will limit ourselves to the leading contact.

We note here that the extension of Lepage's argument from two- to three-body systems becomes also clear when using hyperspherical coordinates. Then, a three-body collision is clearly short ranged as the hyperradius becomes small, and this physics – when integrated out by lacking wavefunction correlations – must be included by renormalizing a hyperspherical contact. This corresponds then to a three-body contact in single-particle coordinates.

We see now why this renormalization is particularly attractive in nuclear physics. Here, a three-body contact already appears at leading order in pion-less effective field theory [68] and at a next-to-leading (next-to-next-to-leading) order in chiral effective field with (without) delta isobars [13, 69]. Thus, restricting the computational solution of the nuclear many-body problem to CCSD simply requires one to renormalize the strength of that contact.

We note finally, that the lack of three-body forces in quantum chemistry probably makes the proposed renormalization scheme much less attractive in that field. Furthermore, three electrons can not interact via a three-body contact and this would require one to employ several contacts with quadratic gradients [66] for the renormalization.

Renormalization of the three-body contact.— We employ the nuclear Hamiltonian

$$H = T_{\rm in} + V_{NN} + V_{NNN} \ . \tag{3}$$

Here, $T_{\rm in}$ denotes the intrinsic kinetic energy (i.e. the total kinetic energy minus that of the center of mass), V_{NN} the nucleon-nucleon interaction, and V_{NNN} the three-nucleon potential. The coupled-cluster computations start from the Hartree-Fock basis, and the Hamiltonian is normal-ordered with respect to the Hartree-Fock reference state. Following the normal-ordered two-body approximation [7, 70], we neglect the residual three-body interaction.

We employ two interactions, namely 1.8/2.0(EM) from Ref. [52] (labelled as interaction A) and ΔNNLO$_{\rm GO}$(394) from Ref. [71] (labelled as B). Interaction A has a cutoff of 1.8 and 2.0 fm^{-1} in the two-body and three-body potential, respectively, while interaction B has a cutoff of 394 MeV in all potentials. Both interactions yield accurate binding energies for medium-mass nuclei. We renormalize their three-body contact c_E in ^{16}O, requiring that CCSD computations of the ground-state energies with the renormalized interactions agree (to four significant digits) with triples results using the original interactions. For the triples computations we use Λ-CCSD(T) [48] for interaction A and CCSDT-1 for interaction B (taken from Ref. [71]). In our computations we use a model space consisting of 15 harmonic oscillator shells with a frequency $\hbar\omega = 16$ MeV. Table I shows the renormalized values of c_E and compares them with the original ones. The

[1] For a formal renormalization of coupled-cluster theory in the frame work of quantum field theory see, e.g., Ref. [64].

[2] This applies also to nucleons as three nucleons can be in an s-wave state that is antisymmetric in spin and isospin.

renormalized values appear to be natural in size, see, e.g., Ref. [72]. The Hartree-Fock energy [73] for symmetric nuclear matter is $\langle V_3 \rangle = -3\Delta c_E \rho^2 A/(16 f_\pi^4 \Lambda_\chi)$ where Δc_E is the change in c_E, $\rho = 0.16$ fm^{-3} the saturation density, $f_\pi = 92.4$ MeV the pion-decay constant, and $\Lambda_\chi = 700$ MeV the spectral-function regulator. This yields $-0.32A$ and $-0.66A$ MeV for interactions A and B, respectively. These simple estimates are about a factor 1.5 larger than what we find below.

TABLE I. Employed interactions are 1.8/2.0(EM) from Ref. [52] (labelled as A) and ΔNNLO$_{\rm GO}$(394) from Ref. [71] (labelled as B). Their renormalized versions only differ by the modified three-body contact c_E from the originals.

Interaction	Name	c_E
A	1.8/2.0(EM)	-0.12 [52]
A renorm.		-0.0665
B	ΔNNLO$_{\rm GO}$(394)	-0.002 [71]
B renorm.		0.11

We perform CCSD computations of other nuclei with the properly renormalized interactions. Results are shown in Table II. The CCSD results with the renormalized interactions are very close to the triples results, with the largest deviation (in ^{40}Ca for interaction B) being less than 2%. This demonstrates that triples indeed account mainly for short-ranged three-body correlations, and that the proposed renormalization is effective.

TABLE II. Binding energies (in MeV) for selected nuclei computed with CCSD using the renormalized interactions and compared to triples results [Λ-CCSD(T) for interaction A and CCSDT-1 for interaction B] using the original interactions. Experimental values are shown in the last column.

