Spurious Isospin Breaking in the In-medium Similarity Renormalization Group

A. Farren
Trinity College, Dublin, Ireland

S. R. Stroberg
Department of Physics and Astronomy, University of Notre Dame Notre Dame, IN, 46556, USA *

(Dated: December 14, 2024)

Robustly quantifying the uncertainty in the isospin-related theoretical correction δ_C to superallowed beta decay rates is vital for a correct assessment of CKM unitarity. To this end, we identify the sources of artificial or *spurious* isospin symmetry breaking introduced by the IMSRG many-body framework at a computational level and provide remedies. We test our best policy for preventing spurious ISB by evaluating δ_C.

I. INTRODUCTION

Superallowed Fermi beta decays provide a stringent test of the Standard Model [1]. These tests require precise measurements, as well as precise calculations of Standard Model effects. A current mild tension with unitarity of the Cabibbo-Kobayashi-Maskawa quark mixing matrix [2, 3], combined with recent progress in *ab initio* nuclear theory has led to increased interest in revisiting these Standard Model corrections with a more rigorous uncertainty quantification [4, 5]. In the present work, we focus on the isospin-breaking correction δ_C, defined as the deviation of the matrix element of the isospin raising operator from the isospin-conserving limit:

$$|\langle\psi_f|T^{\pm}|\psi_i\rangle|^2 = |\langle T_f|T^{\pm}|T_i\rangle|^2(1-\delta_C). \tag{1}$$

For the most extensively studied $T = 1$ cases, the isospin-limit matrix element squared is equal to 2. Deviations from this value are due primarily to the Coulomb interaction between protons, in addition to smaller effects such as the u-d quark mass difference, and the mass difference between the charged and neutral pions.

The precisely-measured superallowed decays range from $A = 10$ to $A = 74$, and in all cases the initial or final nucleus (or both) is open shell, so these decays pose a challenge for *ab initio* theory. The no-core shell model can reach the lightest of these systems [6, 7], but reaching beyond $A \sim 14$ will require a method that scales polynomially with the system size. The in-medium similarity renormalization group (IMSRG), and in particular the valence space formulation (VS-IMSRG), is a polynomially-scaling method capable of reaching all relevant systems. However, as with other polynomially-scaling methods, quantifying uncertainties due to truncations in the many-body solution is non-trivial. In particular, as we will describe below, the truncations usually made in the IMSRG can lead to *spurious* isospin symmetry breaking, directly competing with the authentic and physical signal of interest.

In this paper, we explore the sources and mechanisms of spurious symmetry breaking within the IMSRG, with the eventual goal of reducing these effects to levels needed for precise tests of the Standard Model. While we focus on isospin symmetry breaking, this work also has relevance for the breaking of other symmetries, for example of rotational symmetry in the treatment of deformed systems [8]. Importantly, the usual prescription of projecting onto good symmetries cannot be used in this case because the symmetry-breaking behavior is precisely the desired signal.

A. IMSRG

The details of the IMSRG are presented in several review articles [9–11]. Here we briefly summarize the relevant features.

To simplify *ab initio* many-body calculations, we want to decouple physics at different scales of energy by block-diagonalizing the Hamiltonian with respect to a reference. The IMSRG formalism provides a method to systematically improve such calculations.

Given a many-body system in some eigenstate $|\psi\rangle$ of the original Hamiltonian $H(0)$, we want to use a unitary similarity transformation

$$H(s) \equiv U(s)H(0)U^{\dagger}(s) \tag{2}$$

determined by a flow parameter s to find the energy E of $|\psi\rangle$. We choose a reference $|\Phi_0\rangle$ which is our initial guess of the exact ground state, and so we work 'in-medium' rather than in-vacuum. We think of the exact state as the limit

$$|\psi\rangle = \lim_{s\to\infty} U^{\dagger}(s)\,|\Phi_0\rangle\,. \tag{3}$$

One can freely impose the condition $\frac{d}{ds}U(s) \equiv \eta(s)U(s)$ such the flow equation of the Hamiltonian reads

$$\frac{d}{ds}H(s) = [\eta(s), H(s)]. \tag{4}$$

* rstroberg@.nd.edu

Then, the *generator* of the flow η is chosen such that

$$H(s) \equiv H^{\rm d}(s) + H^{\rm od}(s) \overset{s\to\infty}{\to} H^{\rm d}(s), \tag{5}$$

where $H^{\rm d}(s)$ is diagonal in the *core*. The similarity transformation makes it easy to read off the core's energy via the reference expectation value of the flowed $H(s)$:

$$E = \lim_{s\to\infty} \langle\Phi_0|\, H(s)\, |\Phi_0\rangle = \lim_{s\to\infty} \langle\Phi_0|\, H^{\rm d}(s)\, |\Phi_0\rangle\,. \tag{6}$$

Usually the core is defined as the set of orbitals occupied in $|\Phi_0\rangle$ while the unoccupied orbitals are called *excluded*. As $s\to\infty$ the Hamiltonian becomes diagonal in the state $|\Phi_0\rangle$, i.e., for all non-trivial particle-hole pairs one has

$$\lim_{s\to\infty} \langle\Phi_0|\, H(s)\, \big|\Phi^{ab\cdots}_{ij\cdots}\big\rangle \equiv 0. \tag{7}$$

Our convention is that $a, b, c, ...$ index unoccupied/particle states while $i, j, k, \ldots$ index occupied/hole states in a basis of Slater determinants. Letters $p, q, r, \ldots$ refer to generic states and could be occupied or not. Overlined letters $\overline{a}, \overline{i}, \overline{p}$ refer to the respective nucleon orbitals a, i, p with isospin flipped.

In many-body quantum mechanics [12], it is convenient to work with operators normal-ordered with respect to the reference $|\Phi_0\rangle$. A generic operator A can be written as

$$\begin{aligned} A = {} & \langle\Phi_0|\, A\, |\Phi_0\rangle + \sum_{pr} A_{pr}\{\hat{p}^\dagger \hat{r}\} \\ & + \frac{1}{(2!)^2}\sum_{pqrs} A_{pqrs}\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} \\ & + \frac{1}{(3!)^2}\sum_{pqvrsw} A_{pqvrsw}\{\hat{p}^\dagger\hat{q}^\dagger\hat{v}^\dagger\hat{w}\hat{s}\hat{r}\} + \ldots \end{aligned} \tag{8}$$

where the braces indicate normal-ordering with respect to $|\Phi_0\rangle$, such that

$$\{\hat{p}^\dagger\hat{q}^\dagger\cdots\hat{s}\hat{r}\} = \hat{p}^\dagger\hat{q}^\dagger\cdots\hat{s}\hat{r} - \langle\Phi_0|\, \hat{p}^\dagger\hat{q}^\dagger\cdots\hat{s}\hat{r}\, |\Phi_0\rangle \tag{9}$$

and we use shorthand for creation and annihilation operators $a^\dagger_p \sim \hat{p}^\dagger$. We call the expectation value $A_0 = \langle\Phi_0|\, A\, |\Phi_0\rangle$ the zero-body (0B) part of A, the terms A_{pr} which annihilate and create a single orbital the one-body (1B) part, the terms A_{pqrs} which annihilate and create two orbitals the two-body (2B) part and so on. The combinatorial factors of the form $1/(k!)^2$ appear because the 2B+ matrix elements are anti-symmetrized when working with fermions. The normal-ordered Hamiltonian, up to two-nucleon interactions, is written

$$H = E_0 + \sum_{pr} f_{pr}\{\hat{p}^\dagger\hat{r}\} + \frac{1}{(2!)^2}\sum_{pqrs}\Gamma_{pqrs}\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\}. \tag{10}$$

An important consequence of normal-ordering is that for normal-ordered KB and LB operators the commutator is given by a sum of MB operators, i.e.

$$[K, L] \to M, \tag{11}$$

where $|K-L| \le M \le K+L-1$ [13]. For a simple product of operators that range is $|K-L| \le M \le K+L$. For example, given a one-body operator A and a two-body operator B,

$$\begin{aligned} [A, B] = {} & [A_{\rm 1B}, B_{\rm 1B}]_{\rm 0B} + [A_{\rm 1B}, B_{\rm 1B}]_{\rm 1B} \\ & + [A_{\rm 1B}, B_{\rm 2B}]_{\rm 1B} + [A_{\rm 1B}, B_{\rm 2B}]_{\rm 2B} \end{aligned} \tag{12}$$

and one would refer to $[A_{\rm 1B}, B_{\rm 2B}]_{\rm 1B}$ as the $[1,2]\to 1$ contribution.

The number k in IMSRG(k) indicates the particle rank after which we truncate the induced normal-ordered operators at each calculation in order to avoid prohibitive computational cost. For example, consider evaluating an operator commutator $[A, B] = C$ between 2B operators A and B. At IMSRG(2), we keep at most resulting 2B operators such that

$$C = C_0 + \sum_{pq} C_{pq}\{\hat{p}^\dagger\hat{q}\} + \frac{1}{(2!)^2}\sum_{pqrs} C_{pqrs}\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} \tag{13}$$

where we discard C_{pqvrsw}, in this case coming from the contribution $[2,2]\to 3$. This truncation is an approximation and does not preserve the unitary transformation (2) which is used to evolve all operators along the flow.

