Application of the in-medium similarity renormalization group to a nuclear pairing Hamiltonian

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August 12, 2022

Abstract

We explore a way to utilize the in-medium similarity renormalization group (IMSRG) without the need to first perform a numerically extensive HF calculation to obtain the reference state. This serves to reduce the computational complexity of the IMSRG, which in turn will allow it to study more complicated systems than were previously possible. The system we apply our method to is a special form of the nuclear pairing Hamiltonian in which we assume all nucleons are identical and are in the same j-shell. We utilize the $su(2)$ structure of this Hamiltonian under quasi-spin operators to obtain an optimal seniority-based ground state, and derive analytic expressions for the relevant matrix elements using this state. Doing so in the perturbative limit of strong pairing, we obtain excellent agreement between our IMSRG result and the exact ground state of this system, which is given by numerically solving the Richardson equations. When we instead consider single particle energies that are on the order of the pairing strength, we see that it becomes necessary to further re-diagonalize our Hamiltonian in a reduced subspace.

1 Introduction

1.1 Background

The nucleus is a complicated system to study theoretically. Not only is the nucleus composed of strongly interacting, correlated particles, but the number of nucleons in a nucleus is too numerous for analytic treatment via the Schrodinger equation (with the exception of hydrogen), while simultaneously being too small to confidently apply purely statistical methods. As a result of this, in order to understand and develop models of a multitude of topics within nuclear physics, such as $\beta\beta$-decay and nuclear shape deformation, we must rely on (computationally efficient) many-body methods.

Due to its importance, there are a multitude of existing many-body methods that are used within nuclear physics, such as the coupled-cluster method and many-body perturbation theory. However, many of these methods rely on optimizing parameters using present experimental data, and thus don't offer much insight into the underlying theory. Therefore, it is often more advantageous to use an *ab-initio* method that attempts to describe many-body systems in a "ground-up" way, starting from fundamental nucleon-nucleon interactions and building up to a full many-body method. One such *ab-initio* method that has seen large success is the in-medium similarity renormalization group (IMSRG) [1], which involves utilizing unitary transformations to decouple the ground state of the many-body system from the higher-energy eigenstates, a process referred to as "RG-flow". The IMSRG has proven to be an accurate method for obtaining the ground state energy of many-body nuclear systems, and has been used to study the nuclear structure of elements such as ^{40}Ca [2]. Despite its accuracy, however, the IMSRG has shown to be very computationally expensive, which has hindered its ability to study heavier elements. This is because the IMSRG can be interpreted as a variational method [1], thus the choice of a reference state is crucial for obtaining accurate ground-state results. This is typically done by performing a Hartree-Fock (HF) calculation to obtain the optimal slater determinant state for a given system, which takes a considerable amount of computation time for large systems.

1.2 Project overview

In this paper, we explore a way to utilize the IMSRG without performing an HF calculation, thus reducing the computational complexity of the method, and in turn allowing it to be used on increasingly large systems without the need for more computing power. The system we will be applying the IMSRG to is a special form of the nuclear pairing

Hamiltonian – namely, we assume all nucleons are identical (ie, we don't introduce isospin as a degree of freedom), and assume all the nucleons are in the same j-shell, where j is the combined angular momentum of a given nucleon. To circumvent the need for an HF calculation to compute the reference state, as well as the need to numerically calculate matrix elements with respect to this state that are needed for normal ordering (which is an essential part of the IMSRG), we utilize the $su(2)$ structure of this Hamiltonian under quasi-spin operators to obtain an optimal ground state and derive analytic expressions for the relevant matrix elements using the Wigner-Eckart theorem.

It should be noted that the Hamiltonian we have chosen to analyze has an exact solution given by the Richardson equations [3]. Thus, we are not attempting to introduce a novel way to find the ground state of this specific system– rather, our intention is to introduce a method of utilizing the IMSRG without needing to numerically compute both the reference state and the normal ordered operators, with the Richardson solutions being used to check the accuracy of our work.

Section 2 contains an introduction to the IMSRG, with special attention being given to the process of normal-ordering. The seniority model, which used for obtaining an analytic, approximate ground state for our IMSRG calculations, is outlined in Section 3. This section also introduces the specific form of the pairing Hamiltonian that we took to be our model system. How we applied the IMSRG to obtain the ground state energy of our pairing Hamiltonian is detailed in Section 4, while Section 5 contains the results of our calculations. Finally, a detailed discussion of our results and future work is given in Section 6.

2 IMSRG

2.1 General concept

Let us consider a Hamiltonian H that describes the many-body nuclear system we are interested in. For any realistic nuclear model, H will have a complicated structure arising from strong particle correlations, such as nucleon-nucleon pairing. Therefore, to obtain information regarding the spectrum of H, it is useful to transform H via a similarity transformation $U(s)$, where s is an arbitrary variable that parameterizes the transformation, into a basis in which H takes on a simpler form. As similarity transformations preserve eigenvalues, determining the ground state energy of the transformed Hamiltonian, $H(s) = U(s)HU^\dagger(s)$, gives us the ground state of our desired system. The easiest way to obtain the eigenvalues is to transform H into a basis in which $H(s)$ is diagonal, in which case the eigenvalues can be simply read-off. To facilitate this process, we take $U(s)$ to be unitary so that we can define it as

$$U(s) = \mathcal{S}\left\{\exp\left(\int_0^s ds'\eta(s)\right)\right\} \tag{1}$$

where $\mathcal{S}$ denotes the "s-ordering" operator (completely analogous to the time-ordering operator used in quantum field theory) and $\eta(s)$ is the generator of $U(s)$. It is useful to define $U(s)$ in this way as it allows us to construct a differential equation for H that can be integrated to obtain $H(s)$, which avoids the need to compute the path-ordered exponential. Obtaining the differential equation is done by differentiating the expression for the transformed Hamiltonian, $H(s) = U(s)HU^\dagger(s)$, and using the fact that $\eta(s) = U'U^\dagger(s)$ (the prime here denotes differentiation with respect to s). This gives us the operator flow equation

$$\frac{\mathrm{d}}{\mathrm{d}s}H(s) = [\eta(s), H(s)] \tag{2}$$

Our goal of diagonalizing H now amounts to choosing $\eta(s)$ such that the off-diagonal terms of $H(s)$, which are obtained from integrating Equation (2), vanish as $s \to \infty$. Of course, for most applications we only care about the ground state energy, thus we really only need $\eta(s)$ to decouple the ground state of $H(s)$ from its higher-energy excited states. Possible choices of generators that accomplish this task are discussed in Reference [1].

To actually solve Equation (2) on a computer we need to express our operators in matrix-form, thus we have to choose a basis of states to represent them in. For fermionic systesms, a natural choice of basis is the basis formed by slater determinants, which are states of the form

$$|\Phi\rangle = \prod_i^N a_{j_i}^\dagger |\phi\rangle \tag{3}$$

where $a_{j_i}^\dagger$ is the creation operator for a fermion with some single-particle quantum number j_i and $|\phi\rangle$ is the vacuum state. Using a Hartree-Fock (HF) procedure, we can numerically obtain the slater determinant $|\Phi\rangle$ that is the closest approximation to the true ground state, from which we can obtain the other states in our basis through the application

of particle-hole excitations. We refer to such $|\Phi_0\rangle$ as the reference state. Of course, we don't have to construct our basis from slater determinants; we can instead consider a more general basis comprised of an N-body reference state $|\Phi_0\rangle$, which is typically chosen to be such that it is a close approximation to the true ground state, and all of its possible excitations. The reason for choosing $|\Phi_0\rangle$ close to the true ground state, which is generally done perturbatively (i.e, we know the exact ground state of some H_0 and use this as the reference state of $H = H_0 + \epsilon H_1$ for a suitable choice of ϵ) is two-fold: 1) it reduces the computational effort needed to obtain the ground state via the IMSRG, and 2) it ensures that the eigenvalue associated with the reference state as $s \to \infty$ is the ground state energy and not an excited state energy. Typically, we refer to non-slater determinant reference states as multi-reference states.

With our reference state defined, we can now state the broad goal of the IMSRG as follows: evolve H via Equation (2) with an appropriately chosen η such that we decouple our reference state $|\Phi_0\rangle$ from the other excited states that define our basis (i.e, the states formed by performing excitations of $|\Phi_0\rangle$).

