How to renormalize coupled cluster theory

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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 16O and obtain accurate CCSD results for 24O, 20–34Ne, 40,48Ca, 78Ni, 90Zr, and 100Sn.

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 208Pb [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 excitation 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 \(A^2 u^4\) 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 \(A^3 u^6\), which is significant because \(A = O(10)\) to \(O(100)\) 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 wave function.

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 \(\Lambda\) 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 \(\Lambda\) 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 Gamow-Teller decay of 100Sn 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 \(\Lambda_{UV} \gtrsim \Lambda\) [63].) However, the CCSD approximation 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 the Schrödinger equation. In other words, the CCSD approximation removes (or excludes) short-range physics in the three-body sector from the wave function. This then requires the renormalization of the Hamiltonian, which in this case introduces a short-range three-body potential.
To see this, we consider the coupled-cluster energy

\[ E = \langle \phi | e^{-T_1 - T_2 - T_3} H e^{T_1 + T_2 + T_3} | \phi \rangle = \langle \phi | e^{-T_1 - T_2} (e^{-T_3} H e^{T_3}) e^{T_1 + T_2} | \phi \rangle \]

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],

\[ e^{-T_3} H e^{T_3} \approx H + V_3 . \]

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. Systematic corrections consist of derivatives acting on the contact, see Ref. [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 [64] and at a next-to-leading (next-to-next-to-leading) order in chiral effective field with (without) delta isobars [13, 65]. Thus, restricting the computational solution of the nuclear many-body problem to CCSD simply requires one to renormalize the strength of that contact.

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

\[ H = T_{in} + V_{NN} + V_{NNN} . \]

Here, \( T_{in} \) 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, 66], 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 \( \Delta NNLO_{GO}(394) \) from Ref. [67] (labelled as B). We renormalize their three-body contact \( c_E \) in \(^{16}\text{O}\), 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 \( \Lambda\text{-CCSD(T)} \) [48] for interaction A and CCSDT-1 for interaction B (taken from Ref. [67]). Table I shows the renormalized values of \( c_E \) and compares them with the original ones. In our computations we use a model space consisting of 15 harmonic oscillator shells with a frequency \( \hbar \omega = 16 \) MeV.

**TABLE I.** Employed interactions are 1.8/2.0(EM) from Ref. [52] (labelled as A) and \( \Delta NNLO_{GO}(394) \) from Ref. [67] (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.   | 1.8/2.0(EM)   | -0.0665  |
| B           | \( \Delta NNLO_{GO}(394) \) | -0.002 [67] |
| B renorm.   | \( \Delta NNLO_{GO}(394) \) | 0.11     |

We turn to computations of other nuclei, performing CCSD computations with the properly renormalized interactions. Results are shown in Table II. The CCSD results based on the renormalized interactions are very close to the triples results, with the largest deviation (in \(^{40}\text{Ca}\) 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 [\( \Lambda\text{-CCSD(T)} \) for interaction A and CCSDT-1 for interaction B] using the original interactions. Experimental values are shown in the last column.

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

How systematic is the improvement coming from renormalization? To address this question, 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 (holow) 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. (We also see that interaction A is softer than interaction B because it is closer to the triples benchmark for Hartree Fock and CCSD.) 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. As already seen in Table II, 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.

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. We attribute this to the fact that triples corrections in $^4$He are much smaller than the usual 10% of the correlation energy obtained for heavier nuclei.

How are the triples contributions accounted for in the renormalized interaction? 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 Figs. 2 for both interactions.

**Power counting.**—The approach via renormalization 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 three-body contact terms with two derivatives. Girlanda *et al.* [68] showed that there are 13 such terms with different spin-isospin structures, and this would require one to adjust as many low-energy coefficients to data. While one could, for example, accomplish this in mass-table computations, such an approach is beyond the scope of this work. The important point here is that 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. A derivative on the three-body contact yields a momentum $\min(k_3, k_{typ})$, where $k_3$ is a small three-body momentum (because we lack short-ranged three-body correlations) and $k_{typ}$ is the typical momentum which could be of the scale of the Fermi momentum. We have $k_3 \ll k_{typ}$ when three-body correlations are short ranged. The derivative’s contribution fails to be small (compared to the leading three-body contact) if $k_3 \approx k_{typ}$, i.e. for low-density nucleons without short-range three-body correlations. We therefore propose that the power counting is in the ratio $k_3/k_{typ}$. 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. This makes it interesting to study dripline nuclei. Us-

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**FIG. 1.** Absolute difference of energies per nucleon with respect to triples benchmarks as a function of nucleon number for $^{16,24}$O, $^{40,44}$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.

**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.
ing the renormalized interaction B, we also computed neutron-rich neon isotopes and compared with the triples results [69] of the original interaction. The calculations are based on an axially-symmetric deformed Hartree-Fock state, and they 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. The trend of reduced gains from renormalization as the dripline is approached is consistent with the arguments made for the power counting. Thus, our calculations of neon nuclei show that the renormalization proposed in this work 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 [69]. This is consistent with what is found for the RG evolution of long-ranged operators [70].

We finally turn to symmetric nuclear matter and perform the computations following Refs. [67, 71], taking CCD(T) as the benchmark. The calculations use $A = 132$ nucleons on a momentum-space lattice (with $n_{\text{max}} = 4$) 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 $\rho$ 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. Inspection also shows that the Hartree-Fock energy for the renormalized interaction differs from that of the original one by a contribution proportional to $\rho^2$. 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. 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).](image)

**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 our discussions 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]. In the IMSRG, for instance, capturing three-body correlations comes at a very high cost [72]. Including three-body correlations in the trial wave functions of variational Monte Carlo is also a challenging task [73, 74]. This suggests that the renormalization proposed in this paper could also be useful for these methods.

The insights presented in this paper also explain why triples correlations play a smaller role in neutron matter [71] 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.

One might also consider to take the renormalization proposed in this paper to its extreme: Hartree-Fock computations even exclude two-body correlations. This suggests that one could also employ Hamiltonians from effective field theories using properly renormalized two- and three-body contacts (and derivatives acting on them).
This somewhat resembles the expansions \cite{75, 76} for density functionals but would be for Hamiltonians \cite{77}.

The proposed renormalization scheme significantly lowers the computational cost for nuclear binding energies and thereby puts Hamiltonian-based massstable computations of atomic nuclei \cite{78} in closer reach of various \textit{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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