Looking at (11), if we sum over a basis N states during the matrix multiplication, the product's computational complexity would scale as N^{K+L+M}. For IMSRG(3) we have $M \le 3$ so that $[2,2]\to 3$, $[2,3]\to 3$ and $[3,3]\to 3$ are all possible commutator scenarios. We usually use shell model spin-orbitals with $N \ge 20$ so the scalings N^7, N^8 and N^9 differ significantly [14]. To limit computational cost while maintaining the increased accuracy, we will also use IMSRG(3N7) which limits the surviving 3B operators of IMSRG(3) to commutator and product diagram topologies of complexity N^7.

We work in a basis of spherical harmonic oscillators and truncate this basis by limiting the quantum number $(2n+\ell) \le e_{\rm max}$ and typically choose $e_{\rm max} = 2, 3$ for the purpose of demonstrating isospin symmetry breaking.

1. *Magnus formulation*

One choice of unitary transformation is defined by the Magnus formulation [15] where $U(s) \equiv e^{\Omega(s)}$. From $\frac{d}{ds}U(s)$, one finds the flow equation for the anti-hermitian Magnus operator $\Omega(s)$

$$\frac{d}{ds}\Omega(s) = \sum_{n=0}^{\infty}\frac{B_n}{n!}c^n_\Omega(\eta), \tag{14}$$

where B_n are the Bernoulli numbers and c_Ω^n are nested commutators

$$c_\Omega^0(\eta) \equiv \eta, \qquad c_\Omega^n(\eta) \equiv \big[\Omega, c_\Omega^{n-1}(\eta)\big]. \tag{15}$$

Operators evolve as $\hat{\mathcal{O}}(s) = e^{\Omega(s)}\hat{\mathcal{O}}(0)e^{-\Omega(s)}$ so that we can numerically evolve $\Omega(s)$ using (14) and then transform any number of operators along the IMSRG flow. Here we will exclusively use the Magnus formulation.

2. *Choice of generator*

We have the freedom to chose $\eta(s)$ as long as it drives $H^{\rm od}(s) \to 0$ along the flow. Here we introduce three appropriate generators for the single reference case. Note $H^{\rm od}$ connects the reference to excitations and so has the normal-ordered form

$$H^{\rm od} = \sum_{ai} f_{ai}\{\hat{a}^\dagger\hat{i}\} + \frac{1}{4}\sum_{abij}\Gamma_{abij}\{\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\} + \dots \ . \tag{16}$$

The *White generator* [16] is defined as

$$\begin{aligned}\eta_{\rm W}(s) &\equiv \frac{H^{\rm od}(s)}{\Delta(s)} \\ &= \sum_{ai}\frac{f_{ai}}{\Delta_{ai}}\{\hat{a}^\dagger\hat{i}\} + \frac{1}{4}\sum_{abij}\frac{\Gamma_{abij}}{\Delta_{abij}}\{\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\} + \dots\end{aligned} \tag{17}$$

where we introduce an energy denominator Δ. The *arctangent generator* [16] is

$$\begin{aligned}\eta_{\rm A}(s) &\equiv \frac{1}{2}\,\mathrm{atan}\left(2\frac{H^{\rm od}(s)}{\Delta}\right) \\ &= \frac{1}{2}\sum_{ai}\mathrm{atan}\left(2\frac{f_{ai}}{\Delta_{ai}}\right)\{\hat{a}^\dagger\hat{i}\} \\ &\quad + \frac{1}{8}\sum_{ai}\mathrm{atan}\left(2\frac{\Gamma_{abij}}{\Delta_{abij}}\right)\{\hat{a}^\dagger\hat{b}\hat{j}\hat{i}\} + \dots\end{aligned} \tag{18}$$

while the *imaginary time generator* [10] is

$$\begin{aligned}\eta_{\rm IT}(s) &\equiv \frac{H^{\rm od}(s)}{\mathrm{sgn}(\Delta)} \\ &= \sum_{ai}\mathrm{sgn}(\Delta_{ai})f_{ai}\{\hat{a}^\dagger\hat{i}\} \\ &\quad + \frac{1}{4}\sum_{abij}\mathrm{sgn}(\Delta_{abij})\Gamma_{abij}\{\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\} + \dots \ .\end{aligned} \tag{19}$$

The solution to the flow equation (4) for all three choices of η leads to suppressed $H^{\rm od}$ [10]. In IMSRG calculations, we primarily use denominators based on Epstein-Nesbet or Møller-Plesset partitioning. The Epstein-Nesbet partitioning (EN) of an energy denominator $\Delta_{ab\dots ij\dots}$ is defined as follows, up to a particle rank of 2,

$$\begin{aligned}\Delta_{ai} &= \langle\Phi_i^a|\,H\,|\Phi_i^a\rangle - \langle\Phi|\,H\,|\Phi\rangle \\ &= f_{aa} - f_{ii} + \Gamma_{aiai},\end{aligned} \tag{20}$$

and

$$\begin{aligned}\Delta_{abij} &= \big\langle\Phi_{ij}^{ab}\big|\,H\,\big|\Phi_{ij}^{ab}\big\rangle - \langle\Phi|\,H\,|\Phi\rangle \\ &= f_{aa} + f_{bb} + \Gamma_{abab} - f_{ii} - f_{jj} - \Gamma_{ijij} \\ &\quad - \Gamma_{aiai} - \Gamma_{bjbj} - \Gamma_{ajaj} - \Gamma_{bibi}.\end{aligned} \tag{21}$$

The generator is manifestly anti-hermitian since $\Delta_{ia} = -\Delta_{ai}$, $\Delta_{ijab} = -\Delta_{abij}$. The Møller-Plesset partitioning (MP) of an energy denominator is the same as EN but this time omitting the two-body matrix elements Γ_{pqrs}.

The Hamiltonian flows with the parameter s and thus so do the normal-ordered components f, $\Gamma, \dots$ and Δ.

3. *Valence space*

In contrast to the single-reference decoupling described above, in the valence space IMSRG (VS-IMSRG) [17] one treats a subset of orbitals as *valence* orbitals, whose excitations should capture much of the physics. Typically, the nearest closed shell is used to redefine the inert core. Details can be found in the review article [11]. For the specific case studied in this work, we use a valence space defined by the $0p$ orbits on top of a ^{4}He core, illustrated in Fig. 1.

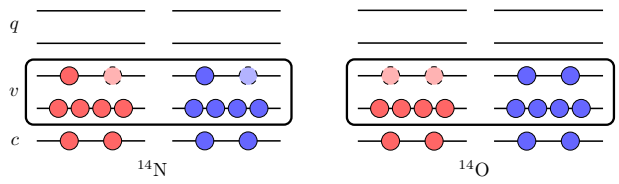


FIG. 1. p-shell valence space configuration of ^{14}N and ^{14}O.

B. Spurious breaking of isospin symmetry

To illustrate the spurious symmetry-breaking in the IMSRG, we begin with an isospin-conserving Hamiltonian and compute the ground-state expectation value of the isospin-squared operator T^2 with the IMSRG. In this case, any deviation from the exact answer indicates the extent to which truncations made in solving the IMSRG flow equations break isospin symmetry. The choice of isospin-conserving Hamiltonian we make is

$$H = T_{\rm rel} + V_{\rm iso} \tag{22}$$

where $T_{\rm rel}$ is the relative kinetic energy, and $V_{\rm iso}$ is an isospin-conserving NN potential. Here we use the NNLOΔ_{GO} potential of Ref. [18], without the Coulomb

interaction. This interaction includes isospin-breaking strong interactions, as well as a 3N force. For convenience, we normal-order with respect to a ^{16}O reference state built from a single Slater determinant of harmonic oscillator wave functions, and discard the residual 3N force. Then we isospin-average the resulting NN potential to yield an isospin-conserving potential $V_{\rm iso}$, which we use for our subsequent investigation.

We take as initial reference state a single Slater determinant $|\Phi_0\rangle$ built from harmonic oscillator states or Hartree-Fock states [12]. We specify this reference to be the ground state of ^{14}O and, using this Hamiltonian, we flow the IMSRG to decouple $|\Phi_0\rangle$ from excitations and consistently evolve the T^2 operator. For $s \to \infty$, the zero-body piece of $T^2(s)$ gives the ground-state expectation value, which for ^{14}O with an isospin symmetric interaction should be equal to 2. We also compute the commutator of the flowing operators $[H(s), T^2(s)]$. The operators commute at $s = 0$, and to the extent that the IMSRG transformation is unitary, these operators should commute throughout the flow. For comparison, we repeat the calculation with a ^{14}N reference, which has $N = Z$ The results of the calculation are shown in Fig. 2 [19].

We observe that isospin symmetry is broken in the ground state, and at the level of operators. The breaking is significantly worse for the isospin-asymmetric ^{14}O reference. The choice of a harmonic oscillator or Hartree-Fock single-particle basis appears to have very little effect on the final result, while there is some dependence on the choice of the generator η. In the following section, we will enumerate and investigate these various sources of isospin symmetry breaking in the IMSRG.

