Nuclear entanglement and deformation

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Abstract

The single-j model is a simple toy Hamiltonian which captures certain phenomenological properties of a nuclear shell with fixed angular momentum j, namely, *nucleon pairing* and *quadrupole deformation*.

We characterize the ground and excited states of this Hamiltonian, in light of its symmetries, for a shell with an even number of nucleons, building up an intuitive picture of the exact solutions. We see that, while the ground state is a rotationally-symmetric state with zero total angular momentum and vanishing deformation, the excited states are organized into multiplets with definite total angular momentum J^2 and are in general deformed states. The effect of the quadrupole term is to break the degeneracy between multiplets with distinct J^2.

Narrowing our attention to the ground state, we next investigate entanglement between single-particle nuclear orbitals via the tools of quantum information: reduced density matrices, mutual information, entanglement entropy, and entanglement of formation. Along the way we consider how "entanglement" should be defined for systems of indistinguishable fermions, meeting tools such as the natural basis of single-particle states, the Jordan-Wigner isomorphism, and the fermionic partial trace, and considering subtleties including particle number conservation and "fluffy-bunny" entanglement which complicate the much more familiar picture of entanglement in systems of distinguishable particles.

Ultimately, we find that quantum correlations in the ground state of the single-j model arise from entanglement involving four orbitals, which perhaps can be thought of as entanglement between pairs of "Cooper pairs". For $j \geq \frac{9}{2}$, and with $N = 4$ nucleons, the Cooper pairs are disrupted by the quadrupole term, leading to a more complicated entanglement structure.

Finally, we compare the ground state of the single-j model with the ground state of a more realistic phenomenological nuclear Hamiltonian and find a surprisingly close fit, suggesting that the single-j model is an excellent starting point for understanding entanglement in real nuclei.

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Contents

Chapter 1 || Entanglement in many-body quantum systems

Introductory texts in quantum mechanics treat entanglement of spin-$\frac{1}{2}$ states of distinguishable particles. In the study of quantum information, these spin states are abstracted to the notion of distinguishable qubits. In many-body quantum mechanics—and, in particular, in nuclear physics—we must confront the fact that particles, in our case, nucleons, are indistinguishable in principle.

In the discussion which follows, we seek an understanding of entanglement in systems of indistinguishable particles. It's important to begin by emphasizing that entanglement is not an observable. The claim that a state is entangled is always a basis-dependent statement—the canonical Bell states are not entangled states when written in the Bell basis! Nevertheless, entanglement is indeed "physical", because not every change of basis involves only *local* transformations. The unitary transformation which takes the computational basis to the Bell basis mixes states of physically-distinguishable particles, and is therefore considered non-local.

Thus, the set of states we consider "entangled" depends sensitively on how we understand *locality*, and on which transformations we consider local. In a system of distinguishable particles, we call a transformation local if and only if it preserves the identity of the individual particles. Clearly, this breaks down when particles are indistinguishable.

1.1 Entanglement for distinguishable particles

A pure state $|\psi\rangle$ involving two distinguishable particles A, B is considered *separable* if it can be written as a tensor product of states of the individual particles, that is, if:

$$|\psi\rangle \equiv |\psi\rangle_{AB} = |\psi\rangle_A \otimes |\psi\rangle_B .$$

If no such factorization exists, the system is considered *entangled*. For example, the state $|10\rangle = |1\rangle \otimes |0\rangle$ of two qubits is separable, while the Bell state $|\Psi^-\rangle \equiv \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ is entangled.

Equivalently, a system of two distinguishable particles is separable if any pair of local observables acting on opposite sides of the bipartiation (A, B) is uncorrelated. To see the equivalence, consider that a necessary condition for independence of two classical random variables X, Y is that their covariance vanishes, that is:

$$\langle XY\rangle - \langle X\rangle \langle Y\rangle = 0.$$

Now, if O_A, P_B are local observables and $|\psi\rangle_{AB}$ is a separable state of the bipartite system, then:

$$\langle\psi|O_A \otimes P_B|\psi\rangle = \langle\psi|_A \otimes \langle\psi|_B \cdot O_A \otimes P_B \cdot |\psi\rangle_A \otimes |\psi\rangle_B = \langle\psi|_A O_A |\psi\rangle_A \cdot \langle\psi|_B P_B |\psi\rangle_B , \tag{1.1}$$

and so the local observables have vanishing covariance—they are uncorrelated.

