Proton-neutron entanglement in the nuclear shell model

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Abstract. We compute the proton-neutron entanglement entropy in the interacting nuclear shell model for a variety of nuclides and interactions. Some results make intuitive sense, for example that the shell structure, as governed by single-particle and monopole energies, strongly affects the energetically available space and thus the entanglement entropy. We also find a surprising result: that the entanglement entropy at low excitation energy tends to decrease for nuclides when $N \neq Z$. While we provide evidence this arises from the physical nuclear force by contrasting with random two-body interactions which shows no such decrease, the exact mechanism is unclear. Nonetheless, the low entanglement suggests that in models of neutron-rich nuclides, the coupling between protons and neutrons may be less computationally demanding than one might otherwise expect.

Submitted to: J. Phys. G: Nucl. Part. Phys.
1. Introduction

The structure of atomic nuclei exhibits a mixture of simple and complex behaviors. What is meant by ‘simple’ can be subtle, but typically it means the behavior can be described by far fewer degrees of freedom than that required by modeling the nucleus as a collection of $A$ interacting nucleons; examples of simplicity include algebraic models \[1\] and mean-field pictures \[2\]. Of course, one must acknowledge that models themselves are not physical observables. Furthermore, complex models can mimic simpler ones, for example quasidynamic symmetries \[3, 4, 5\], where a Hamiltonian mixes symmetries yet observables such as spectra and ratios of transition strengths are consistent with ‘simpler’ symmetry-respecting models.

Entanglement is a concept describing whether the observable coordinates of a quantum system are independent; whether measurement of one generalized coordinate $q_1$ influences future measurements of another coordinate $q_2$ of a system $\psi(q_1, q_2, ...)$ \[6, 7\]. Such correlations can be described by the entanglement entropy, a concept which has become popular in recent years due to increasing interest in quantum information and the potential of quantum computing \[8, 9\]. It is trivial to write down states which are either separable (not entangled) or in a superposition of separable states (entangled), but the creation of entangled states in nature relies on the existence of an interaction that mixes the relevant degrees of freedom.

Here we consider the entanglement between the proton components and neutron components of configuration-interaction models of nuclei. Other recent work in entanglement entropy in nuclei addressed single-particle and seniority-mode entanglement \[10, 11\] as well as orbital entanglement revealing shell closures \[12\]; we note the first two papers reference unpublished versions of the research reported here.

Although it does not directly correspond to the work here, we point out previous analyses of nuclear configuration-interaction wave functions using ‘entropy,’ such as the configuration information entropy \[13, 14\], which is simple but basis dependent, and the invariant correlation entropy \[15\], which is much more complicated to compute. By contrast, because of the way our configuration interaction code constructs the wave functions, extraction of the wave function amplitudes in terms of proton-neutron coefficients is straightforward, a significant motivation for our approach.

In section 2 we lay out the basic framework of shell-model configuration-interaction calculations. In section 3 we define entanglement entropy as well as related concepts. We then provide examples of entanglement entropies for a variety of cases and show how much of the behavior for ground state entropies can be understood through standard concepts in nuclear structure physics. A persistent phenomenon, however, is not so easily explained: realistic ground states of nuclides with $N \neq Z$ tend to have significantly smaller entanglement entropies than those with $N = Z$.

We also show trends for entropies for all states. We can show this is related to some components of realistic nuclear forces by contrasting them with results using random interactions. While the mechanism for suppressing the entanglement eludes us, it is nonetheless worth reporting, not only as an apparently robust yet unexplained phenomenon, but also because it has a practical consequence: the low-lying states of neutron-rich nuclides have fewer nontrivial correlations between the proton and neutron components. This, in turn, suggests a practical approach for such nuclides, one which we are currently developing.
2. The nuclear configuration-interaction shell model

We find low-lying states of a nuclear Hamiltonian by the configuration-interaction method in a shell-model basis \[16, 17, 18\]. Any many-body Hamiltonian can be written in second quantization formalism as a polynomial in creation and annihilation operators \[2\]:

\[
\hat{H} = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{4} \sum_{ijkl} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k, \tag{1}
\]

where \(\epsilon_i\) are single particle energies and \(V_{ijkl}\) are the two-body interaction matrix elements. The single-particle operators \(\hat{a}_i^\dagger\) create spin-1/2 nucleons in simple harmonic oscillator states with quantum numbers: \(n_i\) (radial quantum number), \(l_i\) (orbital angular momentum), and \(j_i\) (total angular momentum). Many-body states are constructed as antisymmetrized products of these single particle states.