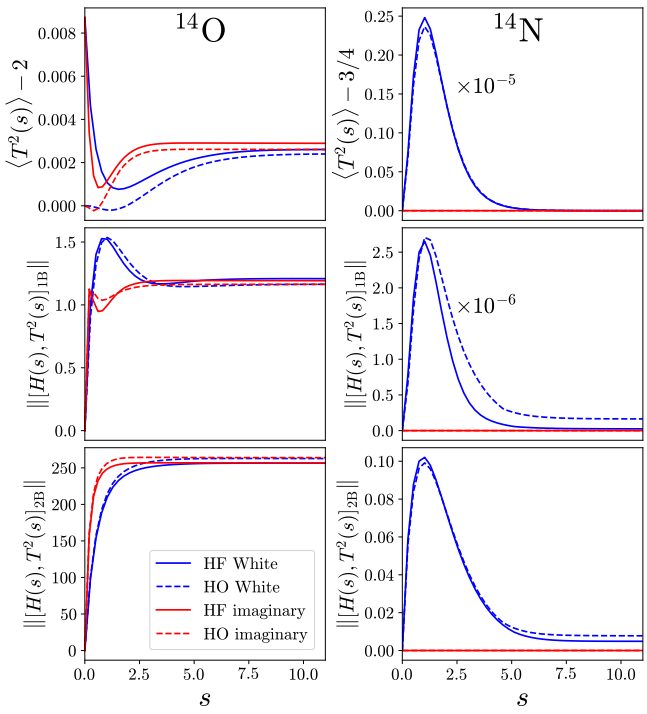


FIG. 2. Isospin symmetry breaking along the IMSRG(2) flow for ^{14}O and ^{14}N with the interaction $V_{\rm iso}$ at $e_{\rm max} = 3$. Epstein-Nesbet partitioning was used for the generator.

II. SOURCES OF SPURIOUS ISOSPIN BREAKING

It has been long known that the Hartree-Fock ground state for $N \neq Z$ spuriously breaks isospin symmetry [20], even if the fully correlated ground state has good isospin. This is because, even with good isospin, the pn interaction is stronger than the pp or nn interaction, so for an asymmetric system with $N \neq Z$, the protons and neutrons see a different mean field. In this case, the Hartree-Fock ground state is not an eigenstate of T^2, but the Hamiltonian expressed in the Hartree-Fock basis still commutes with T^2 . Including correlations beyond the mean field then restores the symmetry [20].

Because it serves as an advantageous starting point, a Hartree-Fock ground state is typically used as the reference state for IMSRG calculations. If the IMSRG could be performed without truncation, then the symmetry of the ground state would be restored. However, the IMSRG flow is usually truncated at the IMSRG(2) level, in which flowing three-body operators are discarded. This truncation may break isospin symmetry, and since the truncation depends on the reference, different choices of reference may will lead to different degrees of symmetry breaking.

In Fig. 2 we see at $s = 0$ that the Hartree-Fock reference breaks isospin in the ground state, while the oscillator reference preserves it. The IMSRG evolution brings the Hartree-Fock result closer to the exact value, while it introduces symmetry-breaking for the oscillator reference, eventually leading to a larger error for $s \to \infty$.

Our goal being to calculate δ_C and its uncertainty, it is a necessary first step to characterize the baseline accuracy of the IMSRG framework by considering the degree of spurious isospin breaking in the case of an isospin conserving interaction. We inspect in detail how the ^{14}O calculation of FIG. 2 breaks isospin symmetry through truncation of operators in the flow of s, and by proxy through the choice of generator.

A. Isospin breaking in the flow

The commutator of the Hamiltonian with the isospin-squared is an operator that obeys the flow equation

$$\begin{aligned}\frac{d}{ds}[H, T^2] &= [\eta, [H, T^2]] \\ &= [[\eta, H], T^2] + [H, [\eta, T^2]].\end{aligned} \tag{23}$$

where all operators are evaluated at flow parameter s. If the initial Hamiltonian $H(0)$ commutes with T^2, then the

first equality in (23) shows that they should commute for all s, assuming no truncation is made. However, what is actually evaluated in the calculation corresponds to the second equality; the H and T^2 operators are separately evolved, and then we take the commutator of the evolved operators. The two terms on the right hand side of (23) should cancel against each other. However, when we discard three-body operators induced by the commutator, the two terms no longer cancel. This can be seen by expanding the right hand side into eight terms

$$\frac{d}{ds}\big[H,T^2\big] = \Big(H(\eta T^2) - H(T^2\eta) - (\eta T^2)H + (T^2\eta)H + (\eta H)T^2 - (H\eta)T^2 - T^2(\eta H) + T^2(H\eta)\Big), \tag{24}$$

where the parentheses indicate which operator product is to be evaluated first. Without truncation, each term in the first row of (24) should cancel against a corresponding term in the second row. For example, the $H(\eta T^2)$ term should cancel against $(H\eta)T^2$. The one-body pieces of these terms are illustrated diagrammatically in Fig. 3, where we label diagrams according to the particle rank of the intermediate operator indicated by parentheses. We see that the diagram labeled (a) in Fig. 3 will be included in the IMSRG(2) approximation of $H(\eta T^2)$, but *not* in $(H\eta)T^2$, where it involves a three-body intermediate; the IMSRG(2) approximation spoils the cancellation.

This artifact resulting from the order of operator multiplication is precisely what the factorized IMSRG($3f_2$) method [21] exploits in the Magnus formulation to more efficiently calculate double commutators $[\Omega,[\Omega,A]]$ in the evolution of an operator A.

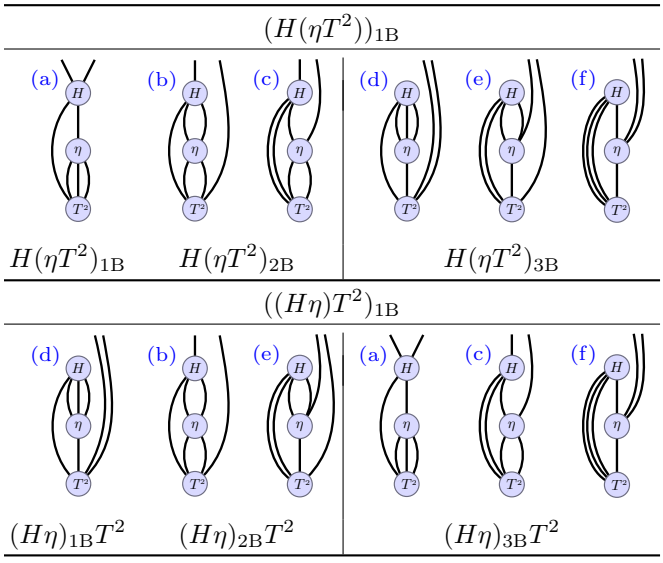


FIG. 3. Diagrams with two-body parts of operators contributing to the one-body matrix elements of $\big[H(ds),T^2(ds)\big]$ according to the flow equation (25). The top row should cancel exactly with the bottom but, because of particle rank truncation at IMSRG(2), isospin symmetry is broken since some cancelling pairs have different intermediate particle rank.

The straightforward solution would be to include flowing three-body operators at the IMSRG(3N7) level or at the cheaper IMSRG($3f_2$) level. However, relaxing the particle-rank truncation fixes the issue for just one numerical flow step. In the next step, there will be cancellations involving intermediate four-body operators, and so on. We may still hope that the importance of these terms will be small, so that going from IMSRG(2) to IMSRG(3) reduces the magnitude of the spurious breaking. This is confirmed in Fig. 4, which shows the flowing ground-state expectation $\langle T^2(s)\rangle$ and commutator $[T^2(s),H(s)]$ computed with IMSRG(2), IMSRG(3N7) and IMSRG(3) truncations.

Alternatively, we may observe that if the generator η commutes with T^2, then the second term in the right hand side of (23) vanishes and the two terms are individually zero; no cancellation is needed. In this case, $\frac{d}{ds}T^2 = [\eta,T^2] = 0$, so that the T^2 operator is unchanged throughout the flow. In practical applications we are interested in, η should at some point break isospin to suppress the isospin-breaking pieces of the Hamiltonian. However, this suggests that we should minimize the isospin breaking in η as much as possible. We discuss this in more detail in the next section.