2.2 Normal Ordering

While we defined the broad goal of the IMSRG in Section 2.1, we need to do more work before actually being able to implement the IMSRG numerically. Let us start by first defining the notion of a (generalized) normal-ordered operator. Analogous to QFT, where normal ordering of an operator is performed such that the operator's expectation value with respect to the vacuum state is 0, generalized normal ordering makes it such that the expectation value with respect to the chosen reference state is 0. For a generic 1-body operator $a_i^\dagger a_j$ (note that we will only ever consider operators that preserve particle number), we can see that it can be normal ordered by considering

$$: a_i^\dagger a_j := a_i^\dagger a_j - \langle\Omega|a_i^\dagger a_j|\Omega\rangle\,, \tag{4}$$

where $: O :$ denotes a (generalized) normal-ordered operator O, and $|\Omega\rangle$ is now defined to be our reference state. This clearly satisfies the required property $\langle\Omega| : a_i^\dagger a_j : |\Omega\rangle = 0$. For 2-body operators $a_i^\dagger a_j^\dagger a_k a_l$ we have the normal-ordered operator being

$$\begin{aligned} : a_i^\dagger a_j^\dagger a_k a_l : = {} & a_i^\dagger a_j^\dagger a_k a_l - \langle\Omega|a_i^\dagger a_j^\dagger a_k a_l|\Omega\rangle \\ & - \langle\Omega|a_i^\dagger a_l|\Omega\rangle : a_j^\dagger a_k : + \langle\Omega|a_i^\dagger a_k|\Omega\rangle : a_j^\dagger a_l : \\ & - \langle\Omega|a_j^\dagger a_l|\Omega\rangle : a_i^\dagger a_k : + \langle\Omega|a_i^\dagger a_k|\Omega\rangle : a_i^\dagger a_l : \end{aligned} \tag{5}$$

Using Equation (4), we have that $\langle\Omega| : a_i^\dagger a_j^\dagger a_k a_l : |\Omega\rangle = 0$, with the added benefit that we can define a more general form of Wick's theorem for decomposing the product of normal-ordered operators into a sum of normal-ordered operators, which is given in Reference [1]. We can further define 3-body normal-ordered operators analogously to Equation (5), with the explict form being displayed in Reference [1].

Let us now reconsider our Hamiltonian, and assume that it can be appropriately described in terms of 1, 2, and 3 body operators (ie, we assume at most $3N$ interactions). If we now re-write our Hamiltonian such that all of the operators are replaced with their normal-ordered counterparts, then we pick up a 0 body term that contains the 1, 2, and 3-body density matrix elements $\langle\Omega|a_a^\dagger a_b|\Omega\rangle\,, \langle\Omega|a_a^\dagger a_b^\dagger a_c a_d|\Omega\rangle$, and $\langle\Omega|a_a^\dagger a_b^\dagger a_c^\dagger a_d a_e a_f|\Omega\rangle$ (matrix elements with respect to the reference state are referred to as "in-medium" contributions), while the 1 and 2 body operators contain the remaining 1 and 2 body in-medium contributions. This ensures that even though applying the commutator from Equation (2) induces higher order operators, we can safely truncate our normal-ordered Hamiltonian to contain only 0, 1, and 2 body normal-ordered operators, as these elements contain all of the 1, 2, and 3-body in-medium contributions. We can then write our truncated, normal-ordered Hamiltonian most generally as

$$H = E + \sum_{i,j} f_j^i : a_i^\dagger a_j : + \sum_{i,j,k,l} \Gamma_{kl}^{ij} : a_i^\dagger a_j^\dagger a_l a_k : \tag{6}$$

To construct explicit forms for E, f_j^i, and Γ_{kl}^{ij}, we must first specify our Hamiltonian so that we can calculate the relevant matrix elements in Equations (4) and (5). This truncation scheme is referred to as the IMSRG(2), and it has been shown to be very effective for many systems in nuclear physics [2]. If we also require that

$$\eta = \eta^{(0)} + \eta^{(1)} \tag{7}$$

and plug Equations (6) and (7) into the operator flow equation (2), then we obtain a system of ODEs for $E(s)$, $f_j^i(s)$ and $\Gamma_{kl}^{ij}(s)$ that can be numerically solved and used to obtain $H(s)$. Solving this system of equations, which are commonly referred to as the IMSRG "flow equations", to decouple the reference state, i.e. ensure that

$$\langle\Omega|H(s)|\varphi\rangle = E\,\langle\Omega|\varphi\rangle + \sum_{i,j} f_j^i(s)\,\langle\Omega| : a_i^\dagger a_j : |\varphi\rangle + \sum_{i,j,k,l} \Gamma_{kl}^{ij}(s)\,\langle\Omega| : a_i^\dagger a_j^\dagger a_l a_k : |\varphi\rangle = 0 \tag{8}$$

where $|\varphi\rangle$ are the excited states of our basis, is precisely what the IMSRG attempts to do. Note that, by definition of normal-ordered operators, the expectation value of $H(s)$ with respect to the reference state is $\langle\Omega|H(s)|\Omega\rangle = E(s)$. Thus, in the case of true decoupling of the reference state at $s = \infty$, we have the ground state energy being $E(\infty)$. Therefore, our interest is in the convergence of $E(s)$ at large s.

3 Nuclear pairing Hamiltonian

3.1 Quasi-spin Formalism

Consider a system of N nucleons contained within angular momentum shells $j = j_1, ...$ that are interacting via a constant pairing force G. This yields the standard pairing Hamiltonian

$$H = \sum_{j,m} \epsilon_{j,m} a^\dagger_{j,m} a_{j,m} - \frac{G}{4} \sum_{j,j',m,m'} (-1)^{j+j'-m-m'} a^\dagger_{j,m} a^\dagger_{j,m-} a_{j',-m'} a_{j',m'} \tag{9}$$

where $\epsilon_{j,m}$ is the single particle energy of a nucleon with quantum numbers j, m, where $m = -j, ...j$.

Let us focus our attention on the two-body component of our Hamiltonian, which incorporates the pairing interaction between nucleons. We will refer top this as H_{pair}, and it is given by

$$H_{pair} = -\frac{G}{4} \sum_{j,j',m,m'} (-1)^{j+j'-m-m'} a^\dagger_{j,m} a^\dagger_{j,m-} a_{j',-m'} a_{j',m'} \tag{10}$$

Following the analysis presented in Chapter 6 of Ring and Schuck [4], we are led to define the operators

$$\begin{aligned} S_+ &= \frac{1}{2} \sum_{j,m} (-1)^{j-m} a^\dagger_{j,m} a^\dagger_{j,-m} \\ S_- &= \frac{1}{2} \sum_{j,m} (-1)^{j-m} a_{j,-m} a_{j,m} \\ S_0 &= \frac{1}{4} \sum_{j,m} \left(a^\dagger_{j,m} a_{j,m} + a^\dagger_{j,-m} a_{j,-m} - 1 \right) = \frac{1}{2}(N - \Omega) \end{aligned} \tag{11}$$

where

$$\Omega = \frac{1}{4} \sum_{j,m} 1 = \sum_j (j + \frac{1}{2}) \tag{12}$$

represents the maximum number of paired nucleons that are allowed within our system (each j-shell has at most $2j+1$ nucleons, corresponding to a maximum of $j + 1/2$ possible pairs for each shell). From the commutation relations derived in Appendix 1 (Section 7.3), we can see that $S_0, S_\pm$ correspond precisely to the generators of an $su(2)$ algebra, which we call the "quasi-spin" algebra. We can clearly see that these operators allow us to write H_{pair} as

$$H_{pair} = -GS_+S_- = G(S^2 - S_0^2 + S_0) \tag{13}$$

where $\mathbf{S} = S_0^2 + S_1^2 + S_2^2$ is the quadratic Casimir operator of our algebra. We thus have the eigenstates of H_{pair} for a given N being states with definite quasi-spin, denoted S, and $S_0 = 1/2(N - \Omega)$, where Ω is determined by the number of j-shells present. We denote these states $|S, S_0\rangle$ and can see that it has an eigenvalue under H_{pair} of

$$E(S) = -G \left[S(S+1) - \frac{1}{4}(N - \Omega)^2 + (N - \Omega) \right] \tag{14}$$

Finally, for a state of definite quasi-spin S we can define the seniority of the state as $s = 2S - \Omega$, which corresponds to the number of unpaired nucleons, i.e, $s = 0$ means all pairs (m,-m) are full, $s = 1$ means one such pair is empty, etc. With this definition, our energy becomes

$$E(s) = -\frac{G}{4} (N - s) (2\Omega - s - N + s) \tag{15}$$

which is a minimum when $s = 0$. Therefore, the seniority 0 state is the ground state of H_{pair}.

3.2 Our Model Hamiltonian

For the purposes of this analysis, let us look at a simplified version of the pairing Hamiltonian (10) in which all nucleons are in the same j-shell. In this case, we have our Hamiltonian being

$$H = \sum_m \epsilon_m a_m^\dagger a_m + \frac{1}{4}\sum_{m,m'} g_{m,m'}(-1)^{-m-m'} a_m^\dagger a_{-m}^\dagger a_{-m'} a_{m'} \tag{16}$$

If we further assume that the single particle energies are equally spaced by some value ϵ such that $\epsilon_m = |m|\epsilon$, then we have

$$\begin{aligned} H &= \epsilon \sum_m |m| a_m^\dagger a_m + \frac{1}{4}\sum_{m,m'} g_{m,m'}(-1)^{-m-m'} a_m^\dagger a_{-m}^\dagger a_{-m'} a_{m'} \\ &= \epsilon H_1 + H_{pair} \end{aligned} \tag{17}$$

where $H_1 = \sum_m |m| a_m^\dagger a_m$.