	Interaction and method				
	A renorm. CCSD	A Λ-CCSD(T)	B renorm. CCSD	B CCSDT-1	Exp.
^{16}O	127.8	127.8	127.5	127.5	127.62
^{24}O	166	165	169	169	168.96
^{40}Ca	346	347	341	346	342.05
^{48}Ca	420	419	419	420	416.00
^{78}Ni	642	638	636	639	641.55
^{90}Zr	798	795	777	782	783.90
^{100}Sn	842	836	816	818	825.30

To check that improvements from the renormalization are systematic, we take the triples values from Table II as benchmarks and compute the absolute differences (with respect to the benchmark) of the energy per particle for Hartree Fock and for CCSD using the original interactions A and B. We also compute the absolute differences of the CCSD energy per particle using the renormalized interactions. The results are shown in Fig. 1 for interaction A (B) as full (hollow) markers, using black circles and blue squares for Hartree Fock and CCSD, respectively, with the original interactions, and red diamonds for CCSD with the renormalized interactions. For the original interactions, CCSD gives an order-of-magnitude improvement in accuracy over Hartree Fock. The CCSD computations with the renormalized interactions improve the accuracy by another order of magnitude. This shows that the renormalization indeed yields a systematic improvement. The nucleus ^{40}Ca is a bit an outlier for interaction B; however, the improvement in accuracy is still about a factor of four also here.

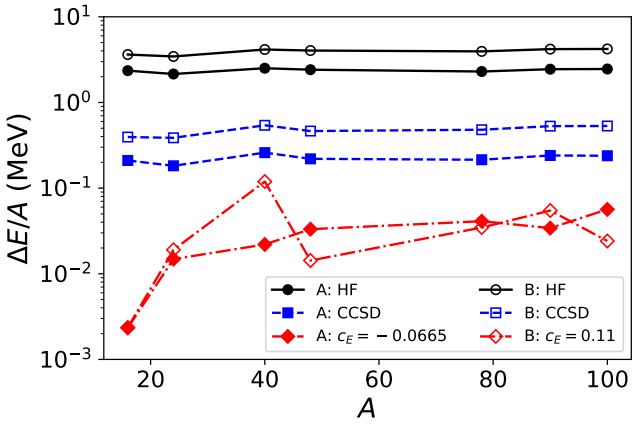

FIG. 1. Absolute difference of energies per nucleon with respect to triples benchmarks as a function of nucleon number for ^{16,24}O, ^{40,48}Ca, ^{78}Ni, ^{90}Zr, and ^{100}Sn using Hartree Fock (HF, black circles) and CCSD (blue squares) for the interactions A (full markers) and B (hollow markers) and for CCSD computations with the renormalized interactions (red diamonds) where the three-body contact has c_E as labelled.

Two comments are in order. First, changing the renormalized c_E value about 5-10% does not reduce the systematic improvement. Thus, c_E is not finely tuned (and could probably be also renormalized in a nucleus different from ^{16}O). Second, performing the renormalization in ^{4}He does not yield accurate results for heavier nuclei, because triples corrections in ^{4}He are much smaller than the usual 10% of the correlation energy obtained for heavier nuclei. The renormalized interaction B yields a binding energy of 29.63 MeV for ^{4}He. Alternatively, we used a three-body contact with a higher cutoff of 450 MeV and strength $\tilde{c}_E = 0.0425$ for the renormalization of interaction B in ^{16}O. This yields a binding energy of 29.41 MeV for ^{4}He (we checked that heavier nuclei such as ^{24}O and ^{40}Ca are unchanged). We speculate that it might be possible to reproduce binding energies for ^{4}He and ^{16}O by optimizing the cutoff of the three-body counter term.

We found that essentially the whole triples contributions to the binding energies using the original interactions become part of the Hartree-Fock energies when using the renormalized interactions, i.e. the energy contributions from CCSD using the original or the renormalized interactions are virtually the same. This is shown in Fig. 2 for both interactions.