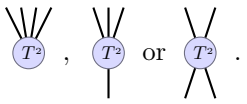
After one step in SRG flow, the commutator is

$$\begin{aligned}\big[H(ds),T^2(ds)\big] = \big[H(0),T^2(0)\big] + ds\big(&\big[[\eta(0),H(0)],T^2(0)\big] \\ &+ \big[H(0),\big[\eta(0),T^2(0)\big]\big]\big) \\ &+ ds^2\big[[\eta(0),H(0)],\big[\eta(0),T^2(0)\big]\big].\end{aligned} \tag{25}$$

If indeed the generator at $s=0$ is isospin symmetric, for both ^{14}O and ^{14}N this reduces to

$$\big[H(ds),T^2(ds)\big] = ds\big[[\eta(0),H(0)],T^2(0)\big]. \tag{26}$$

To compare symmetric and asymmetric references, we can gain insight by looking at the diagrammatic form of $T^2(0)$. Distinctly for an isospin asymmetric reference such as ^{14}O, the $T^{\mp}T^{\pm}$ part of $T^2(0)$ can connect states with different occupation numbers, which means $T^2(0)_{2B}$ permits $[\eta(0),H(0)]_{3B}$ to contribute to $\big[H(ds),T^2(ds)\big]_{2B}$. In this case $T^2(0)_{2B}$ could look like

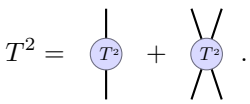


(27)

At IMSRG(2), this $[3,2]\to 2$ contribution is discarded and the expected cancellation shown in FIG. 3 does not happen. Thus for ^{14}O one must work at IMSRG(3N7) to ensure $\big[H(ds),T^2(ds)\big]_{2B} = 0$. Meanwhile this issue does not arise for an isospin symmetric reference such as ^{14}N since $T^2(0)$ only connects states with the same occupation numbers which restricts the operator's diagrammatic

form to

$$T^2 = \quad + \quad . \tag{28}$$



In this case $T^2(0)$ cannot reduce the particle rank of an operator via a commutator, which guarantees all contributions to $\left[H(ds), T^2(ds)\right]_{2\mathrm{B}}$ are captured at IMSRG(2).

Letting $A = [\eta, H]$, to see explicitly where the cancellation happens for ^{14}N we should look at why

$$\left[A_{1\mathrm{B}}, T^2_{1\mathrm{B}}\right]_{1\mathrm{B}} = -\left[A_{1\mathrm{B}}, T^2_{2\mathrm{B}}\right]_{1\mathrm{B}} \neq 0, \tag{29}$$
$$\left[A_{1\mathrm{B}}, T^2_{1\mathrm{B}}\right]_{2\mathrm{B}} = -\left[A_{1\mathrm{B}}, T^2_{2\mathrm{B}}\right]_{2\mathrm{B}} = 0 \tag{30}$$

while

$$\left[A_{2\mathrm{B}}, T^2_{1\mathrm{B}}\right]_{1\mathrm{B}} = -\left[A_{2\mathrm{B}}, T^2_{2\mathrm{B}}\right]_{1\mathrm{B}} = 0, \tag{31}$$
$$\left[A_{2\mathrm{B}}, T^2_{1\mathrm{B}}\right]_{2\mathrm{B}} = -\left[A_{2\mathrm{B}}, T^2_{2\mathrm{B}}\right]_{2\mathrm{B}} \neq 0, \tag{32}$$

and why same is not true for ^{14}O. Observe that, for example, (29) is equivalent to showing the equality for the expressions

$$\left[A_{1\mathrm{B}}, T^2_{1\mathrm{B}}\right]_{pq} = +\frac{3}{2}(n_p - n_q)A_{pq} \tag{33}$$
$$\left[A_{1\mathrm{B}}, T^2_{2\mathrm{B}}\right]_{pq} = -\frac{1}{2}(n_p - n_q)\left(A_{pq} + 2A_{\overline{pq}}\right) \tag{34}$$

derived from explicit commutators with T^2 (A9a), (A9c). Here we used $N = Z$ and $n_{\overline{p}} = n_q$ for an isospin symmetric reference, and $|t_{z,p} + t_{z,q}| - 1/2 = +1/2$ for $A \sim [\eta, H]$ which preserves the nucleon type. These expressions indeed satisfy (29) *as long as* $A_{pq} = A_{\overline{pq}}$. In turn, to see why this equality is only guaranteed for isospin symmetric references, we should look at commutators of the form

$$[\eta_{1\mathrm{B}}, H_{2\mathrm{B}}]_{pq} = \sum_{ab}(n_r - n_s)\eta_{rs}H_{sprq}, \tag{35}$$
$$[\eta_{1\mathrm{B}}, H_{2\mathrm{B}}]_{\overline{pq}} = \sum_{rs}(n_r - n_s)\eta_{rs}H_{s\overline{p}r\overline{q}}. \tag{36}$$

Although (35) and (36) don't cancel exactly term by term, for ^{14}N the terms offset by isospin, i.e.

$$(n_p - n_q)\eta_{pq}H_{qppq}, \tag{37}$$
$$(n_{\overline{p}} - n_{\overline{q}})\eta_{\overline{pq}}H_{\overline{qppq}} \tag{38}$$

are equal for a symmetric reference with isospin symmetric η and H *as long as*

$$(n_p - n_q) = (n_{\overline{p}} - n_{\overline{q}}). \tag{39}$$

A similar story holds for (32) setting $c_{pq} = c_{rs} = 1/2$ in (A10a) and (A10c), (A10d).

We stress that for more than one step in the flow the evolved commutator $\left[H(s), T^2(s)\right]$ will involve intermediate particle ranks greater than 3, so that currently implemented IMSRG truncation schemes will introduce ISB even for symmetric references.

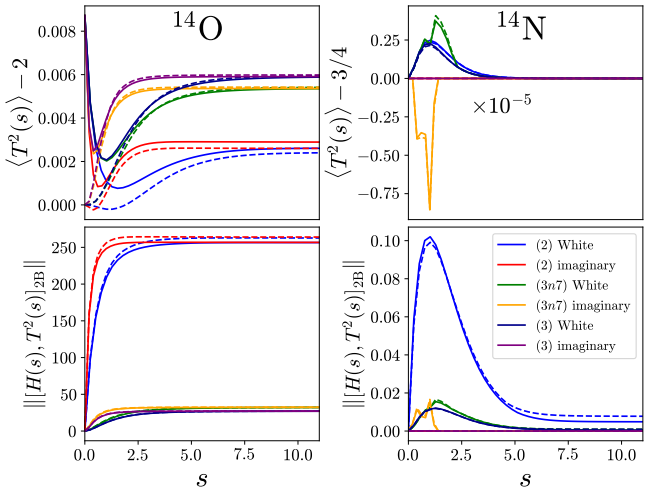


FIG. 4. ISB for ^{14}O and ^{14}N with the isospin-symmetric interaction V_{iso} at $e_{\max} = 3$ with a reference in the HF (full) and HO (dashed) bases for different truncations of the IMSRG. As the truncation is relaxed, the error $\left[H(s), T^2(s)\right]$ is systematically reduced.

Finally, we comment on the 'bumps' of spurious ISB seen in the flow for ^{14}N in FIG. 2 and FIG. 4. It is tempting to interpret this behavior as a temporary isospin breaking which is then repaired by further IMSRG evolution. But this cannot be the case; to the extent that the transformation is unitary, isospin should be conserved throughout the flow. Once it is broken due to a truncation error, the information about the symmetry is lost and there is no reason why further flow should somehow restore it. Instead, this behavior is the result of multiple terms which are not canceled due to the truncation of operators. These terms have different s dependence, and coincidentally have similar magnitudes and opposite signs.

B. Isospin breaking in the generator

In the absence of truncations, *any* anti-hermitian generator η, even one that breaks isospin symmetry, will yield a unitary transformation which preserves the symmetry $[H, T^2] = 0$. However, as we discussed in the previous section, truncations of the IMSRG flow can lead to spurious isospin symmetry breaking. We expect this symmetry breaking will be reduced if we minimize the symmetry breaking of the generator. Here, we enumerate the various ways in which η can violate isospin symmetry, and strategies to mitigate this breaking.

1. ISB due to the definition of off-diagonal

As described in (5), we partition the Hamiltonian into diagonal and off-diagonal pieces $H = H^{\rm d} + H^{\rm od}$, and design a flow to suppress $H^{\rm od}$, typically by making $\eta \sim H^{\rm od}$. Even if the total Hamiltonian has isospin symmetry, the individual pieces $H^{\rm d}$ and $H^{\rm od}$ may not.

To illustrate, we consider the example of a single-reference calculation of ^{14}O, where the reference consists of the proton orbits $\{\pi 0s_{1/2}, \pi 0p_{3/2}, \pi 0p_{1/2}\}$ and the neutron orbits $\{\nu 0s_{1/2}, \nu 0p_{3/2}\}$. Excitations $\nu 0p_{3/2} \to \nu 0p_{1/2}$ connect the reference to excited configurations, and are included in $H^{\rm od}$, while $\pi 0p_{3/2} \to \pi 0p_{1/2}$ does not cause an excitation of the reference. Consequently, for standard choices of generator we will have $\langle \pi 0p_{1/2}|\eta|\pi 0p_{3/2}\rangle = 0$ and $\langle \nu 0p_{1/2}|\eta|\nu 0p_{3/2}\rangle \neq 0$. This leads to $[\eta, T^2] \neq 0$ and consequently, as described in the previous section, involves cancellations which are spoiled when we truncate the flow.

One way to mitigate this source of isospin breaking is to use a valence space which is isospin symmetric, such as the $0p$ shell for both protons and neutrons. In this case, the definition of off-diagonal is the same for protons and neutrons, so that $[H^{\rm od}, T^2] \approx 0$. The equality is not exact if we use a Hartree-Fock reference state with $N \neq Z$ because the effective one-body part of the Hamiltonian will still break isospin, corresponding to protons and neutrons feeling different mean fields. Even for a reference with $N = Z$, the equality will also not be exact due to genuine isospin-breaking terms in the Hamiltonian yielding different single-particle wave functions for protons and neutrons.