4 Applying the IMSRG

4.1 Normal-Ordering the Hamiltonian

As we showed in Section 3.1, the ground state of H_{pair} is the seniority 0 state $|0, S_0\rangle = |0, \frac{1}{2}N - \frac{1}{2}\Omega\rangle$, where now $\Omega = j + 1/2$ as a result of our model Hamiltonian 16 having only a single j-shell. Thus, for $G >> \epsilon_m$ we can safely define the reference state for our IMSRG calculations to simply be $|0, S_0\rangle$.

With our reference state defined, we now need to normal order our Hamiltonian, as detailed in Section 2.2. To do so we need to compute the matrix elements shown in Equations (4) and (5). Typically this is done numerically, but the advantage to using the seniority 0 state is that we have $su(2)$ structure present. From Sections 7.2 and 7.1 in Appendix I, we can see that $a_{j,m}^\dagger$ and $\tilde{a}_m = (-1)^{j-m} a_{-m}$ are spinors under the quasi-spin operators. As $|0, S_0\rangle$ is a state of definite quasi-spin, we can thus use the Wigner-Eckart theorem to compute the 1 and 2 body matrix elements that are necessary for normal ordering. This is done explicitly in Appendix II (Sections 8.1 and 8.2), giving us

$$\begin{aligned} :a_m^\dagger a_{m'}: &= a_m^\dagger a_{m'} - \langle \Omega/2, S_0 | a_m^\dagger a_{m'} | \Omega/2, S_0\rangle \\ &= a_m^\dagger a_{m'} - \frac{N}{2\Omega}\delta_{m,m'} \end{aligned} \tag{18}$$

and

$$\begin{aligned} :a_m^\dagger a_{m'}^\dagger a_{m''} a_{m'''}: &= a_m^\dagger a_{m'}^\dagger a_{m''} a_{m'''} - \langle \Omega/2, S_0 | a_m^\dagger a_{m'}^\dagger a_{m''} a_{m'''} | \Omega/2, S_0\rangle + \text{singles} + \text{doubles} \\ &= a_m^\dagger a_{m'}^\dagger a_{m''} a_{m'''} - \frac{1}{4\Omega(\Omega-1)}[N(N-2)(\delta_{-m,-m'''}\delta_{-m',-m''} - \delta_{-m,-m''}\delta_{-m',-m'''}) \\ &+ N(N-2\Omega)(-1)^{m+m'''}\delta_{m,-m'}\delta_{m'',-m'''}] + \frac{N}{2\Omega}(-\delta_{m,m'''}:a_{m'}^\dagger a_{m''}: + \delta_{m,m''}:a_{m'}^\dagger a_{m'''}: \\ &- \delta_{m',m''}:a_m^\dagger a_{m'''}: + \delta_{m',m'''}:a_m^\dagger a_{m''}:) \end{aligned} \tag{19}$$

Substituting these normal-ordered operators into our Hamiltonian then gives us a Hamiltonian of the form of Equation (6)

$$H = E + \sum_m f_m :a_m^\dagger a_m: + \frac{1}{4}\sum_{m,m'} \Gamma_{m,m'} :a_m^\dagger a_{-m}^\dagger a_{-m'} a_{m'}: \tag{20}$$

where here we have

$$\begin{aligned} \Gamma_{m,m'} &= g_{m,m'}(-1)^{-m-m'} \\ f_m &= \epsilon_m - \frac{N}{4\Omega}(g_{-m,-m} + g_{m,-m}) \\ E &= \frac{N}{2\Omega}\sum_m \epsilon_m - \frac{1}{4}\left[\frac{N(N-2)}{4\Omega(\Omega-1)}\left(\sum_m g_{m,m} + \sum_m g_{m,-m}\right) - \frac{N(N-2\Omega)}{4\Omega(\Omega-1)}\sum_{m,m'} g_{m,m'}\right] \end{aligned} \tag{21}$$

These are the quantities to which we will apply the IMSRG flow equations.

4.2 IMSRG Flow Equations

The result of plugging Equation (20) into the operator flow equation (2) is a set of coupled differential equations given by

$$\begin{aligned}\frac{dE}{ds} &= \frac{1}{4}\sum_{m,m'}\left[\left(\eta^m_{m'}\Gamma_{m,m'} - \Gamma_{m',m}\eta^{m'}_m\right)\left(\frac{N}{2\Omega}\left(1-\frac{N}{2\Omega}\right)\right)^2 + \left(\frac{d}{ds}\Gamma_{m,m'}\right)\lambda^{m,-m}_{m',-m'}\right] \\ &+ \frac{1}{4}\sum_{a,b,c,d,e}\left(\eta^{b,c}_{d,e}\Gamma_{a,b}\lambda^{c,a,-a}_{d,e,-b} - \Gamma_{a,b}\eta^{c,d}_{a,e}\lambda^{-a,c,d}_{b,-b,e}\right),\end{aligned} \tag{22}$$

$$\begin{aligned}\frac{d}{ds}f_m &= (\eta^m_m f_m - f_m\eta^m_m) + \left(1-\frac{N}{2\Omega}\right)\frac{N}{4\Omega}\sum_a\left(\eta^{m,-m}_{a,-a}\Gamma_{m,a} - \Gamma_{a,m}\eta^{a,-a}_{m,-m}\right) + \frac{1}{4}\sum_{a,b,c}\left(\eta^{m,-m}_{b,c}\Gamma_{a,m}\lambda^{a,-a}_{b,c} - \Gamma_{m,a}\eta^{b,-a}_{m,-m}\lambda^{b,c}_{a,-a}\right) \\ &+ \sum_{a,b,c}\left(\eta^{m,b}_{a,c}\Gamma_{a,m}\lambda^{b,-a}_{c,-m} - \Gamma_{m,a}\eta^{a,b}_{m,c}\lambda^{-m,b}_{-a,c}\right) - \frac{1}{2}\sum_{a,b,c}\left(\eta^{m,a}_{m,b}\Gamma_{c,a}\lambda^{c,-c}_{b,a} - \Gamma_{m,m}\eta^{b,c}_{-m,a}\lambda^{b,c}_{-m,a}\right) \\ &+ \frac{1}{2}\sum_{a,b,c}\left(\eta^{m,c}_{m,a}\Gamma_{a,b}\lambda^{c,-a}_{b,-b} - \Gamma_{m,m}\eta^{-m,a}_{b,c}\lambda^{-m,a}_{b,c}\right)\end{aligned} \tag{23}$$

$$\begin{aligned}\frac{d}{ds}\Gamma_{m,m'} &= \left(\eta^m_m + \eta^{-m}_{-m} - \eta^{m'}_{m'} - \eta^{-m'}_{-m'}\right)\Gamma_{m,m'} - \left(f_m + f_{-m} - f_{m'} - f_{-m'}\right)\eta^{m,-m}_{m',-m'} \\ &+ \frac{1}{2}\left(1-\frac{N}{\Omega}\right)\sum_a\left(\eta^{m,-m}_{a,-a}\Gamma_{a,m'} - \Gamma_{m,a}\eta^{a,-a}_{m',-m'}\right)\end{aligned} \tag{24}$$

where

$$\eta = \sum_{i,j}\eta^i_j a^\dagger_i a_j + \sum_{i,j,k,l}\eta^{i,j}_{k,l}a^\dagger_i a^\dagger_j a_l a_k \tag{25}$$

is our generator and λ are the irreducible matrix elements, which are given by

$$\begin{aligned}\lambda^{a,b}_{c,d} &= \langle N|a^\dagger_a a^\dagger_b a_d a_c|N\rangle - \langle N|a^\dagger_a a_c|N\rangle\langle N|a^\dagger_b a_d|N\rangle + \langle N|a^\dagger_a a_d|N\rangle\langle N|a^\dagger_b a_c|N\rangle \\ &= \left(\frac{1}{4\Omega(\Omega-1)}[N(N-2)(\delta_{-a,-c}\delta_{-b,-d} - \delta_{-a,-d}\delta_{-b,-c}) + N(N-2\Omega)(-1)^{a+c}\delta_{-a,b}\delta_{-d,c}]\right) + \left(\frac{N}{2\Omega}\right)^2(\delta_{a,d}\delta_{b,c} - \delta_{a,c}\delta_{b,d})\end{aligned} \tag{26}$$

and

$$\lambda^{a,b,c}_{d,e,f} = \langle N|a^\dagger_a a^\dagger_b a^\dagger_c a_f a_e a_d|N\rangle - \mathcal{A}\{\lambda^a_d\lambda^{b,c}_{e,f}\} - \mathcal{A}\{\lambda^a_d\lambda^b_e\lambda^c_f\} \tag{27}$$

where $\mathcal{A}$ is the antisymmetrization operator.