For entangled states, such factorization of the expectation value is not possible, leading to statistical correlations between local observables. It's possible to choose observables O_A, P_B with nonzero covariance, showing that these observables are not independent random variables. [1]

[1] This is not in itself a violation of local realism, nor of classical probability theory.

More profoundly, so-called "Bell inequalities" such as the CSHS inequality introduced in [1] and also discussed in [2] demonstrate that covariance of such quantum observables can violate bounds which apply to classical random variables, that is, that the joint distribution of such observables cannot be represented using a classical probability distribution.

The notions just introduced extend naturally to mixed states. For distinguishable particles A, B, a state ρ_{AB} is called separable if it can be written as a convex combination of separable pure states, that is, if:

$$\rho_{AB} = \sum_i p_i \, \rho_A^{(i)} \otimes \rho_B^{(i)}, \qquad\qquad 1 \geq p_i > 0, \quad \sum_i p_i = 1.$$

Otherwise, ρ_{AB} is an entangled state.

Equivalently, the state is separable if, for any pair of local observables O_A, P_B acting on opposite sides of the bipartiation (A, B), we have:

$$\mathrm{Tr}\{\rho_{AB} \cdot O_A \otimes P_B\} = \sum_i p_i \, \mathrm{Tr}\Big\{\rho_A^{(i)} \, O_A\Big\} \cdot \mathrm{Tr}\Big\{\rho_B^{(i)} \, P_B\Big\}, \qquad 1 \geq p_i > 0, \quad \sum_i p_i = 1. \tag{1.2}$$

That is, if correlations between local observables can be viewed as arising from a completely classical source.

1.2 Entanglement for indistinguishable particles

For a system with two indistinguishable fermions, we must work in a basis of antisymmetric states of form:

$$|\alpha\beta\rangle = |\alpha\rangle \wedge |\beta\rangle = \tfrac{1}{\sqrt{2}}\Big(|\alpha\rangle_A \otimes |\beta\rangle_B - |\beta\rangle_A \otimes |\alpha\rangle_B\Big).$$

Notice that, according to what we saw in the previous section, this state looks superficially entangled. But indistinguishability has undermined the notion of locality we used for distinguishable particles, and so the superficial appearance is misleading.

Similarly, a single-particle operator must take the form:

$$O = O_A \otimes \mathbb{1}_B + \mathbb{1}_A \otimes O_B.$$

Notice that this operator is non-local in the sense of the previous section, where a local observable was understood to be an observable which depended on the state of a single distinguishable particle.

We wish to revise our definition of entanglement to cover such fermionic systems. As argued by [3], we must revisit our notion of "locality", looking for a definition which satisfies the following properties:

- entanglement should correspond to the existence of non-local correlations, according to the revised definition of locality,
- considering the limiting case where indistinguishable particles become effectively distinguishable by freezing an additional degree of freedom—for example, by localizing the particles in traps—the definition of entanglement should agree with the definition for distinguishable particles, and
- local operators acting on separable states should not violate classical bounds on the performance of information processing tasks.

After considering various approaches taken in the literature to entanglement in many-body systems, [3] concluded that the only approach which satisfied all three criteria was one based on the occupation of single-particle states.[2]

In particular, given a bipartition (A, B) of the singe-particle states of the system, the local observables are operators of form $P(a_1, a_2)Q(b_1, b_2)$ where P, Q are polynomials and:

$$a_1, a_2 \in \{a_m : m \in A\} \cup \{a_m^\dagger : m \in A\}, \qquad\qquad b_1, b_2 \in \{a_m : m \in B\} \cup \{a_m^\dagger : m \in B\}.$$

In this work, we accept this definition, mindful of the following caveat.

[2] We will hereon use the terms "orbital" and "single-particle state" completely interchangeably.

1.3 Entanglement and particle number conservation

In closed, non-relativistic quantum systems, particle number is often conserved. In this case, we often work in a subspace with given definite particle number N of the full many-body Fock space. For example, to study the Hydrogen nucleus, we need only consider the subpace with $N = 1$. Particle number conservation undermines the picture presented in [3], or at least obligates us to treat this understanding of entanglement with caution.

Consider the Fock space for identical nucleons with total angular momentum $j = \frac{1}{2}$. A basis for this space is:

$$|0\rangle\,, \qquad a^\dagger_\uparrow |0\rangle\,, \qquad a^\dagger_\downarrow |0\rangle\,, \qquad a^\dagger_\uparrow a^\dagger_\downarrow |0\rangle\,.$$

Under the Jordan-Wigner transformation defined below in 1.6, these states map respectively to the following two-qubit states:

$$|00\rangle\,, \qquad |01\rangle\,, \qquad |10\rangle\,, \qquad |11\rangle\,,$$

where 0, 1 may be interpreted as occupation numbers for the single-particle states $|\uparrow\rangle$ and $|\downarrow\rangle$.