2. ISB due to energy denominators

The White, arctangent and imaginary-time generators all feature energy denominators (20) defined in the introduction. In the J-coupled scheme of matrix element storage, we use the monopole definition of the two-body elements

$$\Gamma_{pqpq} \to \bar{\Gamma}_{pqpq} \equiv \frac{\sum_J (2J+1)\Gamma^J_{pqpq}}{\sum_J (2J+1)}. \tag{40}$$

This choice breaks isospin symmetry, as can be seen by considering the denominators for η^J_{abij} with $a = b$ up to isospin projection. If a and b are both neutrons, then only even J will contribute to the $\bar{\Gamma}_{abab}$ term, but if a, b are proton-neutron, then odd J will also contribute, leading to a different denominator. Similar effects modify the other monopole terms. In principle, one could take more care and maintain isospin in the averaging, but it is much easier to simply use the MP denominators for which the elements Γ_{pqrs} do not appear in the first place. Fig. 5, shows $\langle T^2(s)\rangle$ and $[T^2(s), H(s)]$ for different choices of generator, revealing a reduced symmetry breaking with the MP denominators when using a ^{14}N reference.

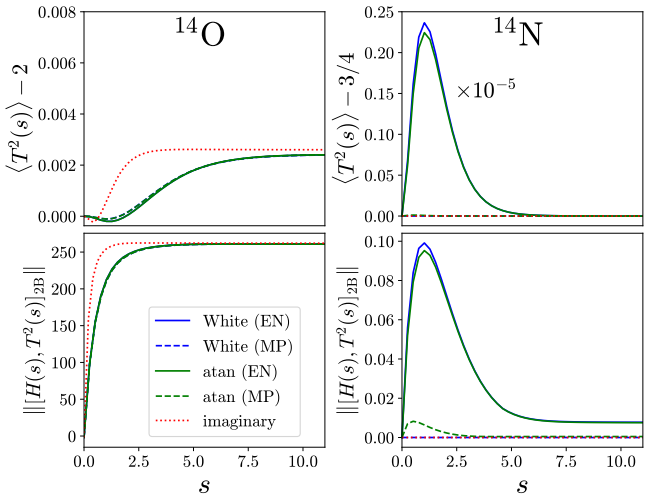


FIG. 5. ISB along the IMSRG(2) flow for ^{14}O and ^{14}N with the interaction $V_{\rm iso}$ at $e_{\rm max} = 3$ in the HO basis, this time with different energy denominators in η. In contrast to the MP partitioning, the EN partitioning spoils isospin for two-body elements because of the monopole definition (40). The arctangent generator slightly breaks isospin because of the non-linear mixing shown in (42).

3. ISB due to non-linear mixing

The arctangent generator, along with any generator defined as a formal power series of an argument of the form $H^{\rm od}/\Delta$, leads to spurious ISB due to non-linear terms in its definition

$$\mathrm{atan}(x) = x - \frac{1}{3}x^3 + \frac{1}{5}x^5 + \dots\ . \tag{41}$$

Because the expansion is matrix-element-wise, rather than a definition in terms of powers of operators, the non-linear terms spoil the linear relationship between the coupled and uncoupled isospin bases. For example, if a given $T_z = 0$ element is a superposition of $T = 0, 1$, the cubic term gives

$$\eta^3_{pnpn} = (\eta_{T=1} + \eta_{T=0})^3 = \eta^3_{T=1} + \eta^3_{T=0} + \eta^2_{T=1}\eta_{T=0} + \dots \tag{42}$$

Because of the cross terms like $\eta^2_{T=1}\eta_{T=0}$ we cannot extract the $\eta^{T=1}$ component by the usual linear combination of pn matrix elements, and we have $[\eta, T^2] \neq 0$.

III. BENCHMARKING

A. Prescription to remedy spurious isospin breaking

Having identified the sources of spurious ISB, we can now present a best practice to minimize the spurious contamination of calculations in the context of δ_C.

First, it is preferable to take a reference with $N = Z$ so

that terms which should cancel are either both included or both omitted at a given truncation level. Second, it is preferable to use a valence space with the same orbits for protons and neutrons, to minimize isospin breaking due to the partitioning $H = H^{\mathrm{d}} + H^{\mathrm{od}}$.

In addition, there are some further choices which have a smaller impact: We should use either the White generator with Møller-Plesset partitioning of the energy denominators, or the imaginary time generator. For the initial decoupling stage of the IMSRG flow, we should isospin average the generator. This average should be performed on the elements of η before normal-ordering such that, for example,

$$\begin{aligned}\langle \pi 0p_{1/2}|\,\eta\,|\pi 1p_{1/2}\rangle \to \frac{1}{2}\big(\,&\langle \pi 0p_{1/2}|\,\eta\,|\pi 1p_{1/2}\rangle \\ &+ \langle \nu 0p_{1/2}|\,\eta\,|\nu 1p_{1/2}\rangle\,\big)\end{aligned} \tag{43}$$

while for 2B matrix elements the $T = 0$ and $T = 1$ channels are averaged separately. This initial decoupling should be followed by a second stage without isospin averaging which suppresses the isovector components of H^{od} that were previously averaged.

B. Application to δ_C

Thus far, the investigation has focused on the T^2 operator as a measure of symmetry breaking. For application to the δ_C correction for superallowed Fermi decays, we are interested in the isospin raising/lowering operator $T^{\pm}$. With an isospin-conserving interaction, we should obtain $\delta_C = 0$; any nonzero value is due to truncation error.

We are also interested in the accuracy of a calculation with an isospin breaking interaction. For this, we add a Coulomb potential to the isospin-conserving interaction. In this case, the exact result can no longer be trivially obtained from symmetry. We perform a configuration diagonalization in a space of three major oscillator shells ($e_{\max} = 2$) with a further truncation on the total oscillator quanta $N_{\max} = 12$ beyond the oscillator ground state. We find $\delta_C \approx 0.03\%$.

Our results for δ_C, with and without the Coulomb potential, obtained with IMSRG(2), IMSRG($3f_2$), and IMSRG(3N7) are listed in Tabs. III, IV, and V, respectively.

With the symmetric interaction, we find a pattern similar to that observed for the T^2 operator. In the worst case, IMSRG(2) with a ^{14}O Hartree-Fock reference, we obtain $\delta_C \sim 0.27$ when we should find $\delta_C = 0$. This constitutes an unacceptably large error. In contrast, using the ^{14}N reference we obtain $\delta_C = 0$, supporting our preference for the $N = Z$ reference.

When the Coulomb potential is turned on, we find $\delta_C \approx 0.015$ for the ^{14}N reference, which is off by a factor ~ 2 from the CI result. With the ^{14}O reference we find $\delta_C \sim 0.3$, which is off by a factor 10. While the symmetric $N = Z$ reference is superior, it is clear that some significant source of error remains, which we will investigate in future work.

IV. CONCLUSION

We have used a toy model to investigate how truncations made in the IMSRG lead to spurious breaking of isospin symmetry. After investigating the various mechanisms, we have identified strategies to minimize the spurious breaking, and demonstrated them in calculations of the correction δ_C for superallowed Fermi decays. In the case of a isospin conserving interaction, we successfully eliminated the spurious contributions to δ_C. However, when isospin breaking is introduced with the Coulomb potential, we still find a discrepancy with the quasi-exact result. This should be investigated further. It will also be interesting to explore the spurious breaking of other symmetries, especially of rotational symmetry when using a deformed reference.

ACKNOWLEDGMENTS

We thank Bingcheng He and Heiko Hergert for helpful discussions. SRS is supported by the National Science Foundation under award PHY-2340834. AF was supported by the Naughton Fellowship.

[1] J. C. Hardy and I. S. Towner, Superallowed $0^+ \to 0^+$ nuclear β decays: 2020 critical survey, with implications for V_{ud} and ckm unitarity, Phys. Rev. C **102**, 045501 (2020).
[2] N. Cabibbo, Unitary Symmetry and Leptonic Decays, Phys. Rev. Lett. **10**, 531 (1963).
[3] M. Kobayashi and T. Maskawa, CP Violation in the Renormalizable Theory of Weak Interaction, Prog. Theor. Phys. **49**, 652 (1973).
[4] V. Cirigliano, A. Crivellin, M. Hoferichter, and M. Moulson, Scrutinizing ckm unitarity with a new measurement of the k3/k2 branching fraction, Physics Letters B **838**, 137748 (2023).
[5] B. Chakraborty, A. Gilman, M. Hoferichter, and M. Koval, Working group 1 summary: v_{ud}, v_{us}, v_{cd}, v_{cs} and semileptonic/leptonic d decays (2024), arXiv:2406.13703 [hep-ph].
[6] B. R. Barrett, P. Navrátil, and J. P. Vary, Ab initio no core shell model, Progress in Particle and Nuclear Physics **69**, 131 (2013).
[7] E. Caurier, P. Navrátil, W. E. Ormand, and J. P. Vary, Ab initio shell model for $a = 10$ nuclei, Phys. Rev. C **66**, 024314 (2002).

[8] Q. Yuan, S. Q. Fan, B. S. Hu, J. G. Li, S. Zhang, S. M. Wang, Z. H. Sun, Y. Z. Ma, and F. R. Xu, Deformed in-medium similarity renormalization group, Phys. Rev. C **105**, L061303 (2022).