All that is left in order to solve the ODE system given by Equations (22)-(24) is to define a generator that will decouple our seniority 0 reference state as $s\to\infty$, in accordance with Equation (8), so that we can obtain the ground state energy $E(\infty)$.

4.3 Generator

There is lots of freedom when it comes to choosing a generator, with an extensive discussion of popular choices being given in Reference [1]. For the purposes of a multi-reference state, which we have here, the most commonly used generator is the Brillouin generator, defined by

$$\begin{aligned}\eta^i_j &= \langle\Phi_0|[H,:a^\dagger_i a_j]|\Phi_0\rangle \\ \eta^{i,j}_{k,l} &= \langle\Phi_0|[H,:a^\dagger_i a^\dagger_j a_l a_k]|\Phi_0\rangle\end{aligned} \tag{28}$$

For our given choice of Hamiltonian and reference state, we have

$$\begin{aligned}\eta^i_j &= -1/2\sum_m(\Gamma_{j,m}\lambda^{i,-j}_{m,m} - \Gamma^{m,-m}_{i,-i}\lambda^{m,-m}_{j,-i}) \\ \eta^{i,j}_{k,l} &= f_i\lambda^{i,j}_{k,l} - f_j\lambda^{j,i}_{k,l} - f_k\lambda^{i,j}_{k,l} + f_l\lambda^{i,j}_{l,k} \\ &+ \frac{1}{2}\left(\Gamma^{k,-k}_{m,-m}\lambda^{-k,i,j}_{m,-m,l} - \Gamma^{l,-l}_{m,-m}\lambda^{-l,i,j}_{m,-m,k} - \Gamma^{m,-m}_{i,-i}\lambda^{m,-m,j}_{-i,k,l} + \Gamma^{m,-m}_{j,-j}\lambda^{m,-m,i}_{-j,k,l}\right)\end{aligned} \tag{29}$$

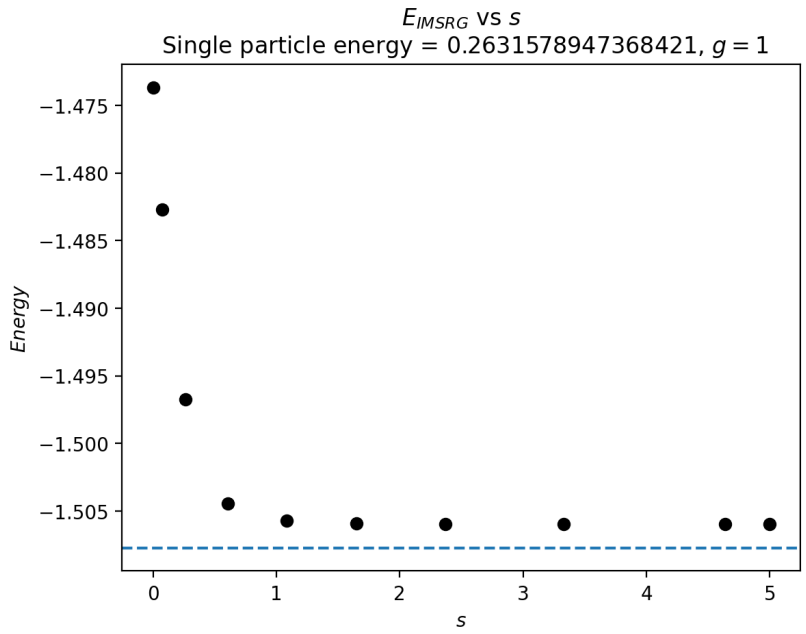

Figure 1: The output of the IMSRG for $E(s)$ at $\epsilon \approxeq 0.26$ and $N = 2$, which was obtained by solving Equations (22)-(24) for $0 \leq s \leq 5$. The blue dashed line corresponds to the true ground state energy of this configuration, which was obtained by numerically solving the Richardson equations.

Having derived analytic expressions for all of the quantities contained in our flow equations, we can now solve them to obtain the ground state of our system.

5 Results

Numerical implementation of the IMSRG flow equations was carried out using Python, with the package `scipy.integrate.solve_ivp` being used to actually solve the system of ODE's. We chose a system comprised of two indistinguishable nucleons, and integrated s from 0 to 5, which proved to be sufficient in allowing the numerical solver to converge. Furthermore, when solving the flow equations we took the pairing strength to be $G = 1$ and solved the equations for 20 values of ϵ that ranged from 0 to 1. This was done to test the performance of our numerical scheme both at points in the perturbative regime $\epsilon << G$ as well as the non-perturbative regime $\epsilon \to G$. The output of our numerical solver for $E(s)$ at $\epsilon \approx 0.26$ is shown in Figure 1. The ground state energy of our pairing Hamiltonian (17) at all of the chosen values of ϵ is displayed in Figure 2, where we took the ground state energy to be $E(s = \infty) \approx E(s = 5)$. Displayed alongside our results from the IMSRG is the exact ground state energy of our simplified pairing Hamiltonian at these various values of ϵ, which were found by numerically solving the Richardson equations [3]. To ensure the numerical implementation of the Richardson equations was working properly, we analytically diagonalized the Hamiltonian (16) to obtain the true ground state of the system for 2 nucleons.

6 Conclusion

6.1 Discussion

It is evident from Figure 2 that the IMSRG scheme we developed yields accurate ground state energies in the perturbative regime $\epsilon << G$, with the relative error between our IMSRG output and the true ground state energy being close to 0 for $0 \leq \epsilon \approxeq 0.4$, where G was taken to be 1. Outside of this perturbative regime, however, we can see that the relative error increases exponentially. As the Richardson equations were accurately solved, which is evidenced by the agreement between the Richardson solutions and our analytic expression for the true ground state energy in Figure 2, this suggests that our reference state becomes a worse approximation to the ground state as $\epsilon \to G$, which is exactly as we would expect from the way it was constructed. Furthermore, we can see from Figure 1 that even within the perturbative regime we don't have full decoupling of the reference state, as the converged value of the IMSRG lies above the dashed line corresponding to the true ground state energy (exact decoupling would give us the true ground

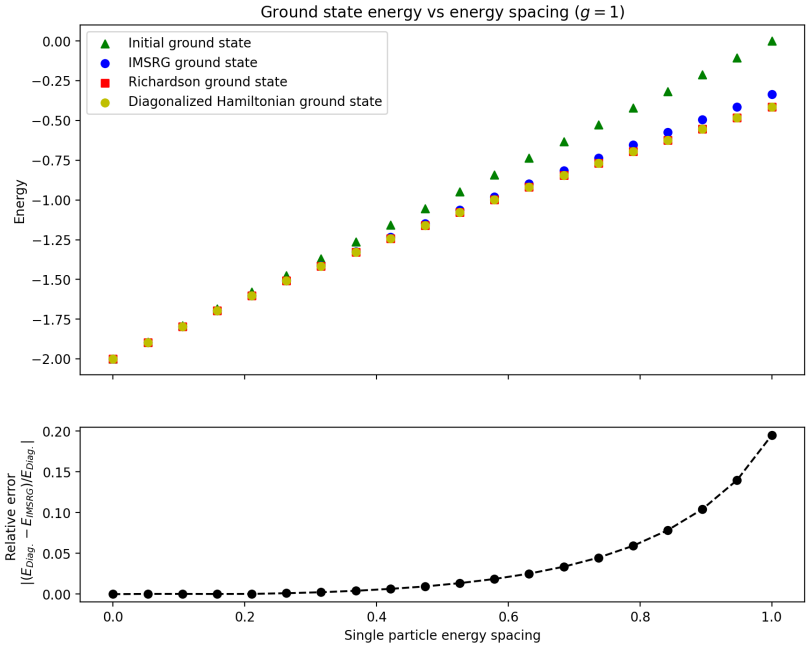

Figure 2: The ground state energy and relative error of the IMSRG for twenty different values of ϵ, i.e. the single particle energy spacing. Plotted alongside the IMSRG ground state energy is the exact ground state energy given by the Richardson equations (alongside our analytic calculation of the true ground state), and our initial value for $E(s)$, given by Equation (21). Note that with the way we constructed our reference state, $E(0) = \langle H \rangle$ corresponds precisely to the pure pairing Hamiltonian ground state + first order perturbative correction. Note that for $\epsilon << G$, we see excellent agreement between our IMSRG and the exact ground state energy, while for $\epsilon \sim G$ we see the relative error increasing exponentially.

state energy, thus it should lie precisely on this line). This is a consequence of our choice to use a multi-reference state as opposed to a slater determinant, as discussed in Reference [1]. To obtain more effective decoupling, as well as extend the accuracy of the IMSRG farther into the non-perturbative regime of $\epsilon \sim G$, we can perform a re-diagonalization routine of the Hamiltonian in a reduced subspace. This is done by taking the Hamiltonian that is outputted by the IMSRG, projecting it onto a subspace spanned by, for example, the seniority 0 and seniority 2 states (i.e, the reference state and first excited state, respectively) and obtaining the exact eigenvalues of this new matrix using a numerical routine such as `numpy.linalg.eig`. If we assume that the first excited state couples the strongest to the reference state, then this would serve to increase the accuracy of our obtained ground state energy. This type of re-diagonalization procedure is commonly performed in IMSRG applications, such as in Reference [2].