Power counting.— The approach via renormalization

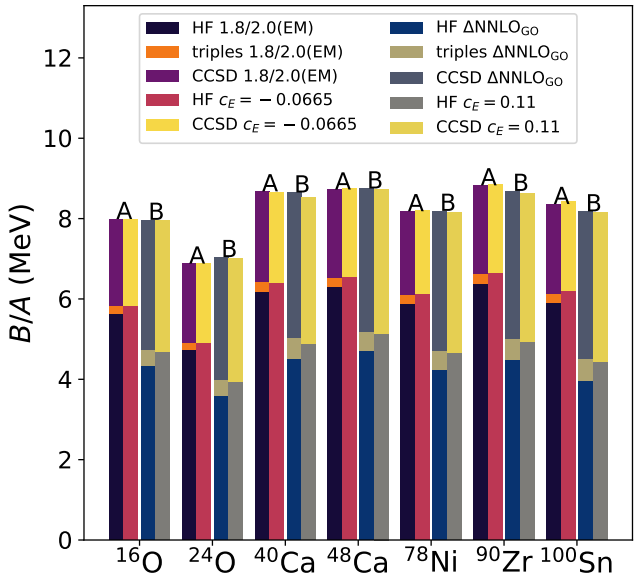

FIG. 2. Energy contributions from Hartree Fock (HF), triples, and CCSD to the binding energy per nucleon, B/A, of various nuclei, computed with the original interactions A and B (three stacked left bars in pairs of columns) and compared with Hartree-Fock and CCSD energies from the renormalized interactions (two stacked right bars in pairs of columns). For each nucleus the left and right pairs of columns show the results for the interaction A and B, respectively.

makes it clear how one would further improve these results, i.e. bring the CCSD calculations with renormalized interactions closer to the triples benchmarks [1]: The subleading corrections consist of 13 three-body contact terms with two derivatives [66]. This would require one to adjust as many low-energy coefficients to data, and such an approach is beyond the scope of this work. Thus, renormalization offers us a way to systematically improve the results. The key question then concerns the power counting, i.e. by how much would one expect the subleading corrections to get closer to the triples benchmark?

The proposed renormalization scheme must break down when triples correlations are not dominantly short ranged. In CCSD, the three-body hypermomentum k_3 is small because we lack short-ranged three-body correlations. A derivative three-body contact yields k_3 and we have $k_3 \ll k_{\rm typ}$, where $k_{\rm typ}$ is the typical momentum (which could be of the scale of the Fermi momentum). The derivative's contribution fails to be small (compared to the leading three-body contact) if $k_3 \approx k_{\rm typ}$, i.e. for low-density nucleons without short-range three-body correlations. We therefore propose that the power counting is in the ratio $k_3/k_{\rm typ}$. This ratio must be small for nuclei, because the leading contact recovers so much of the triples benchmarks.

The arguments proposed below would entail that the renormalization is less effective in low-density matter and dripline nuclei. Using the renormalized interaction B, we also computed neutron-rich neon isotopes and compared with the triples results [74] of the original interaction. The calculations are based on an axially-symmetric Hartree-Fock state and lack angular momentum projection. The results, shown in Fig. 3, demonstrate that the renormalization significantly and systematically improves the ground-state energies. For the most neutron-rich isotopes, though, the accuracy is "only" improved by a factor of about four. These reduced gains are consistent with the arguments made for the power counting. We see that the proposed renormalization is also useful for open-shell nuclei.

We also computed the charge radius of ^{20}Ne and found that the renormalized interaction yields about 1.8% less than the original one [74]. This is consistent in size with what is found for the renormalization group evolution of long-ranged operators [75]. In contrast, magnetic moments and the Gamow-Teller operator also contain significant short-range contributions and the proposed renormalization would also affect the corresponding one- and two-body currents [62, 76].

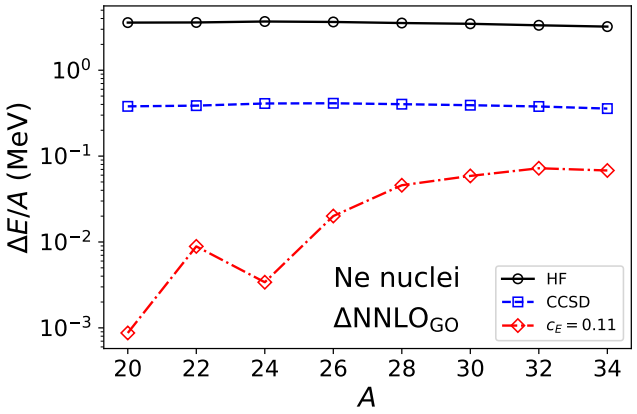

FIG. 3. Absolute difference of energies per nucleon with respect to CCSDT-1 as a function of nucleon number for $^{20-34}$Ne nuclei using Hartree Fock (HF, black circles) and CCSD (blue squares) for the interaction B and for CCSD computations with the renormalized interaction where the three-body contact has been renormalized with $c_E = 0.11$ (red diamonds).