[9] H. Hergert, In-medium similarity renormalization group for closed and open-shell nuclei, Physica Scripta **92**, 023002 (2016).

[10] H. Hergert, S. Bogner, T. Morris, A. Schwenk, and K. Tsukiyama, The in-medium similarity renormalization group: A novel ab initio method for nuclei, Physics Reports **621**, 165 (2016), memorial Volume in Honor of Gerald E. Brown.

[11] S. R. Stroberg, H. Hergert, S. K. Bogner, and J. D. Holt, Nonempirical interactions for the nuclear shell model: an update, Annual Review of Nuclear and Particle Science **69**, 307 (2019).

[12] I. Shavitt and R. Bartlett, *Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory* (2009).

[13] H. Hergert, S. K. Bogner, J. G. Lietz, T. D. Morris, S. J. Novario, N. M. Parzuchowski, and F. Yuan, In-medium similarity renormalization group approach to the nuclear many-body problem, An Advanced Course in Computational Nuclear Physics: Bridging the Scales from Quarks to Neutron Stars , 477 (2017).

[14] M. Heinz, A. Tichai, J. Hoppe, K. Hebeler, and A. Schwenk, In-medium similarity renormalization group with three-body operators, Phys. Rev. C **103**, 044318 (2021).

[15] T. D. Morris, N. M. Parzuchowski, and S. K. Bogner, Magnus expansion and in-medium similarity renormalization group, Physical Review C **92**, 10.1103/physrevc.92.034331 (2015).

[16] S. R. White, Numerical canonical transformation approach to quantum many-body problems, The Journal of Chemical Physics **117**, 7472 (2002).

[17] S. R. Stroberg, A. Calci, H. Hergert, J. D. Holt, S. K. Bogner, R. Roth, and A. Schwenk, Nucleus-dependent valence-space approach to nuclear structure, Phys. Rev. Lett. **118**, 032502 (2017).

[18] W. G. Jiang, A. Ekström, C. Forssén, G. Hagen, G. R. Jansen, and T. Papenbrock, Accurate bulk properties of nuclei from $a = 2$ to ∞ from potentials with Δ isobars, Phys. Rev. C **102**, 054301 (2020).

[19] The s-axis of imaginary time generator flows was rescaled by 20 for illustrative purposes. Note that s also has different units by the definition of $U(s)$ and η.

[20] D. Brink and J. Svenne, Isospin mixing of hartree-fock solutions, Nuclear Physics A **154**, 449 (1970).

[21] B. C. He and S. R. Stroberg, Factorized approximation to the in-medium similarity renormalization group imsrg(3), Phys. Rev. C **110**, 044317 (2024).

[22] S. R. Stroberg, T. D. Morris, and B. C. He, In-medium similarity renormalization group with flowing 3-body operators, and approximations thereof, Phys. Rev. C **110**, 044316 (2024).

Appendix A: Isospin commutators

In this appendix we collect useful expressions for the matrix elements of the unflowed isospin operator $T^2(0)$, as well as its commutators. If T^2 acts on a two-particle state, then

$$T^2 = \underbrace{T_1^2 \otimes \mathbb{1} + \mathbb{1} \otimes T_2^2}_{\text{1B}} + \underbrace{2T_1^z \otimes T_2^z + T_1^+ \otimes T_2^- + T_1^- \otimes T_2^+}_{\text{2B}}. \tag{A1}$$

The normal-ordered antisymmetrized two-body matrix elements are

$$T^2_{pqrs} = c_{pq}\left(\delta_{pr}\delta_{qs} - \delta_{ps}\delta_{qr}\right) + \left(\frac{1}{2} - c_{pq}\right)\left(\delta_{p\overline{r}}\delta_{q\overline{s}} - \delta_{p\overline{s}}\delta_{q\overline{r}}\right), \tag{A2}$$

where we defined the quantity

$$c_{pq} = |t_{z,p} + t_{z,q}| - \frac{1}{2} = |T_z| - \frac{1}{2}, \tag{A3}$$

and in turn the normal-ordered one-body matrix elements are

$$T^2_{pq} = \frac{3}{4}\delta_{pq} + \sum_r n_r T^2_{prqr} = \left(\frac{3}{4} + t_{z,p}(N-Z) - \frac{1}{2}n_p - n_{\overline{p}}\right)\delta_{pq}. \tag{A4}$$

Using expressions in [22], a normal-ordered three-body operator A gives the commutators

$$\left[A, T^2\right]_0 = \frac{1}{2}\sum_{pq} n_p n_{\overline{p}} n_q n_{\overline{q}}\left(A_{pq\overline{pq}} - A_{\overline{pq}pq}\right), \tag{A5}$$

$$[A_{1\mathrm{B}}, T^2_{1\mathrm{B}}]_{pq} = \left((t_{z,p} - t_{z,q})(N - Z) + \frac{1}{2}(n_p - n_q) + (n_{\overline{p}} - n_{\overline{q}})\right) A_{pq}, \tag{A6a}$$

$$[A_{2\mathrm{B}}, T^2_{1\mathrm{B}}]_{pq} = 0, \tag{A6b}$$

$$\begin{aligned}[A_{1\mathrm{B}}, T^2_{2\mathrm{B}}]_{pq} = &-(n_p - n_q)c_{pq}A_{pq} - (n_{\overline{p}} - n_{\overline{q}})\left(\frac{1}{2} + c_{pq}\right) A_{\overline{pq}} \\ &+ \delta_{p\overline{q}} \sum_r (n_r - n_{\overline{r}})\left(\frac{1}{2} + c_{pr}\right) A_{r\overline{r}},\end{aligned} \tag{A6c}$$

$$\begin{aligned}[A_{2\mathrm{B}}, T^2_{2\mathrm{B}}]_{pq} = \sum_r n_r \overline{n}_{\overline{r}} \Bigg(&\left(\frac{1}{2} + c_{rq}\right) n_{\overline{q}} A_{\overline{r}pr\overline{q}} + \left(\frac{1}{2} - c_{rq}\right) \overline{n}_{\overline{q}} A_{rp\overline{rq}} \\ &- \left(\frac{1}{2} + c_{rp}\right) n_{\overline{p}} A_{r\overline{pr}q} + \left(\frac{1}{2} - c_{rp}\right) \overline{n}_{\overline{p}} A_{\overline{rpr}q}\Bigg),\end{aligned} \tag{A6d}$$

$$[A_{3\mathrm{B}}, T^2_{2\mathrm{B}}]_{pq} = \frac{1}{2} \sum_{rs} n_r n_s \overline{n}_{\overline{r}} \overline{n}_{\overline{s}} \left(\frac{1}{2} - c_{rs}\right) \left(A_{rsp\overline{rs}q} - A_{\overline{rs}prsq}\right), \tag{A6e}$$

$$\begin{aligned}[A_{2\mathrm{B}}, T^2_{1\mathrm{B}}]_{pqrs} = \Big[&\frac{1}{2}(n_p + n_q - n_r - n_s) + (n_{\overline{p}} + n_{\overline{q}} - n_{\overline{r}} - n_{\overline{s}}) \\ &- (t_{z,p} + t_{z,q} - t_{z,r} - t_{z,s})\,(N - Z)\Big] A_{pqrs},\end{aligned} \tag{A7a}$$

$$[A_{3\mathrm{B}}, T^2_{1\mathrm{B}}]_{pqrs} = 0, \tag{A7b}$$

$$\begin{aligned}[A_{1\mathrm{B}}, T^2_{2\mathrm{B}}]_{pqrs} = &\,(c_{rs} - c_{pq})\,(\delta_{qs}A_{pr} - \delta_{qr}A_{ps} - \delta_{ps}A_{qr} + \delta_{pr}A_{qs}) \\ &+ \left(\frac{1}{2} - c_{rs}\right)(\delta_{q\overline{s}}A_{p\overline{r}} - \delta_{q\overline{r}}A_{p\overline{s}} - \delta_{p\overline{s}}A_{q\overline{r}} + \delta_{p\overline{r}}A_{q\overline{s}}) \\ &- \left(\frac{1}{2} - c_{pq}\right)(\delta_{\overline{q}s}A_{\overline{p}r} - \delta_{\overline{q}r}A_{\overline{p}s} - \delta_{\overline{p}s}A_{\overline{q}r} + \delta_{\overline{p}r}A_{\overline{q}s}),\end{aligned} \tag{A7c}$$

$$\begin{aligned}[A_{2\mathrm{B}}, T^2_{2\mathrm{B}}]^{\mathrm{pphh}}_{pqrs} \overset{\dagger}{=} &\left[(\overline{n}_r \overline{n}_s - n_r n_s)\, c_{rs} - (\overline{n}_p \overline{n}_q - n_p n_q)\, c_{pq}\right] A_{pqrs} \\ &+ (\overline{n}_{\overline{r}} \overline{n}_{\overline{s}} - n_{\overline{r}} n_{\overline{s}})\left(\frac{1}{2} - c_{rs}\right) A_{pq\overline{rs}} - (\overline{n}_{\overline{p}} \overline{n}_{\overline{q}} - n_{\overline{p}} n_{\overline{q}})\left(\frac{1}{2} - c_{pq}\right) A_{\overline{pq}rs},\end{aligned} \tag{A7d}$$