6.2 Concluding Thoughts

We have presented here a method of performing the IMSRG by utilizing the algebraic structure of the pairing Hamiltonian to obtain analytic expressions for relevant matrix elements. Doing so eliminates the need to numerically calculate these matrix elements, in turn greatly reducing the computational time needed to perform IMSRG calculations, which will allow the IMSRG to be applied to more complicate physical systems. Applying our method to a simplified pairing model that assumes a single j-shell and indistinguishable nucleons, we saw that our method had excellent agreement with the exact ground state energy, which is given by solving the Richardson equations, in the regime of $\epsilon << G$, where ϵ is the single particle energy spacing and G is the pairing strength. However, as is true for all multi-reference states, we did not obtain true decoupling of the ground state, especially in the limit of $\epsilon \to G$. To mitigate this, we proposed a method to project the outputted Hamiltonian onto the seniority 0 and seniority 2 subspace, and then perform a diagonalization routine on the resulting matrix to obtain a more accurate approximation of the ground state energy.

7 Appendix I: Commutation Relations

7.1 Relations for $a^\dagger$

$$
\begin{aligned}
(1)\quad [S_+, a^\dagger_{j,m}] &= \frac{1}{2}\sum_{j',m'} (-1)^{j'-m'} [a^\dagger_{j',m'} a^\dagger_{j',-m'}, a^\dagger_{j,m}] \\
&= \boxed{0} \\
(2)\quad [S_-, a^\dagger_{j,m}] &= \frac{1}{2}\sum_{j',m'} (-1)^{j'-m'} [a_{j',-m'} a_{j',m'}, a^\dagger_{j,m}] \\
&= \frac{1}{2}\sum_{j',m'} (-1)^{j'-m'} \delta_{j',j}(\delta_{m,m'} a_{j,-m'} - \delta_{m,-m'} a_{j,m'}) \\
&= \frac{1}{2}\sum_{m'} (-1)^{j-m'} (\delta_{m,m'} a_{j,-m'} - \delta_{m,-m'} a_{j,m'}) \\
&= \frac{1}{2}((-1)^{j-m} a_{j,-m} - (-1)^{j+m} a_{j,-m}) \\
&= \frac{1}{2}(\tilde{a}_{j,m} - ((-1)^{2m}(-1)^{j-m} a_{j,-m})) \\
&= \frac{1}{2}(\tilde{a}_{j,m} + \tilde{a}_{j,m}) \\
&= \boxed{\tilde{a}_{j,m}} \\
(3)\quad [S_0, a^\dagger_{j,m}] &= \frac{1}{4}\sum_{j',m'} ([a^\dagger_{j',m'} a_{j',m'}, a^\dagger_{j,m}] + [a^\dagger_{j',-m'} a_{j',-m'}, a^\dagger_{j,m}] + [1, a^\dagger_{j,m}]) \\
&= \frac{1}{4}\sum_{j',m'} (a^\dagger_{j',m'} \delta_{m',m} \delta_{j',j} + a^\dagger_{j',-m'} \delta_{m',-m} \delta_{j',j}) \\
&= \frac{1}{4}\sum_{m'} (a^\dagger_{j,m'} \delta_{m',m} + a^\dagger_{j,-m'} \delta_{m',-m}) \\
&= \frac{1}{4}(a^\dagger_{j,m} + a^\dagger_{j,m}) \\
&= \boxed{\frac{1}{2} a^\dagger_{j,m}}
\end{aligned}
$$

7.2 Relations for $\tilde{a}$

$$
\begin{aligned}
(1)\quad [S_-, \tilde{a}_{j,m}] &= \frac{1}{2}\sum_{j',m'} (-1)^{j'-m'} [a_{j',-m'} a_{j',m'}, \tilde{a}_{j,m}] \\
&= \boxed{0} \\
(2)\quad [S_+, \tilde{a}_{j,m}] &= \frac{1}{2}\sum_{j',m'} (-1)^{j'-m'} [a^\dagger_{j',m'} a^\dagger_{j',-m'}, \tilde{a}_{j,m}] \\
&= \frac{1}{2}\sum_{j',m'} (-1)^{j'-m'}(-1)^{j'-m} [a^\dagger_{j',m'} a^\dagger_{j',-m'}, a_{j,-m}] \\
&= \frac{1}{2}\sum_{j',m'} (-1)^{j'-m'}(-1)^{j-m} \delta_{j',j}(\delta_{-m,-m'} a^\dagger_{j',m'} - \delta_{-m,m'} a^\dagger_{j',-m'}) \\
&= \frac{1}{2}((-1)^{j-m}(-1)^{j-m} a^\dagger_{j,m} - (-1)^{j+m}(-1)^{j-m} a^\dagger_{j,m}) \\
&= \frac{1}{2}(a^\dagger_{j,m} + a^\dagger_{j,m}) \\
&= \boxed{a^\dagger_{j,m}} \\
(3)\quad [S_0, \tilde{a}_{j,m}] &= \frac{1}{4}\sum_{j',m'} ([a^\dagger_{j',m'} a_{j',m'}, \tilde{a}_{j,m}] + [a^\dagger_{j',-m'} a_{j',-m'}, \tilde{a}_{j,m}] + [1, \tilde{a}_{j,m}]) \\
&= -\frac{1}{4}\sum_{j',m'} ((-1)^{j-m} a_{j',m'} \delta_{m',-m} \delta_{j',j} + (-1)^{j-m} a_{j',-m'} \delta_{-m',-m} \delta_{j',j}) \\
&= -\frac{1}{4}((-1)^{j-m} a_{j,-m} + (-1)^{j-m} a_{j,-m}) \\
&= -\frac{1}{4}(\tilde{a}_{j,m} + \tilde{a}_{j,m}) \\
&= \boxed{-\frac{1}{2}\tilde{a}_{j,m}}
\end{aligned}
$$

7.3 Generator Association

$$
\begin{aligned}
(1)\quad [S_0, S_+] &= [\frac{1}{4}\sum_{j',m'} (a^\dagger_{j',m'} a_{j',m'} + a^\dagger_{j',-m'} a_{j',-m'} - 1), S_+] \\
&= \frac{1}{4}\left(\sum_{j',m'} [a^\dagger_{j',m'} a_{j',m'}, S_+] + [a^\dagger_{j',-m'} a_{j',-m'}, S_+]\right) \\
&= \frac{1}{4}\left(\sum_{j',m'} -(-1)^{j'+m'} a^\dagger_{j',m'} a^\dagger_{j',-m'} + \sum_{j',m'} -(-1)^{j'-m'} a^\dagger_{j',-m'} a^\dagger_{j',m'}\right) \\
&= \frac{1}{4}\left(\sum_{j',m'} (-1)^{j'-m'} a^\dagger_{j',m'} a^\dagger_{j',-m'} + \sum_{j',m'} (-1)^{j'+m'} a^\dagger_{j',-m'} a^\dagger_{j',m'}\right)
\end{aligned}
$$