To make calculations tractable, we limit the number of single particle valence states. For example, several of our calculation assume a fixed \(^{16}\)O core and allows valence nucleons in the \(1s_{1/2}-0d_{3/2}-0d_{5/2}\) orbits, colloquially known as the \(sd\) shell; we also work in the \(pf\)-shell (\(^{40}\)Ca core with valence orbits \(1p_{1/2}, 3/2-0f_{5/2}, 7/2\)) and the combined \(sd-pf\) shells. Starting from a finite single-particle valence space yields a finite many-body basis \[18\]:

\[
|\Psi\rangle = \sum_{\alpha} c_{\alpha}|\alpha\rangle, \tag{2}
\]

where we use the occupation representation of Slater determinants, that is, of the form \(|\alpha\rangle = \prod_i \hat{a}_i^\dagger|0\rangle\). In particular we work in the \(M\)-scheme, which means the total \(J_z\) or \(M\) of all basis states is fixed to the same value. For our calculations here we construct all possible valence configurations with fixed \(M\). Furthermore, we factorize the basis into proton (\(\pi\)) and neutron (\(\nu\)) components, so that we can write:

\[
|\alpha\rangle = |\mu_\pi\rangle \otimes |\sigma_\nu\rangle. \tag{3}
\]

This enables calculation of the proton-neutron entanglement entropy.

The parameters \(\epsilon_i\) and \(V_{ijkl}\) in Eq. (1) are input parameters of the Hamiltonian. For details see the reviews in \[16, 17, 18\]. For our calculations we used both high-quality empirical interactions fitted separately in each model space to experimental spectra, as well as schematic interactions known to capture many features of nuclear structure, and randomly generated parameters. Using Eq. (1) and the factorized basis (2) one can compute \[18, 19\] the matrix elements of the Hamiltonian in the many-body basis, \(H_{\alpha,\beta} = \langle \alpha | H | \beta \rangle\). Then the time-independent Schrödinger equation becomes a simple matrix eigenvalue problem: \(\mathbf{H}\vec{c} = E\vec{c}\).

3. Entanglement entropy

The entanglement entropy is a fundamental tool in quantum information science \[2, 8, 9\]. Here we briefly review the development found in those sources.

For a pure quantum state \(|\Psi\rangle\), the density operator is \(\hat{\rho} = |\Psi\rangle \langle \Psi|\); in a basis \(\{|\alpha\rangle\}\), i.e., Eq. (2), the density matrix elements are \(\rho_{\alpha'\alpha} = c_{\alpha'}^* c_{\alpha}\). Because this is idempotent, \(\rho^2 = \rho\), and thus has either 0 or 1 as eigenvalues, the von Neumann entropy, \(S = -\text{tr}(\rho \log \rho)\) vanishes.
Suppose we work in a bipartite Hilbert space, e.g. \( \mathcal{H} = \mathcal{H}_\pi \otimes \mathcal{H}_\nu \), with basis states such as (3); we can then write Eq. (2) explicitly as
\[
|\Psi\rangle = \sum_{\mu,\sigma} c_{\mu,\sigma} |\mu_\pi\rangle \otimes |\sigma_\nu\rangle. \tag{4}
\]
An unentangled state is one where one can transform to a basis where the amplitudes are separable, that is \( c_{\mu,\sigma} = a_\mu b_\sigma \); in this case the state could be written as a simple product: \( |\Psi\rangle = \left( \sum_\mu a_\mu |\mu_\pi\rangle \right) \otimes \left( \sum_\sigma b_\sigma |\sigma_\nu\rangle \right) \). States which do not satisfy this are entangled.