$$\begin{aligned}[A_{2\mathrm{B}}, T^2_{2\mathrm{B}}]^{\mathrm{ph}}_{pqrs} = &\,(1 - P_{pq})\,(1 - P_{rs})\Bigg((n_r - n_p)c_{pr}A_{pqrs} + (n_{\overline{r}} - n_{\overline{p}})\left(\frac{1}{2} + c_{pr}\right) A_{\overline{pq}\overline{rs}} \\ &- \sum_m (n_m - n_{\overline{m}})\left(\frac{1}{2} - c_{pm}\right) \delta_{p\overline{r}} A_{\overline{m}qms}\Bigg),\end{aligned} \tag{A7e}$$

$$\begin{aligned}[A_{3\mathrm{B}}, T^2_{2\mathrm{B}}]_{pqrs} = &-(1 - P_{pq}) \sum_m (n_{\overline{p}} n_{\overline{m}} \overline{n}_m + \overline{n}_{\overline{p}} \overline{n}_{\overline{m}} n_m)\left(\frac{1}{2} - c_{pm}\right) A_{\overline{pm}qrsm} \\ &+ (1 - P_{rs}) \sum_m (n_{\overline{r}} n_{\overline{m}} \overline{n}_m + \overline{n}_{\overline{r}} \overline{n}_{\overline{m}} n_m)\left(\frac{1}{2} - c_{rm}\right) A_{pqm\overline{rm}s}.\end{aligned} \tag{A7f}$$

In the case of a symmetric reference, where $N = Z$ and $n_p = n_{\overline{p}}$, these expressions reduce to

$$\left[A, T^2\right]_0 = \frac{1}{2} \sum_{pq} n_p n_q \left(A_{pq\overline{pq}} - A_{\overline{pq}pq}\right), \tag{A8}$$

$$[A_{1\mathrm{B}}, T^2_{1\mathrm{B}}]_{pq} = \frac{3}{2}(n_p - n_q)A_{pq}, \tag{A9a}$$

$$[A_{2\mathrm{B}}, T^2_{1\mathrm{B}}]_{pq} = 0, \tag{A9b}$$

$$[A_{1\mathrm{B}}, T^2_{2\mathrm{B}}]_{pq} = -(n_p - n_q)\left(c_{pq}A_{pq} + \left(\frac{1}{2} + c_{pq}\right)A_{\overline{pq}}\right), \tag{A9c}$$

$$[A_{2\mathrm{B}}, T^2_{2\mathrm{B}}]_{pq} = 0, \tag{A9d}$$

$$[A_{3\mathrm{B}}, T^2_{2\mathrm{B}}]_{pq} = 0, \tag{A9e}$$

$$[A_{2\mathrm{B}}, T^2_{1\mathrm{B}}]_{pqrs} = \frac{3}{2}(n_p + n_q - n_r - n_s)A_{pqrs}, \tag{A10a}$$

$$[A_{1\mathrm{B}}, T^2_{2\mathrm{B}}]_{pqrs} = (1 - P_{pq})(1 - P_{rs})\,\delta_{qs}\left(c_{rs}(A_{pr} - A_{p\overline{r}}) - c_{pq}(A_{pr} - A_{\overline{p}r}) + \frac{1}{2}(A_{p\overline{r}} - A_{\overline{p}r})\right), \tag{A10b}$$

$$\begin{aligned}[A_{2\mathrm{B}}, T^2_{2\mathrm{B}}]^{\mathrm{pphh}}_{pqrs} = (\overline{n}_r\overline{n}_s - n_r n_s)\left[c_{rs}A_{pqrs} + \left(\frac{1}{2} - c_{rs}\right)A_{pq\overline{rs}}\right] \\ - (\overline{n}_p\overline{n}_q - n_p n_q)\left[c_{pq}A_{pqrs} + \left(\frac{1}{2} - c_{pq}\right)A_{\overline{pq}rs}\right],\end{aligned} \tag{A10c}$$

$$[A_{2\mathrm{B}}, T^2_{2\mathrm{B}}]^{\mathrm{ph}}_{pqrs} = (1 - P_{pq})(1 - P_{rs})(n_r - n_p)\left(c_{pr}A_{pqrs} + \left(\frac{1}{2} + c_{pr}\right)A_{\overline{p}q\overline{r}s}\right), \tag{A10d}$$

$$[A_{3\mathrm{B}}, T^2_{2\mathrm{B}}]_{pqrs} = 0. \tag{A10e}$$

Appendix B: Data tables

DeltaGO_isoavg HF

^{14}O

$s = 0$						$s \to \infty$					
SR						SR					
η	$\langle T^2 \rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$	$[\eta,T^2]_{1B}$	$[\eta,T^2]_{2B}$	η	$\langle T^2 \rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$		
White (EN)	0.0087	1.259e-09	3.938e-08	0.2352	3.0895	White (EN)	0.0026	1.2054	256.3086		
White (MP)	–	–	–	0.2205	2.9574	White (MP)	0.0026	1.2042	256.3364		
imaginary	–	–	–	8.7259	126.7682	imaginary	0.0029	1.1954	256.7812		
Iso White (EN)	–	–	–	0.0074	0.1161	Iso White (EN)	0.0021	0.9142	58.5530		
Iso White (MP)	–	–	–	0.0071	0.1122	Iso White (MP)	0.0021	0.9171	58.6564		
Iso imaginary	–	–	–	0.4698	7.7513	Iso imaginary	0.0020	0.8268	58.1933		
VS						VS					
η	$\langle T^2 \rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$	$[\eta,T^2]_{1B}$	$[\eta,T^2]_{2B}$	η	$\langle T^2 \rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$		
SMW (EN)	0.0086	–	–	0.2343	3.3873	SMW (EN)	0.0063	1.0071	58.8213		
SMW (MP)	–	–	–	0.2197	3.3057	SMW (MP)	0.0061	1.0002	58.7619		
SMit	–	–	–	8.6819	122.6028	SMit	0.0040	0.8143	57.9623		
Iso SMW (EN)	–	–	–	0.0153	0.2578	Iso SMW (EN)	0.0032	0.7730	57.9876		
Iso SMW (MP)	–	–	–	0.0150	0.2507	Iso SMW (MP)	0.0031	0.7704	58.0141		
Iso SMit	–	–	–	0.6993	12.4497	Iso SMit	0.0026	0.6611	57.3887		

^{14}N

$s = 0$						$s \to \infty$					
SR						SR					
η	$\langle T^2 \rangle - \frac{3}{4}$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$	$[\eta,T^2]_{1B}$	$[\eta,T^2]_{2B}$	η	$\langle T^2 \rangle - \frac{3}{4}$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$		
White (EN)	1.332e-15	7.477e-15	2.021e-08	2.407e-16	0.0297	White (EN)	-5.688e-10	2.556e-08	0.0050		
White (MP)	–	–	–	2.417e-16	1.202e-10	White (MP)	1.332e-15	8.970e-15	2.036e-08		
imaginary	–	–	–	1.111e-14	7.964e-09	imaginary	1.332e-15	7.690e-15	2.036e-08		
Iso White (EN)	–	–	–	4.700e-18	2.444e-15	Iso White (EN)	1.332e-15	8.801e-15	2.027e-08		
Iso White (MP)	–	–	–	4.587e-18	2.440e-15	Iso White (MP)	1.332e-15	7.379e-15	2.027e-08		
Iso imaginary	–	–	–	3.757e-16	1.408e-13	Iso imaginary	1.332e-15	8.564e-15	2.027e-08		
VS						VS					
η	$\langle T^2 \rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$	$[\eta,T^2]_{1B}$	$[\eta,T^2]_{2B}$	η	$\langle T^2 \rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$		
SMW (EN)	8.882e-16	–	–	2.536e-16	0.0584	SMW (EN)	-3.102e-04	4.415e-06	0.1698		
SMW (MP)	–	–	–	2.562e-16	1.452e-10	SMW (MP)	1.332e-14	8.465e-15	2.051e-08		
SMit	–	–	–	1.111e-14	8.638e-09	SMit	-4.619e-14	9.003e-15	2.050e-08		
Iso SMW (EN)	–	–	–	8.165e-17	3.993e-15	Iso SMW (EN)	8.882e-16	8.884e-15	2.040e-08		
Iso SMW (MP)	–	–	–	2.627e-17	3.256e-15	Iso SMW (MP)	8.882e-16	9.846e-15	2.040e-08		
Iso SMit	–	–	–	1.224e-15	1.674e-13	Iso SMit	8.882e-16	9.836e-15	2.040e-08		

TABLE I. Spurious ISB for isospin-averaged DeltaGO interaction in the **Hartree-Fock basis**, with various generators (IMSRG($3f_2$), magnus, complete decoupling with IsoAv generators, $\hbar\omega = 16$, cLS$= -2$, $e_{\max} = 3$)