As these two sums run from $m' = -j$ to $m' = j$, the two summations are equivalent, thus we have

$$
\begin{aligned}
[S_0, S_+] &= \frac{1}{2}\sum_{j',m'} (-1)^{j'-m'} a^\dagger_{j',m'} a^\dagger_{j',-m'} \\
&= \boxed{S_+}
\end{aligned}
$$

$$
\begin{aligned}
(2)\quad [S_0, S_-] &= [\frac{1}{4}\sum_{j',m'}(a^\dagger_{j',m'}a_{j',m'} + a^\dagger_{j',-m'}a_{j',-m'} - 1), S_0] \\
&= \frac{1}{4}(\sum_{j',m'}[a^\dagger_{j',m'}a_{j',m'}, S_0] + [a^\dagger_{j',-m'}a_{j',-m'}, S_0]) \\
&= \frac{1}{4}(\sum_{j',m'} -\tilde{a}_{j',m'}a_{j',m'} + \sum_{j',m'} -\tilde{a}_{j',-m'}a_{j',-m'}) \\
&= -\frac{1}{4}(\sum_{j',m'}(-1)^{j'-m'}a_{j',-m'}a_{j',m'} + \sum_{j',m'}(-1)^{j'+m'}a_{j',m'}a_{j',-m'}) \\
&= -\frac{1}{2}\sum_{j',m'}(-1)^{j'-m'}a_{j',-m'}a_{j',m'} \\
&= \boxed{-S_-}
\end{aligned}
$$

$$
\begin{aligned}
3)\quad [S_+, S_-] &= [\frac{1}{2}\sum_{j',m'}(-1)^{j-m}a^\dagger_{j',m'}a^\dagger_{j',-m'}, S_-] \\
&= \frac{1}{2}\sum_{j',m'}(-1)^{j-m}[a^\dagger_{j',m'}a^\dagger_{j',-m'}, S_-] \\
&= \frac{1}{2}\sum_{j',m'} -(-1)^{j'-m'}(\tilde{a}_{j',m'}a^\dagger_{j',-m'} + a^\dagger_{j',m'}\tilde{a}_{j',-m'}) \\
&= \frac{1}{2}\sum_{j',m'} -(-1)^{j'-m'}((-1)^{j'-m'}a_{j',-m'}a^\dagger_{j,-m'} + (-1)^{j'+m'}a^\dagger_{j',m'}a_{j',m'}) \\
&= \frac{1}{2}\sum_{j',m'}(a^\dagger_{j',m'}a_{j',m'} + a^\dagger_{j',-m'}a_{j',-m'} - 1) \\
&= \boxed{2S_0}
\end{aligned}
$$

This tells us that S_+, S_- and S_0 are the generators of $SU(2)$, allowing us to interpret the commutation relations of $a^\dagger$ and $\tilde{a}$ with these generators as those of a spinor with $s = 1/2$

8 Appendix II: Matrix Element Calculations

As $a^\dagger_{j,m}$ and $\tilde{a}_{j,m}$ are spinors under the quasi-spin operators, we know they have a quasi-spin of $1/2$, meaning we can treat them as up/down "states".

8.1 One-Body Operators

In the pairing model (10), one-body operators are of the form $a^\dagger_{j,m}a_{j,m} = (-1)^{j+m}a^\dagger_{j,m}\tilde{a}_{j,-m}$. Using the fact that $a^\dagger_{j,m} \cong |+\rangle$ and $\tilde{a}_{j,-m} \cong |-\rangle$, we can decompose the product $a^\dagger_{j,m}\tilde{a}_{j,-m}$ into a sum of spin 0 and spin 1 operators,

$$a^\dagger_{j,m}\tilde{a}_{j,-m} = \frac{1}{\sqrt{2}}(\hat{O}_{1,0} + \hat{O}_{0,0}),$$

where $\hat{O}_{i,j}$ denotes an operator with quasi-spin i and projection j. For the seniority scheme we are interested in one-body matrix elements of the form $\langle\Omega/2, S_0|a^\dagger_{j,m}\tilde{a}_{j,-m}|\Omega/2, S_0\rangle$, where $|\Omega/2, S_0\rangle$ is a state of seniority 0, and thus has quasi spin $S = \Omega/2$ and projection $S_0 = N/2 - \Omega/2$. Using our above decomposition, we have this being

$$\langle\Omega/2, S_0|a^\dagger_{j,m}\tilde{a}_{j,-m}|\Omega/2, S_0\rangle = \frac{1}{\sqrt{2}}(\langle\Omega/2, S_0|\hat{O}_{1,0}|\Omega/2, S_0\rangle + \langle\Omega/2, S_0|\hat{O}_{0,0}|\Omega/2, S_0)\rangle),$$

We can determine these matrix elements by using the Wigner-Eckart theorem, which yields

$$\langle \Omega/2, S_0 | a^\dagger_{j,m} \tilde{a}_{j,-m} | \Omega/2, S_0 \rangle = \frac{1}{\sqrt{2}} (\alpha(1) \langle \Omega/2 | \, | \hat{O}_1 | \, | \Omega/2 \rangle + \alpha(0) \langle \Omega/2 | \, | \hat{O}_0 | \, | \Omega/2 \rangle),$$

where $\alpha(i) = \langle \Omega/2, S_0; i, 0 | \Omega/2, S_0 \rangle$ are the Clebsch–Gordan coefficients, with $\alpha(0) = 1$. To find the reduced matrix elements $\langle \Omega/2 | \, | \hat{O}_i | \, | \Omega/2 \rangle$, we can exploit their invariance with respect to S_0 to choose the vacuum case of $N = 0 \implies S_0 = -\Omega/2$. Doing so for the case of $\hat{O}_1 = \hat{O}_{1,0}$, where we denote $|\Omega/2, -\Omega/2\rangle = |\emptyset\rangle$ as the vacuum state, yields

$$\begin{aligned}
\langle \emptyset | \hat{O}_{1,0} | \emptyset \rangle &= \frac{1}{\sqrt{2}} \langle \emptyset | (a^\dagger_{j,m} \tilde{a}_{j',m'} + \tilde{a}_{j,m} a^\dagger_{j',m'}) | \emptyset \rangle \\
&= \frac{1}{\sqrt{2}} \langle \emptyset | \tilde{a}_{j,m} a^\dagger_{j',m'} | \emptyset \rangle \\
&= \frac{(-1)^{j-m}}{\sqrt{2}} \langle j, -m | j', m' \rangle \\
&= \frac{(-1)^{j-m}}{\sqrt{2}} \delta_{j,j'} \delta_{m',-m}
\end{aligned}$$

Thus, $\langle \Omega/2, -\Omega/2; 1, 0 | \Omega/2, -\Omega/2 \rangle \langle \Omega/2 | \, | \hat{O}_1 | \, | \Omega/2 \rangle = \frac{(-1)^{j-m}}{\sqrt{2}} \delta_{j,j'} \delta_{m',-m}$. An analogous calculation gives

$$\begin{aligned}
\langle \emptyset | \hat{O}_{0,0} | \emptyset \rangle &= \frac{1}{\sqrt{2}} \langle \emptyset | (a^\dagger_{j,m} \tilde{a}_{j',m'} - \tilde{a}_{j,m} a^\dagger_{j',m'}) | \emptyset \rangle \\
&= -\frac{1}{\sqrt{2}} \langle \emptyset | \tilde{a}_{j,m} a^\dagger_{j',m'} | \emptyset \rangle \\
&= -\frac{(-1)^{j-m}}{\sqrt{2}} \langle j', -m | j', m' \rangle \\
&= -\frac{(-1)^{j-m}}{\sqrt{2}} \delta_{j,j'} \delta_{-m,m'}
\end{aligned}$$

meaning $\langle \Omega/2, -\Omega/2; 0, 0 | \Omega/2, -\Omega/2 \rangle \langle \Omega/2 | \, | \hat{O}_0 | \, | \Omega/2 \rangle = -\frac{(-1)^{j-m}}{\sqrt{2}} \delta_{j,j'} \delta_{-m,m'}$. Of course, $\langle \Omega/2, -\Omega/2; 0, 0 | \Omega/2, -\Omega/2 \rangle = 1$.

Combining this with our previous result thus tells us that

$$\langle \Omega/2, S_0 | a^\dagger_{j,m} \tilde{a}_{j',m'} | \Omega/2, S_0 \rangle = \frac{(-1)^{j-m}}{2} \delta_{j,j'} \delta_{-m,m'} \left(\frac{\langle \Omega/2, S_0; 1, 0 | \Omega/2, S_0 \rangle}{\langle \Omega/2, -\Omega/2; 1, 0 | \Omega/2, -\Omega/2 \rangle} - 1 \right)$$

For the case of the pairing model, where $m' = -m$ and $j' = j$, we have the one-body matrix elements being

$$\begin{aligned}
\langle \Omega/2, S_0 | a^\dagger_{j,m} a_{j,m} | \Omega/2, S_0 \rangle &= (-1)^{j+m} \langle \Omega/2, S_0 | a^\dagger_{j,m} \tilde{a}_{j',-m} | \Omega/2, S_0 \rangle \\
&= -\frac{1}{2} \left(\frac{\langle \Omega/2, S_0; 1, 0 | \Omega/2, S_0 \rangle}{\langle \Omega/2, -\Omega/2; 1, 0 | \Omega/2, -\Omega/2 \rangle} - 1 \right)
\end{aligned}$$