Now, consider, for example, the canonical two-qubit Bell state $|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$. Viewed as representing an element of the full Fock space, it's perfectly reasonable to interpret this state as entangled. But in a system with particle number conservation, this is a state with definite particle number $N = 1$, and belongs to a two-dimensional Hilbert subspace of the Fock space. As an element of this subspace, the state has an alternative representation as $\frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$, which is a trivial superposition, and certainly not an entangled state.

This situation is an example of what [4]—writing from a quantum information perspective—calls "fluffy bunny" entanglement: a form of entanglement which cannot be operationalized in information processing tasks due to physical superselection rules leaving some states of the full Hilbert space inaccessible.

Whether fluffy bunny entanglement is considered an artefact depends on our purpose: if our goal is to optimize a quantum algorithm which simulates a fermionic system using qubits, then entanglement between qubits—fluffy or otherwise—is always significant, even when it doesn't correspond to nonlocal correlations between fermion states.

1.4 Quantifying quantum correlations

For bipartite pure states, *entanglement entropy* is a well-loved measure of entanglement, and is easy to calculate. Given a bipartition (A, B), the entanglement entropy $T_{AB}(|\psi\rangle)$ of a pure state $|\psi\rangle_{AB}$ measures the number of bits entangled across the bipartition, calculated as:

$$T_{AB}(|\psi\rangle) \equiv H(\mathrm{Tr}_A\, |\psi\rangle\langle\psi|_{AB}) = H(\mathrm{Tr}_B\, |\psi\rangle\langle\psi|_{AB}), \tag{1.3}$$

where $H(\rho) \equiv -\,\mathrm{Tr}\{\rho \log_2 \rho\}$ is the von Neumann entropy of a quantum state ρ. Positivity of this quantity may also be interpreted as the part A having more randomness than the whole AB, a situation which is impossible for separable states or in classical information theory.

In this work, we will need to quantify bipartite entanglement of mixed states obtained by computing a reduced four-body density matrix as the partial trace of a larger pure state. Unfortunately, for a mixed state ρ_{AB}, the quantity $H(\mathrm{Tr}_A\, \rho_{AB}) - H(\rho_{AB})$ can be non-positive even when the state is not separable. Therefore, we consider a quantity known as the *entanglement of formation*—discussed in [5, 6]—which quantifies the number of entangled Bell pairs required to prepare a quantum state. [3] To arrive at the entanglement of formation, we begin with the entanglement entropy, and, employing a general-purpose construction known as the *convex roof*,[4] extend its definition to mixed states by performing an optimization over ensembles of pure states:

$$T_{AB}(\rho) \equiv \min_{\rho = \sum_i p_i |\psi^{(i)}\rangle\langle\psi^{(i)}|} \sum_i p_i\, T_{AB}\left(\left|\psi^{(i)}\right\rangle\right). \tag{1.4}$$

[3] For mixed states, the number of entangled pairs that can be extracted from a state does not necessarily agree with the number of pairs required to prepare the state.

[4] In appendix C. we discuss a related measure of multipartite entanglement known as the *tangle*.

The optimization is in general hard to perform. But when ρ is of form $\rho = p_0 \, |\psi\rangle\langle\psi| + \sum_i p_i \, |i\rangle\langle i|$, that is, when the state is the convex sum of a classically-correlated state with a pure state, the optimization is trivial and we obtain $T_{AB}(\rho) = p_0 \, T_{AB}(|\psi\rangle)$. This case will turn out to be important to us below in 3.3. Details regarding these computations may be found in appendix G.

In [7], the quantum correlations of the single-j model were quantified using the *quantum discord*. Discord—see [8, 9]—is a more sensitive criterion for the existence of quantum correlations than entanglement: entangled systems have nonzero discord, but discordant systems are not necessarily entangled. In any purely classically-correlated system, the discord vanishes. A simple formula for quantum discord for fermionic states involving two orbitals was obtained in [10], but for larger systems the discord is very difficult to compute, involving an optimization over projectors.

1.5 Choice of single-particle states

In the description of a quantum many-body system, the choice of basis for single-particle states is in principle arbitrary, and the choice of basis will affect metrics such as mutual information, discord, or entanglement entropy which seek to quantify classical or quantum correlations.