DeltaGO_isoavg HO

^{14}O

$s = 0$

SR

η	$\langle T^2\rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$	$[\eta,T^2]_{1B}$	$[\eta,T^2]_{2B}$
White (EN)	0.000e+00	2.014e-12	2.314e-08	0.1696	4.8492
White (MP)	–	–	–	0.1651	4.7986
imaginary	–	–	–	5.1353	178.0304
Iso White (EN)	–	–	–	3.025e-17	1.364e-15
Iso White (MP)	–	–	–	1.202e-17	1.539e-15
Iso imaginary	–	–	–	9.679e-16	8.460e-14

VS

η	$\langle T^2\rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$	$[\eta,T^2]_{1B}$	$[\eta,T^2]_{2B}$
SMW (EN)	-1.776e-15	–	–	0.0152	0.3673
SMW (MP)	–	–	–	0.0089	0.3550
SMit	–	–	–	2.014e-12	8.933e-09
Iso SMW (EN)	–	–	–	1.194e-16	2.789e-15
Iso SMW (MP)	–	–	–	1.202e-16	3.164e-15
Iso SMit	–	–	–	4.985e-15	1.411e-13

$s \to \infty$

SR

η	$\langle T^2\rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$
White (EN)	0.0024	1.1649	262.4804
White (MP)	0.0024	1.1632	262.4878
imaginary	0.0026	1.1644	264.0152
Iso White (EN)	0.0032	1.2841	60.1039
Iso White (MP)	0.0032	1.2884	60.2127
Iso imaginary	0.0033	1.2171	59.8850

VS

η	$\langle T^2\rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$
SMW (EN)	0.0061	1.1518	60.0454
SMW (MP)	0.0059	1.1414	59.9322
SMit	0.0040	0.9764	59.2391
Iso SMW (EN)	0.0040	1.0389	58.9400
Iso SMW (MP)	0.0039	1.0377	58.9456
Iso SMit	0.0035	0.9119	58.4581

^{14}N

$s = 0$

SR

η	$\langle T^2\rangle - \frac{3}{4}$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$	$[\eta,T^2]_{1B}$	$[\eta,T^2]_{2B}$
White (EN)	0.000e+00	2.706e-15	2.026e-08	8.940e-17	0.0279
White (MP)	–	–	–	8.994e-17	1.221e-10
imaginary	–	–	–	2.683e-15	8.087e-09
Iso White (EN)	–	–	–	9.813e-18	1.727e-15
Iso White (MP)	–	–	–	9.813e-18	1.848e-15
Iso imaginary	–	–	–	3.140e-16	9.962e-14

VS

η	$\langle T^2\rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$	$[\eta,T^2]_{1B}$	$[\eta,T^2]_{2B}$
SMW (EN)	-1.110e-15	–	–	9.008e-17	0.0621
SMW (MP)	–	–	–	9.048e-17	1.470e-10
SMit	–	–	–	2.706e-15	8.737e-09
Iso SMW (EN)	–	–	–	5.194e-17	2.858e-15
Iso SMW (MP)	–	–	–	6.435e-17	2.463e-15
Iso SMit	–	–	–	2.826e-15	1.286e-13

$s \to \infty$

SR

η	$\langle T^2\rangle - \frac{3}{4}$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$
White (EN)	-5.170e-10	1.552e-07	0.0076
White (MP)	0.000e+00	4.133e-15	2.038e-08
imaginary	0.000e+00	3.737e-15	2.038e-08
Iso White (EN)	0.000e+00	3.682e-15	2.028e-08
Iso White (MP)	0.000e+00	3.844e-15	2.028e-08
Iso imaginary	0.000e+00	3.318e-15	2.028e-08

VS

η	$\langle T^2\rangle - 2$	$[H,T^2]_{1B}$	$[H,T^2]_{2B}$
SMW (EN)	-2.997e-04	5.003e-06	0.1874
SMW (MP)	-1.443e-14	3.789e-15	2.054e-08
SMit	-8.837e-14	4.020e-15	2.053e-08
Iso SMW (EN)	-1.332e-15	3.605e-15	2.041e-08
Iso SMW (MP)	-8.882e-16	3.760e-15	2.041e-08
Iso SMit	-4.441e-16	3.606e-15	2.041e-08

TABLE II. Spurious ISB for isospin-averaged DeltaGO interaction in the **harmonic oscillator basis**, with various generators (IMSRG($3f_2$), magnus, complete decoupling with IsoAv generators, $\hbar\omega = 16$, cLS$= -2$, $e_{\max} = 3$)

δ_C (%)

^{14}O					^{14}N				
$s = 0$					$s = 0$				
η	no HF		HF		η	no HF		HF	
	no Coul	Coulomb	no Coul	Coulomb		no Coul	Coulomb	no Coul	Coulomb
Any	2.220e-14	2.220e-14	-0.00016	-0.00029	Any	2.220e-14	2.220e-14	-2.220e-14	-1.000e-05
$s \to \infty$					$s \to \infty$				
η	no HF		HF		η	no HF		HF	
	no Coul	Coulomb	no Coul	Coulomb		no Coul	Coulomb	no Coul	Coulomb
SMW (EN)	-0.25566	-0.29942	-0.27495	-0.32487	SMW (EN)	4.585e-06	-0.01624	4.683e-06	-0.01626
SMW (MP)	-0.25466	-0.29817	-0.27458	-0.32459	SMW (MP)	4.441e-14	-0.01626	-2.220e-14	-0.01629
SMa (EN)	-0.25572	-0.29949	-0.27500	-0.32492	SMa (EN)	4.827e-06	-0.01624	4.910e-06	-0.01626
SMa (MP)	-0.25471	-0.29824	-0.27463	-0.32463	SMa (MP)	1.020e-08	-0.01626	8.743e-09	-0.01629
SMit	-0.25356	-0.29670	-0.27006	-0.31939	SMit	-2.220e-14	-0.01618	-2.220e-14	-0.01620
Iso SMW (EN)	-0.25498	-0.29369	-0.28461	-0.33482	Iso SMW (EN)	4.441e-14	-0.01573	-2.220e-14	-0.01574
Iso SMW (MP)	-0.25607	-0.29463	-0.28592	-0.33609	Iso SMW (MP)	4.441e-14	-0.01573	-4.441e-14	-0.01574
Iso SMa (EN)	-0.25497	-0.29368	-0.28458	-0.33479	Iso SMa (EN)	4.441e-14	-0.01573	2.220e-14	-0.01574
Iso SMa (MP)	-0.25605	-0.29461	-0.28589	-0.33605	Iso SMa (MP)	2.220e-14	-0.01573	-2.220e-14	-0.01574
Iso SMit	-0.25041	-0.28887	-0.27817	-0.32793	Iso SMit	4.441e-14	-0.01568	-2.220e-14	-0.01570

TABLE III. IMRSG(2) DeltaGo emax 2.

$s \to \infty$					$s \to \infty$				
η	no HF		HF		η	no HF		HF	
	no Coul	Coulomb	no Coul	Coulomb		no Coul	Coulomb	no Coul	Coulomb
SMW (EN)	-0.18470	-0.22160	-0.19991	-0.24026	SMW (EN)	5.599e-06	-0.01399	5.264e-06	-0.01386
SMW (MP)	-0.18452	-0.22144	-0.19962	-0.23997	SMW (MP)	4.441e-14	-0.01401	2.220e-14	-0.01385
SMa (EN)	-0.18474	-0.22165	-0.19994	-0.24029	SMa (EN)	5.706e-06	-0.01399	5.351e-06	-0.01386
SMa (MP)	-0.18456	-0.22148	-0.19966	-0.24000	SMa (MP)	3.740e-09	-0.01401	3.207e-09	-0.01385
SMit	-0.18505	-0.22166	-0.19787	-0.23760	SMit	-2.220e-14	-0.01401	4.441e-14	-0.01387
Iso SMW (EN)	-0.18441	-0.21589	-0.20684	-0.24581	Iso SMW (EN)	4.441e-14	-0.01331	-2.220e-14	-0.01325
Iso SMW (MP)	-0.18451	-0.21600	-0.20693	-0.24594	Iso SMW (MP)	4.441e-14	-0.01331	2.220e-14	-0.01326
Iso SMa (EN)	-0.18441	-0.21589	-0.20683	-0.24580	Iso SMa (EN)	2.220e-14	-0.01332	2.220e-14	-0.01325
Iso SMa (MP)	-0.18451	-0.21599	-0.20692	-0.24593	Iso SMa (MP)	4.441e-14	-0.01331	2.220e-14	-0.01326
Iso SMit	-0.18276	-0.21469	-0.20245	-0.24325	Iso SMit	-2.220e-14	-0.01334	6.661e-14	-0.01329

TABLE IV. IMSRG(3f$_2$) DeltaGO emax 2.

$s \to \infty$					$s \to \infty$				
η	no HF		HF		η	no HF		HF	
	no Coul	Coulomb	no Coul	Coulomb		no Coul	Coulomb	no Coul	Coulomb
SMW (MP)	-0.29796	-0.33639	-0.30217	-0.34159	SMW (MP)	4.441e-14	-0.01342	2.220e-14	-0.01361
Iso SMW (MP)	-0.29122	-0.32810	-0.29781	-0.33668	Iso SMW (MP)	2.220e-14	-0.01294	2.220e-14	-0.01307

TABLE V. IMRSG(3N7) DeltaGo emax 2.