We can simplify this result by considering the number operator

$$\hat{N} = \sum_{j,m} a^\dagger_{j,m} a_{j,m}$$

and noting that

$$\begin{aligned}
\langle \Omega/2, S_0 | \hat{N} | \Omega/2, S_0 \rangle &= \sum_{j,m} \langle \Omega/2, S_0 | a^\dagger_{j,m} a_{j,m} | \Omega/2, S_0 \rangle \\
&= -\frac{1}{2} \sum_{j,m} \left(\frac{\langle \Omega/2, S_0; 1, 0 | \Omega/2, S_0 \rangle}{\langle \Omega/2, -\Omega/2; 1, 0 | \Omega/2, -\Omega/2 \rangle} - 1 \right) \\
&= -\left(\frac{\langle \Omega/2, S_0; 1, 0 | \Omega/2, S_0 \rangle}{\langle \Omega/2, -\Omega/2; 1, 0 | \Omega/2, -\Omega/2 \rangle} - 1 \right) \left(\frac{1}{2} \sum_{j,m} 1 \right) \\
&= -\left(\frac{\langle \Omega/2, S_0; 1, 0 | \Omega/2, S_0 \rangle}{\langle \Omega/2, -\Omega/2; 1, 0 | \Omega/2, -\Omega/2 \rangle} - 1 \right) \Omega,
\end{aligned}$$

where $\frac{1}{2}\sum_{j,m} 1 = \sum_j (j+1/2) = \Omega$. As this summation is simply N (due to $\hat{N}$ being the number-operator acting on an N-particle state), we have that

$$\begin{aligned} -\left(\frac{\langle \Omega/2, S_0; 1, 0 | \Omega/2, S_0\rangle}{\langle \Omega/2, -\Omega/2; 1, 0 | \Omega/2, -\Omega/2\rangle} - 1\right)\Omega &= N \\ \implies -\left(\frac{\langle \Omega/2, S_0; 1, 0 | \Omega/2, S_0\rangle}{\langle \Omega/2, -\Omega/2; 1, 0 | \Omega/2, -\Omega/2\rangle} - 1\right) &= \frac{N}{\Omega}. \end{aligned}$$

Thus, we have the simplifed result

$$\langle \Omega/2, S_0 | a^\dagger_{j,m} a_{j,m} | \Omega/2, S_0\rangle = \frac{N}{2\Omega}$$

The more general form of this simplifed result is

$$\langle \Omega/2, S_0 | a^\dagger_{j,m} a_{j',m'} | \Omega/2, S_0\rangle = \frac{N}{2\Omega}\delta_{j,j'}\delta_{m,m'}$$

Simpler Calculation

Exploiting commutation relations and properties of S_+ and S_- allows us to compute the above matrix elements much more efficiently. Using $|N_i\rangle = |\frac{1}{2}\Omega, \frac{1}{2}(N_i - \Omega)\rangle$, we have

$$\begin{aligned} \langle N | a^\dagger_{j,m} a_{j',m'} | N\rangle &\propto \langle N | a^\dagger_{j,m} a_{j',m'} S_+^{N/2} | 0\rangle \\ &= \langle N | [a^\dagger_{j,m} a_{j',m'}, S_+^{N/2}] | 0\rangle \\ &= \langle N | a^\dagger_{j,m} [a_{j',m'}, S_+^{N/2}] | 0\rangle \\ &= \langle N | a^\dagger_{j,m} (-(-1)^{j'+m'}\frac{N}{2}) a^\dagger_{j',-m'} S_+^{N/2-1} | 0\rangle \\ &= -(-1)^{j'+m'}\frac{N}{2}\langle N | a^\dagger_{j,m} a^\dagger_{j',-m'} S_+^{N/2-1} | 0\rangle \\ &= -(-1)^{j'+m'}\frac{N}{2}\langle N | S_+^{N/2-1} a^\dagger_{j,m} a^\dagger_{j',-m'} | 0\rangle \\ &\propto -(-1)^{j'+m'}\frac{N}{2}\langle 2 | a^\dagger_{j,m} a^\dagger_{j',-m'} | 0\rangle \\ &\propto -(-1)^{j'+m'}\frac{N}{2}\langle 0 | S_- a^\dagger_{j,m} a^\dagger_{j',-m'} | 0\rangle \\ &= -(-1)^{j'+m'}\frac{N}{2}\langle 0 | [S_- a^\dagger_{j,m}] a^\dagger_{j',-m'} | 0\rangle \\ &= -(-1)^{j'+m'}\frac{N}{2}\langle 0 | \tilde{a}_{j,m} a^\dagger_{j',-m'} | 0\rangle \\ &= -(-1)^{j'+m'}(-1)^{j-m}\frac{N}{2}\langle j, -m | j', -m'\rangle \\ &= -(-1)^{j'+m'}(-1)^{j-m}\frac{N}{2}\delta_{j,j'}\delta_{m,m'} \\ &= \frac{N}{2}\delta_{j,j'}\delta_{m,m'} \end{aligned}$$

Thus, we have $\langle N | a^\dagger_{j,m} a_{j',m'} | N\rangle = \alpha\frac{N}{2}\delta_{j,j'}\delta_{m,m'}$. While we could determine the constant of proportionality α by tracking the coefficients induced by repeated applications of S_+ and S_-, a more straightforward way is to utilize the number operator $\hat{N} = \sum_{j,m} a^\dagger_{j,m} a_{j,m}$, which has an expectation value given by

$$\begin{aligned} \langle N | \hat{N} | N\rangle &= \sum_{j,m} \langle N | a^\dagger_{j,m} a_{j,m} | N\rangle \\ &= \alpha\frac{N}{2}\sum_{j,m} 1 \\ &= \alpha\frac{N}{2}(2\Omega) \\ &= \alpha N\Omega \end{aligned}$$

As $\langle N|\hat{N}|N\rangle = N$, we thus have $\alpha N\Omega = N \implies \alpha = 1/\Omega$. Thus, our final result is

$$\langle N|a^\dagger_{j,m}a_{j',m'}|N\rangle = \frac{N}{2\Omega}\delta_{j,j'}\delta_{m,m'}$$

8.2 Two-Body Operators

Now let's consider the two-body matrix elements. In the pairing Hamiltonian, the two-body operators are of the form $a^\dagger_{j,m}a^\dagger_{j',m'}a_{j'',m''}a_{j''',m'''}$. Using associativity of tensor products, we get this being decomposed as

$$\begin{aligned}
a^\dagger_{j,m}a^\dagger_{j',m'}a_{j'',m''}a_{j''',m'''} &= (-1)^{j''+j'''}(-1)^{m''+m'''}a^\dagger_{j,m}a^\dagger_{j',m'}\tilde{a}_{j'',-m''}\tilde{a}_{j''',-m'''} \\
&= (-1)^{j''+j'''}(-1)^{m''+m'''}\hat{O}_{1,1}\hat{O}_{1,-1} \\
&= (-1)^{j''+j'''}(-1)^{m''+m'''}\left(\frac{1}{\sqrt{6}}\hat{O}_{2,0} + \frac{1}{\sqrt{2}}\hat{O}_{1,0} + \frac{1}{\sqrt{3}}\hat{O}_{0,0}\right)
\end{aligned}$$

By linearity of the inner product we thus know that

$$\begin{aligned}
\langle\Omega/2, S_0|a^\dagger_{j,m}a^\dagger_{j',m'}a_{j'',m''}a_{j''',m'''}|\Omega/2, S_0\rangle = (-1)^{j''+j'''}(-1)^{m''+m'''}\Bigg(&\frac{1}{\sqrt{6}}\langle\Omega/2, S_0|\hat{O}_{2,0}|\Omega/2, S_0\rangle + \\
&\frac{1}{\sqrt{2}}\langle\Omega/2, S_0\hat{O}_{1,0}|\Omega/2, S_0\rangle + \langle\Omega/2, S_0\frac{1}{\sqrt{3}}\hat{O}_{0,0}|\Omega/2, S_0\rangle\Bigg)
\end{aligned}$$

meaning our goal is to find $\langle\Omega/2, S_0|\hat{O}_{2,0}|\Omega/2, S_0\rangle$, $\langle\Omega/2, S_0\hat{O}_{1,0}|\Omega/2, S_0\rangle$ and $\langle\Omega/2, S_0\frac{1}{\sqrt{3}}\hat{O}_{0,0}|\Omega/2, S_0\rangle$.