In the basis (4) the density matrix is \( \rho_{\mu',\sigma';\mu,\sigma} = c_{\mu',\sigma'}^* c_{\mu,\sigma} \). This density matrix is idempotent. To get the reduced density matrix, one traces over one of the subspace indices:
\[
\rho_{\mu',\mu}^{\text{red}} = \sum_{\sigma} c_{\mu',\sigma}^* c_{\mu,\sigma}. \tag{5}
\]
If the state is unentangled, the reduced density matrix will also be idempotent. For a general state the reduced density matrix need not be idempotent, and its eigenvalues can be between 0 and 1. Then the entanglement entropy \[6\]
\[
S_{\text{entangled}} = -\text{tr} \rho^{\text{red}} \ln \rho^{\text{red}} \tag{6}
\]
can be nonzero. Because unentangled states must have zero entanglement entropy, non-zero entropy is a measure of entanglement \(6\). The fact that the eigenvalues of \( \rho^{\text{red}} \) are real and non-negative, and independent of which subspace index we trace over, is a result of the singular value decomposition theorem; this is also called the Schmidt decomposition, especially in quantum information science. The maximum entropy possible is the natural logarithm of the smaller subspace dimensions,
\[
S_{\text{max}} = \ln(\min(\text{dim}_\pi, \text{dim}_\nu)). \tag{7}
\]
Because our code is written using an explicit proton-neutron basis, it is easy to extract \( c_{\mu,\sigma} \) for any calculated state and then compute the entanglement entropy.

4. Results

We work in three different model spaces and with several different shell model interactions. All of our calculations are in the \(M\)-scheme, that is, a basis with fixed total \(J_z\). We start with several studies of \(N = Z\) nuclides in the \(sd\)-shell, where our results can be easily understood. We then look at cases in the \(sd, pf\), and \(sd-pf\) spaces with \(N \neq Z\), which leads to a surprise: ground states with \(N \neq Z\) have significantly lower entanglement entropies than those with \(N = Z\). By comparing with randomly generated interactions we provide evidence that this phenomenon has its origin in physical forces; but beyond that, we have yet to understand the specific mechanism. Finally, we look at the behavior of the entropy over the entire spectrum.

4.1. Examples with \(N = Z\) and the role of the shell structure

In this subsection we discuss some introductory results, focusing on \(N = Z\) nuclides.

Our first examples in Fig. [1] are the ground state entanglement entropies for \(N = Z\) nuclides in the so-called \(sd\)-shell, which has a fixed \(^{16}\)O core and valence particles in the \(1s_{1/2} - 0d_{3/2} - 0d_{5/2}\) orbitals. For convenience we give the \(M = 0\) dimensions in Table [1] Here the proton and neutron many-body spaces have equal dimensions. We
Figure 1. Ground state entanglement entropy for $N = Z$ nuclides in the $sd$-shell. Both panels show results for USDB [20], a high-quality empirical interaction, and the maximum possible entanglement entropy. In panel (a) we show results for an attractive isoscalar quadrupole-quadrupole (QQ) interaction; isovector (IV) and isoscalar (IS) pairing. In panel (b) we show results for USDB with single-particle energies and monopole interactions which have been set to zero, eliminating shell structure (’no mono’), and with single-particle energies were inflated by a factor of ten, amplifying shell structure (’s.p.e. x 10’). Additionally, panel (b) gives the average and standard deviation for calculations drawn from a two-body random ensemble [21], also with shell structure eliminated (’TBRE no mono’). See text for discussion.

| Nuclide | dimension |
|---------|-----------|
| $^{20}$Ne, $^{26}$Ar | 640 |
| $^{22}$Na, $^{34}$Cl | 6,116 |
| $^{24}$Mg, $^{32}$S | 28,503 |
| $^{26}$Al, $^{30}$P | 69,784 |
| $^{28}$Si | 93,710 |

Table 1. $M = 0$ dimensions for the $N = Z$ nuclides in Fig. 1 with valence nucleons in the $sd$-shell. Because there are a maximum of 12 valence nucleons of either species, the dimensions have a particle-hole symmetry around N,Z=14.

use a high-quality empirical interaction, the universal $sd$-shell interaction, version B or USDB, which, like all similar empirical interactions, is represented as a list of single-particle energies and two-body matrix elements fitted to data [20]. We also show in Fig. 1(a) the entropies for ground states of the attractive isoscalar quadrupole-
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Figure 2. Ground state entanglement beyond $N = Z$. Here we compare nuclide triplets with the same dimensionality (and thus the same maximum entanglement entropy), with the same number of protons/proton holes and neutrons/neutron holes; not all cases correspond to physical nuclides. Panel (a) is for $sd$-shell nuclides, while panel (b) is for $pf$-shell nuclides. Here USDB [20] is an empirical interaction for the $sd$-shell while GX1A [22, 23, 24] is for the $pf$-shell. We also show the average and standard deviation for interactions drawn from the two-body random ensemble (TBRE). Finally, ‘no mono’ means the single-particle energies and monopole interaction terms have been set to zero, thus eliminating any shell structure [18].