We finally turn to symmetric nuclear matter and perform the computations following Refs. [71, 77], taking CCD(T) as the benchmark. The calculations use $A = 132$ nucleons on a momentum-space lattice (with $n_{\rm max} = 4$) corresponding to periodic boundary conditions in position space. We checked that CCSDT-1 benchmarks are close to the less expensive CCD(T) for $A = 28$. Figure 4 shows the absolute difference to the triples benchmark of the energy per nucleon as a function of the density ρ for Hartree Fock and CCD with the interaction B, and for CCD with the renormalized interaction B. We see that CCD with the interaction renormalized in ^{16}O is very accurate around saturation density. We note that the energy difference changes sign there. In-

spection also shows that the Hartree-Fock energy for the renormalized interaction differs from that of the original one by a contribution proportional to ρ^2. This explains the trend seen for neutron-rich neon nuclei. Figure 4 also shows that the renormalization breaks down at low densities ($\rho \approx 0.06$ fm^{-3}) and high densities ($\rho \approx 0.24$ fm^{-3}).

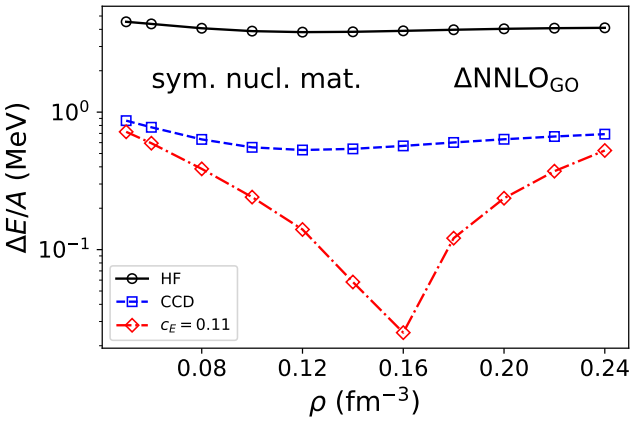

FIG. 4. Absolute difference of energies per nucleon with respect to CCD(T) as a function of density using Hartree Fock (HF, black circles) and CCD (blue squares) for the interaction B and for CCD computations with the renormalized interaction where the three-body contact has been renormalized with $c_E = 0.11$ (red diamonds).

Discussion and summary.— We have seen that the extensive energy contributions from nuclear three-nucleon correlations can be captured in CCSD via a renormalization of the three-body contact. Our results are based on (and consistent with) the assumption that three-nucleon correlations are dominantly short ranged. This suggests that arguments about the universality of short-range two-body correlations [57, 60, 61, 63] extend to three-nucleon correlations.

While we focused on the coupled-cluster theory, this method is closely related to the in-medium similarity renormalization group (IMSRG) [18, 24, 25], Green's function approaches [19], and Gorkov methods [23]. Including three-body correlations in the IMSRG [78] or in the trial wavefunction of variational Monte Carlo is also a challenging task [79, 80]. This suggests that the renormalization proposed in this paper could also be useful for these methods.

This paper also explains why triples correlations play a smaller role in neutron matter [77] than in nuclear matter: the Pauli principle prevents short-ranged three-neutron correlations, and the leading renormalization comes from terms where two derivatives act on a three-body contact. This would require one to adjust several contact terms with derivatives, thus making the proposed renormalization more complicated.

The proposed renormalization does not remove three-body correlations but rather compensates for the lack of three-body correlations in the employed computational method. Thus, the renormalized Hamiltonian must not be solved with triples correlations included. This is similar to nuclear density functional theory where uncorrelated densities must be used. One might consider to take the proposed renormalization to its extreme: Hartree-Fock computations also exclude two-body correlations. This suggests to employ Hamiltonians from effective field theories with properly renormalized two- and three-body contacts [81–84].

The proposed renormalization scheme significantly lowers the computational cost for nuclear binding energies and thereby puts Hamiltonian-based masstable computations of atomic nuclei [85] in closer reach of various *ab initio* methods. It also links correlations in many-body systems to the renormalization group and thereby offers new ways to think about their role.

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