To do so, let us work backwards and decompose our spin 2,1,0 tensors in terms of our original spin-1/2 states (ie, $a^\dagger_{j,m}, a^\dagger_{j',m'}, \tilde{a}_{j'',-m''}$ and $\tilde{a}_{j''',-m'''}$). For $\hat{O}_{2,0}$ we have that

$$\begin{aligned}
\hat{O}_{2,0} &= \frac{1}{\sqrt{6}}\hat{O}_{1,1}\hat{O}_{1,-1} + \sqrt{\frac{2}{3}}\hat{O}_{1,0}\hat{O}_{1,0} + \frac{1}{\sqrt{6}}\hat{O}_{1,-1}\hat{O}_{1,1} \\
&= \frac{1}{\sqrt{6}}a^\dagger_{j,m}a^\dagger_{j',m'}\tilde{a}_{j'',-m''}\tilde{a}_{j''',-m'''} + \sqrt{\frac{2}{3}}\hat{O}_{1,0}\hat{O}_{1,0} + \frac{1}{\sqrt{6}}\tilde{a}_{j,m}\tilde{a}_{j',m'}a^\dagger_{j'',-m''}a^\dagger_{j''',-m'''}
\end{aligned}$$

For the middle term we know that

$$\begin{aligned}
\hat{O}_{1,0}\hat{O}_{1,0} = \frac{1}{2}(&a^\dagger_{j,m}\tilde{a}_{j',m'}\tilde{a}_{j'',-m''}a^\dagger_{j''',-m'''} + a^\dagger_{j,m}\tilde{a}_{j',m'}a^\dagger_{j'',-m''}\tilde{a}_{j''',-m'''} \\
&+ \tilde{a}_{j,m}a^\dagger_{j',m'}a^\dagger_{j'',-m''}\tilde{a}_{j''',-m'''} + \tilde{a}_{j,m}a^\dagger_{j',m'}\tilde{a}_{j'',-m''}a^\dagger_{j''',-m'''})
\end{aligned}$$

The vacuum-state matrix element then is

$$\begin{aligned}
\langle\emptyset|\hat{O}_{2,0}|\emptyset\rangle &= \frac{1}{\sqrt{6}}\langle\emptyset|a^\dagger_{j,m}a^\dagger_{j,-m}\tilde{a}_{j',-m'}\tilde{a}_{j',m'}|\emptyset\rangle + \sqrt{\frac{2}{3}}\frac{1}{2}\langle\emptyset|\tilde{a}_{j,m}a^\dagger_{j',m'}\tilde{a}_{j'',-m''}a^\dagger_{j''',-m'''}|\emptyset\rangle \\
&+ \frac{1}{\sqrt{6}}\langle\emptyset|\tilde{a}_{j,m}\tilde{a}_{j',m'}a^\dagger_{j'',-m''}a^\dagger_{j''',-m'''}|\emptyset\rangle \\
&= 0 + \sqrt{\frac{1}{6}}(-1)^{j-m}(-1)^{j''+m''}\langle j, -m|a^\dagger_{j',m'}a_{j'',m''}|j''', -m'''\rangle \\
&+ (-1)^{j-m}(-1)^{j'-m'}\frac{1}{\sqrt{6}}\langle j, -m|a_{j',-m'}a^\dagger_{j'',-m''}|j''', -m'''\rangle
\end{aligned}$$

Using $a_{j',-m'}a^\dagger_{j'',-m''} = \delta_{j',j''}\delta_{-m'',-m'} - a^\dagger_{j'',-m''}a_{j',-m'}$ gives

$$\begin{aligned}
\langle j, -m|a_{j',-m'}a^\dagger_{-m''}|j''', -m'''\rangle &= \langle j, -m|\delta_{j',j''}\delta_{-m'',-m'}|j''', -m'''\rangle - \langle j, -m|a^\dagger_{j'',-m''}a_{j',-m'}|j''', -m'''\rangle \\
&= \delta_{j,j'''}\delta_{j',j''}\delta_{-m,-m'''}\delta_{-m',-m''} - \delta_{j,j''}\delta_{j',j'''}\delta_{-m',-m'''}\delta_{-m,-m''}
\end{aligned}$$

Now using $\langle j,-m|a^\dagger_{j',m'}a_{j'',m''}|j''',-m'''\rangle = \delta_{j,j'}\delta_{j'',j'''}\delta_{-m,m'}\delta_{m'',-m'''}$, we have

$$\begin{aligned}\langle \Omega/2,S_0|\hat{O}_{2,0}|\Omega/2,S_0\rangle &= \frac{\langle \Omega/2,S_0;2,0|\Omega/2,S_0\rangle}{\langle \Omega/2,-\Omega/2;2,0|\Omega/2,-\Omega/2\rangle}\langle \Omega/2,-\Omega/2|\hat{O}_{2,0}|\Omega/2,-\Omega/2\rangle \\ &= \sqrt{\frac{1}{6}}\frac{\langle \Omega/2,S_0;2,0|\Omega/2,S_0\rangle}{\langle \Omega/2,-\Omega/2;2,0|\Omega/2,-\Omega/2\rangle}((-1)^{j-m}(-1)^{j''+m''}\delta_{j,j'}\delta_{j'',j'''}\delta_{-m,m'}\delta_{m'',-m'''} \\ &+ (-1)^{j-m}(-1)^{j'-m'}(\delta_{j,j'''}\delta_{j',j''}\delta_{-m,-m'''}\delta_{-m',-m''} \\ &- \delta_{j,j''}\delta_{j',j'''}\delta_{-m',-m'''}\delta_{-m,-m''}))\end{aligned}$$

Next, let's consider $\hat{O}_{1,0} = \frac{1}{\sqrt{2}}\left(\hat{O}_{1,1}\hat{O}_{1,-1} - \hat{O}_{1,-1}\hat{O}_{1,1}\right)$. Using our previous work we can easily evaluate this, giving

$$\begin{aligned}\langle \Omega/2,S_0|\hat{O}_{1,0}|\Omega/2,S_0\rangle = -(-1)^{j-m}(-1)^{j'-m'}\frac{1}{\sqrt{2}}\frac{\langle \Omega/2,S_0;2,0|\Omega/2,S_0\rangle}{\langle \Omega/2,-\Omega/2;2,0|\Omega/2,-\Omega/2\rangle}\times \\ (\delta_{j,j'''}\delta_{j',j''}\delta_{-m,-m'''}\delta_{-m',-m''} - \delta_{j,j''}\delta_{j',j'''}\delta_{-m',-m'''}\delta_{-m,-m''})\end{aligned}$$

Finally, we have for $\hat{O}_{0,0} = \frac{1}{\sqrt{3}}\left(\hat{O}_{1,1}\hat{O}_{1,-1} - \hat{O}_{1,0}\hat{O}_{1,0} + \hat{O}_{1,-1}\hat{O}_{1,1}\right)$ that

$$\begin{aligned}\langle \Omega/2,S_0|\hat{O}_{0,0}|\Omega/2,S_0\rangle = \frac{1}{\sqrt{3}}(-\frac{1}{2}(-1)^{j-m}(-1)^{j''+m''}\delta_{j,j'}\delta_{j'',j'''}\delta_{-m,m'}\delta_{m'',-m'''} \\ + (-1)^{j-m}(-1)^{j'-m'}(\delta_{j,j'''}\delta_{j',j''}\delta_{-m,-m'''}\delta_{-m',-m''} \\ - \delta_{j,j''}\delta_{j',j'''}\delta_{-m',-m'''}\delta_{-m,-m''}))\end{aligned}$$

After performing simplifications, we can express our final result as

$$\begin{aligned}\langle \Omega/2,S_0|a^\dagger_{j,m}a^\dagger_{j',m'}a_{j'',m''}a_{j''',m'''}|\Omega/2,S_0\rangle = \frac{(-1)^{j''+j'''-m''-m'''}}{4\Omega(\Omega-1)}[N(N-2)(-1)^{j+j'-m-m'}(\delta_{j,j'''}\delta_{j',j''}\delta_{-m',-m''}\delta_{-m,-m'''} \\ - \delta_{j,j''}\delta_{j',j'''}\delta_{-m',-m'''}\delta_{-m,-m''}) + N(N-2\Omega)(-1)^{j+j''-m+m''} \\ (\delta_{j,j'}\delta_{j'',j'''}\delta_{-m,m'}\delta_{m'',-m'''})]\end{aligned}$$

Defining $a,b,c,d = (j,m),(j',m'),(j'',m''),(j''',m''')$, $\overline{q} = (j_q,-m_q)$ and $p_{q\sigma} = (-1)^{j_q+j_\sigma-m_q-m_\sigma}$, we can simplify this further as

$$\langle \Omega/2,S_0|a^\dagger_a a^\dagger_b a_c a_d|\Omega/2,S_0\rangle = \frac{p_{cd}}{4\Omega(\Omega-1)}[N(N-2)p_{ab}(\delta_{\overline{a},\overline{d}}\delta_{\overline{b},\overline{c}} - \delta_{\overline{a},\overline{c}}\delta_{\overline{b},\overline{d}}) + N(N-2\Omega)p_{a\overline{c}}\delta_{\overline{a},b}\delta_{\overline{c},d}]$$

Utilizing the Kronecker δ's allow us to eliminate some of the phases, yielding

$$\langle \Omega/2,S_0|a^\dagger_a a^\dagger_b a_c a_d|\Omega/2,S_0\rangle = \frac{1}{4\Omega(\Omega-1)}[N(N-2)(\delta_{\overline{a},\overline{d}}\delta_{\overline{b},\overline{c}} - \delta_{\overline{a},\overline{c}}\delta_{\overline{b},\overline{d}}) - N(N-2\Omega)p_{ad}\delta_{\overline{a},b}\delta_{\overline{c},d}]$$

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