quadrupole (QQ) interaction, the attractive isovector (IV) pairing, that is, nucleons paired up to isospin $T = 1$, and the attractive isoscalar (IS) pairing, or nucleons paired up to $T = 0$. These schematic interactions are well-known in nuclear structure physics [16, 2, 25]; we give their exact definitions in the Appendix. Unsurprisingly, isoscalar pairing, which forces protons to pair with neutrons, has nearly maximal entanglement entropy. Isovector pairing shows a strong odd-even effect: odd-odd nuclides, where at least one proton and at least one neutron must pair up, has much higher entropy than the even-even cases. Ground states of the QQ interaction have a
much weaker odd-even staggering, while USDB ground states have the lowest entropies of all and exhibit no odd-even staggering.

In Fig. 1(b), we further investigate the origin of some of these behaviors. The shell structure of nuclei is governed by the single-particle energies and the so-called monopole terms \[ \hat{n}_a \hat{n}_b \] where \( \hat{n}_a \) is the number operator for orbital \( a \). By setting the single-particle energies and monopole terms to zero, the ground state entanglement entropy increases, and shows an odd-even staggering comparable to \( QQ \). Conversely, by inflating the standard USDB values of the single-particle energies (\( \epsilon(1s_{1/2}) = -3.2079 \) MeV, \( \epsilon(0d_{3/2}) = 2.1117 \) MeV, and \( \epsilon(0d_{5/2}) = -3.9257 \) MeV) by a factor of \( \times 10 \), we restrict the space energetically available and dramatically decrease the ground state entanglement entropy, reaching zero at shell closures. Finally, we considered two-body interactions drawn from a random ensemble (TBRE [21]), also removing single-particle energies and monopole terms. We used results from ten different members of the ensemble to get average entropies and corresponding standard deviations. From this we learn that, first, the shell structure, as encoded in single-particle energies and monopole terms, has a strong effect on the entanglement entropy, by energetically restricting the available model space and thus reducing the effective dimension. While the ‘no mono’ USDB results appear consistent with a randomly drawn interaction, it does show a nontrivial odd-even staggering. Later, we will see additional behaviors that strongly differ between USDB and randomly generated interactions.

From these numerical experiments we conclude the lower entanglement of the full USDB wave functions is due to the shell structure, i.e., the monopole terms and single-particle energies. We speculate the lack of odd-even staggering in the entropies of full USDB calculations may be due to many small, quasi-random components in the interaction beyond pairing and QQ.

4.2. Away from \( N = Z \)

In the previous subsection we considered exclusively nuclides with \( N = Z \). Here we compare entropies for nuclides with \( N \neq Z \), and find systematically lower entropies–albeit when using physical forces. Because we use interactions which respect isospin as a good symmetry, we only consider here \( N > Z \).

In Fig. 2 we compare the ground state entropies for ‘triplets’ of nuclides. These triplets are set in the same valence space, either \( sd \) or \( pf \), and all members of a triplet have the same number of valence protons or proton holes, and the same number of valence neutrons or neutron holes. For example, we have \( ^{26}\text{Ne} \), with 2 valence protons and 2 valence neutrons; \( ^{36}\text{Ar} \), with 2 proton holes and 2 neutron holes (since the filled \( sd \) valence orbitals contain 12 particles of a given nuclear species); and \( ^{28}\text{Ne} \), with 2 valence protons and 2 neutron holes. By this construction all members of a triplet have exactly the same dimensionalities. For the \( sd \)-shell cases in Fig. 2(a), following Fig. 1 we compare entanglement entropies from ground states computed with the full USDB interaction, USDB with monopole terms and single-particle energies set to zero, and finally entropies of ground states calculated from the two-body random ensemble (with monopole terms zeroed out). For the \( pf \)-shell cases in Fig. 2(b), we do the same but replace USDB with the GX1A interaction [24].