However, it was shown by [11] that there is a special or "natural" choice of basis which minimizes the sum:

$$S = \sum_\alpha h\big(\rho^{(1)}_{\alpha\alpha}\big), \qquad\qquad h(p) \equiv -p \log_2 p - (1-p)\log_2(1-p), \tag{1.5}$$

where the *one-body density matrix* $\rho^{(1)}_{\alpha\beta}$ is defined by:

$$\rho^{(1)}_{\alpha\beta} = \left\langle a^\dagger_\beta \, a_\alpha \right\rangle_\psi . \tag{1.6}$$

S may be viewed as quantifying of the total entanglement associated with the state $|\psi\rangle$ as measured in the given basis. The natural basis which minimizes S is the basis which diagonalizes the one-body density matrix. Notice that the natural basis depends on the many-body quantum state through the expectation value.

A diagonal one-body density matrix $\rho^{(1)}_{\alpha\beta}$ does not imply that the density matrix $\rho = |\psi\rangle\langle\psi|$ of the full many-body state is diagonal. In particular, an entangled state $|\psi\rangle$ can have a diagonal one-body density matrix.

In appendix F. we show that $\rho_\alpha \equiv \mathrm{Tr}_{\beta\neq\alpha} \, |\psi\rangle\langle\psi|$, the single-orbital reduced density matrix obtained by tracing out every single-particle state except the basis state $|\alpha\rangle$, is also diagonal, and so, in the natural basis:

$$\rho^{(1)}_{\alpha\alpha} = \langle\alpha| \, \rho_\alpha \, |\alpha\rangle \qquad\qquad \Rightarrow \qquad\qquad h\big(\rho^{(1)}_{\alpha\alpha}\big) = H(\rho_\alpha). \tag{1.7}$$

Here, we work in a basis built from single-particle angular momentum eigenstates of form $|j, m\rangle$. We have verified by numerical calculation that our ground states have diagonal one-body densities, and so the angular momentum eigenstates are always the natural basis for the ground state.

Indeed, it's asserted by [7] that, given a state with zero total angular momentum—which is the case for our ground states—the one-body density matrix is always diagonal in the basis of angular momentum eigenstates. It's further argued that quantum correlations between pairs of single-particle states must vanish in such a natural basis, and that therefore all correlations between paired single-particle states must be classical. Entanglement manifests in correlations between three or more single-particle states, and we should therefore look for it in reduced density matrices for selections of three, four, or more orbitals.

1.6 The Jordan-Wigner transformation

The Jordan-Wigner transformation is an isomorphism between Hilbert spaces, namely, between:

- the fermionic Fock space $\bigoplus_{k=0}^{d} \mathcal{A}\big(H^{\otimes k}\big)$ formed from the Hilbert space H with d single-particle states, with $\mathcal{A}$ representing antisymmetrization, and
- the Hilbert space $\big(\mathbb{C}^2\big)^{\otimes d}$ of d qubits.

Each qubit is taken to hold the occupation number of the corresponding single-particle state. For example, in a system with single-particle states $|\alpha\rangle$, $|\beta\rangle$, $|\gamma\rangle$, the state $|\alpha\gamma\rangle = a_\alpha^\dagger a_\gamma^\dagger |0\rangle$ might be represented by the three-qubit state $|101\rangle = |1\rangle_\alpha \otimes |0\rangle_\beta \otimes |1\rangle_\gamma$.

Operators in the Fock space are expressed in terms of annihilation and creation operators a_α, $a_\alpha^\dagger$ obeying fermionic anticommutation relations. For example, a one-body operator T for the many-body system may be expressed via the well-known formula:

$$T = \sum_{\alpha\beta} t_{\alpha\beta}\, a_\alpha^\dagger a_\beta, \qquad\qquad t_{\alpha\beta} = \langle\alpha|t|\beta\rangle\,, \tag{1.8}$$

where t is a single-particle operator and α, β label the single-particle states.

The Jordan-Wigner mapping lets us reexpress such operators as operators on qubits, while preserving the anticommutation relations. Given an integer relabelling $\alpha_i \to i$ of the single-particle states, it is defined by:

$$a_n \to \left(\bigotimes_{i=0}^{n-1} Z_i\right) \otimes |1\rangle\langle 0|_n = \frac{1}{2}\left(\bigotimes_{i=0}^{n-1} Z_i\right) \otimes (X_n - iY_n), \tag{1.9}$$

where X, Y, Z are the Pauli matrices.