We see a strong and persistent trend: ground states of nuclides with \( N \neq Z \) computed with realistic interactions have significantly lower entanglement than those with \( N = Z \), a result we have replicated in other shell model spaces we do not show.
To put this in perspective, an entropy difference of 1 corresponds to a difference in effective dimensionality of $e = 2.71 \ldots$. This trend is stronger for even-even nuclides and when the shell structure is removed. For ground states computed under the TBRE, however, that trend disappears and is even slightly reversed. While we have made attempts to devise a plausible model for these behaviors, for example why the $N \neq Z$ entropy is lower for realistic interactions but is higher for the TBRE, we have not succeeded.

Because this trend suggests a lower entanglement for neutron-rich nuclides (or, because of isospin symmetry for these interactions, proton-rich as well), we continue our investigation in Fig. 3 where we consider cross-shell examples in the $sd$-$pf$ space using the ‘mu-db’ interaction $^{[26]}$. In order to compare with past results, we restrict the space so as to follow the dimensionalities of Fig. 1. Thus we restrict protons to the $sd$-shell, while for neutrons the $sd$-shell and the $0f_{7/2}$ orbitals are filled and frozen, leaving only $0f_{5/2}$-$1p_{3/2}$-$1p_{1/2}$ as the active space for neutrons. Finally, we restrict ourselves to the same number of active protons and neutrons. Thus the nuclides correspond to $^{40}$Ne, $^{42}$Na, $^{44}$Mg, and so on, through $^{56}$Ar. These restrictions are chosen so that the dimensionalities are the same as in Fig. 1. While somewhat artificial—we do not claim all these correspond to physical nuclides—this nonetheless
allows us to make a clean investigation into the entanglement. For ease of comparison, we include the USDB and USDB monopole-subtracted (‘no mono’) results for $N = Z$ nuclides, shifted over by $A = 20$ (so that $^{20,40}\text{Ne}$ are superimposed, etc.). Again we see a low entanglement entropy, even lower than for the $sd$-shell examples in Fig. 1, although the ‘no monopole’ case shows much of this is driven by shell structure. Nonetheless this provides evidence that the low-entanglement for $N \neq Z$ nuclides persists for cross-shell spaces.

It is important to note that this is not simply isospin. Although we do not show it, for a given $N$ and $Z$, states of different $J$ and $T$ nonetheless show very similar trends. In other words, this behavior is related to $T_z$, not $T$. In the next section we investigate further.

4.3. Entanglement entropies of excited levels

In the previous results we focused on ground state entanglement. Here we look at systems where we can fully diagonalize and compute the entanglement entropy across the spectrum.

![Figure 4](image.png)

Figure 4. Entanglement entropies for all levels as a function of excitation energy $E_x$. Panels (a), (b), and (c) are computed in the $sd$-shell using the USDB interaction [20]. Panel (d) is computed in the $sd-pf$ space, using the ‘mu-db’ interaction [26]; certain orbits are frozen in order to make the dimensions for this case the same as the other three cases. The maximum entanglement entropy is at the top of each plot.

In Fig. 4 we present the entanglement entropy for all levels for several nuclides computed with empirical interactions that give a good description of the data.
Specifically we consider $^{20,28}\text{Ne}$ and $^{36}\text{Ar}$, computed in the $sd$-shell with the USDB interaction [20], and $^{40}\text{Ne}$ computed in a truncated $sd-pf$ space, computed with a cross-shell interaction [26]; for the latter, we restricted the valence protons to the $sd$-shell, and froze all neutrons in the $sd$-shell and in the $0f_{7/2}$ orbital, so that we have only two valence neutrons in the $0f_{5/2}-1p_{3/2}-1p_{1/2}$ orbitals. These choices are made so that all four cases have exactly the same dimensionalities. While each plot has considerable scatter, there are a couple of noticeable features. The first is an overall curvature: on average, the entropy rises and then falls. The second feature is that the isospin-asymmetric nuclides, $^{28,40}\text{Ne}$, are noticeably more asymmetric in the distribution of entropies, in particular the low entropy of the ground state as pointed out in the previous section.

![Figure 5. Entanglement entropies for all levels as a function of excitation energy $E_x$. The top panels, (a)-(c), are computed with realistic interactions (USDB for panels (a) and (b), and ‘mu-db’ for panel (c)) but with all single-particle energies and monopole interaction terms set to zero, so as to remove shell effects. The bottom panels, (d)-(f), correspond to the same nuclides, but with a random two-body interaction. The maximum entanglement entropy is the top of each plot.](image-url)
Ne is much reduced. An important lesson we learn is that the $T_z$ dependence of the entropy appears to come out of the physical nuclear force, as it does not appear when using a randomly generated interaction.

5. Conclusions and acknowledgements

We have found that both schematic and realistic nuclear shell model Hamiltonians have low entanglement between the proton and neutron components of the wave function. This is particularly pronounced for states with high isospin. Part of the behavior is governed by the shell structure, which reduces the effective dimensionality, but, by using random two-body matrix elements, we can establish that the low entropy also is a feature of typical nuclear forces. While we have spent considerable effort to construct toy models to understand this behavior, so far none of them have provided convincing illumination.

A low entanglement means that one can get a good approximation to a wave function using a much smaller subset of basis states. This is the driving idea between the density matrix renormalization group methods [27, 28, 29], which have only been used sporadically in nuclear structure physics [12, 30, 31, 32, 33], partitioning on orbitals rather than between protons and neutrons. Closer to the present work is the proton-neutron singular-value decomposition analysis of shell model wave functions [34, 35]; ironically, the latter studies focused on $N \approx Z$ nuclides. One happy conclusion from our work presented here is that reduced basis methods, justified by low entanglement [36], may be even more effective for high-isospin nuclides, such as heavy nuclei, where the need for dimensional reduction is greatest. We have made progress in a systematic implementation of this idea and will present results soon.

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Award Number DE-FG02-03ER41272, and by the Office of High Energy Physics, under Award No. DE-SC0019465, and by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, with support from the ACT-UP award.

Appendix A. Schematic interactions

Schematic interactions are well-known to capture many features of nuclear structure and have long been used in nuclear physics [16, 2, 25]. For completeness we summarize them here.

- Quadrupole-Quadrupole (QQ): We construct a quadrupole operator

$$\hat{Q}_{2M,TM_T} = \sum_{ab} Q_{ab} [\hat{c}_a^\dagger \otimes \hat{c}_b]_{2M,TM_T}$$

(A.1)

where $a, b$ are indices for single-particle orbits defined by $n, l, j$; $[\cdot \otimes \cdot]_{JM,TM_T}$ indicates coupling by Clebsch-Gordan coefficients up to total angular momentum $J$ (here $J = 2$) and $z$-component $M$ and total isospin $T$ and third component $M_T$; $\hat{c}_a^\dagger$ creates a particle in orbit $a$, $\hat{c}_b$ is a time-reversed destruction operators [37] for a particle in orbit $b$; and finally the reduced matrix elements [37] of the quadrupole operator (which we compute in a harmonic-oscillator basis)

$$Q_{ab} = \langle a || r^2 Y_2 || b \rangle,$$

(A.2)
where $Y_{lm}(\theta, \phi)$ is a spherical harmonic. The quadrupole-quadrupole Hamiltonian is

$$V_{QQ} \left[ \hat{Q} \otimes \hat{Q} \right]_{00,00}, \quad (A.3)$$

where $V_{QQ}$ is the strength of the interaction and is taken $< 0$ to make it attractive; because we only focus on the wave functions and not the energies, the magnitude of $V_{QQ}$ is unimportant here. For our calculations we considered only the isoscalar ($T=0$) QQ interaction.

- Pairing. The pairing operator is

$$\hat{P}_{TM}^\dagger = \sum_a \sqrt{2j_a + 1} [c_a^\dagger \otimes c_a^\dagger]_{00,TM_T}, \quad (A.4)$$

where $j_a$ is the angular momentum of orbital $a$. The pairing Hamiltonian is

$$G \sum_{MT} (-1)^{-M_T} \hat{P}_{TM_T}^\dagger \hat{P}_{TM_T}, \quad (A.5)$$

where $G$ is the strength of the pairing Hamiltonian, and is taken $< 0$ to make attractive. Here $T = 1$ yields isovector pairing and $T = 0$ isoscalar pairing.
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