In appendix D. we show that this mapping preserves the standard anticommutation relations between fermionic annihilation and creation operators.

In this work we make use of the Jordan-Wigner mapping according to the following procedure:

- Define an integer labelling of single-particle states, writing states from the fermionic many-body system in the occupation number format, as strings of bits indicating occupation of the labeled orbitals.
- Apply the Jordan-Wigner transformation to the Hamiltonian H, to obtain a Hamiltonian operator H_{qubit} acting on d qubits.
- Restrict the Fock space to states with N occupied orbitals.
- Diagonalize H_{qubit} in the resulting subspace, to obtain the ground state and excited states.
- Apply the Jordan-Wigner transformation to other operators used to compute additional properties such as the deformation β^2.

We would also like to compute reduced density matrices for the ground state, and, from there, obtain quantum information metrics such as entanglement entropy and mutual information. However, there's a wrinkle: the fermionic Fock space does not have a tensor product structure, and so the usual partial trace operation is not quite well-defined. Instead, it was argued in [12] that the partial trace must be understood in terms of a "braided" tensor product.

1.7 The fermionic partial trace

Some authors—see [13]—have analysed fermionic systems simply by taking the usual partial trace in the qubit space isomorphic under the Jordan-Wigner mapping. But this procedure is not quite correct: in systems with more than two particles, the Jordan-Wigner isomorphism does not preserve the partial trace operation of the fermionic system, and so the reduced density matrices obtained in qubit space—and metrics computed from them—do not necessarily agree with results obtained when reduced densities are calculated directly in the fermionic Fock space. [5]

Again, it matters what our purpose is. If our goal is to find entanglement between qubits in a quantum algorithm which simulates a fermionic system, then this is all perfectly acceptable, and the usual partial trace is quite the right thing to use, as long as we don't over-interpret our results. But here we're more interested in the entanglement structure of the physical nucleus.

[5] The root source of this problem is an ambiguity in the Jordan-Wigner mapping. In a fermionic Fock space, the states $|\alpha\beta\rangle = \alpha^\dagger\beta^\dagger|0\rangle$ and $|\beta\alpha\rangle = \beta^\dagger\alpha^\dagger|0\rangle$ differ by a sign. We must therefore fix the sign by imposing an ordering of the single-particle states, by, for example, specifying that $|\alpha\beta\rangle = -|\beta\alpha\rangle \to |11\rangle$.

Fortunately, [14] proposes a definition of a *fermionic partial trace*, which is consistent with the anticommuting algebra of the Fock space. Since the partial trace is a linear operation, we need only define its action on basis states. We begin by specifying that:

$$\begin{aligned} &\mathrm{Tr}_\alpha^{\text{fermionic}} |0\rangle\langle 0| = |0\rangle\langle 0|, && \mathrm{Tr}_\alpha^{\text{fermionic}} |\alpha\rangle\langle\alpha| = \mathrm{Tr}_\alpha^{\text{fermionic}} a_\alpha^\dagger |0\rangle\langle 0| a_\alpha = |0\rangle\langle 0|, \\ &\mathrm{Tr}_\alpha^{\text{fermionic}} |\alpha\rangle\langle 0| = \mathrm{Tr}_\alpha^{\text{fermionic}} a_\alpha^\dagger |0\rangle\langle 0| = 0, && \mathrm{Tr}_\alpha^{\text{fermionic}} |0\rangle\langle\alpha| = \mathrm{Tr}_\alpha^{\text{fermionic}} |0\rangle\langle 0| a_\alpha = 0. \end{aligned} \tag{1.10}$$

We then extend the fermionic partial trace to basis states containing more than one occupied orbital according to the following prescription: when computing $\mathrm{Tr}_\alpha^{\text{fermionic}}$, first anticommute operators involving α so that they act directly on the vacuum state, and then apply one of the rules above. For example:

$$\mathrm{Tr}_\alpha^{\text{fermionic}} a_\alpha^\dagger a_\beta^\dagger |0\rangle\langle 0| a_\alpha = -\mathrm{Tr}_\alpha^{\text{fermionic}} a_\beta^\dagger a_\alpha^\dagger |0\rangle\langle 0| a_\alpha = -a_\beta^\dagger |0\rangle\langle 0| = -|\beta\rangle\langle 0|.$$

Or, written in occupation number representation with $|11\rangle_{01} \equiv a_1^\dagger a_0^\dagger |0\rangle$:

$$\mathrm{Tr}_1^{\text{fermionic}} |11\rangle\langle 01|_{01} = \mathrm{Tr}_1^{\text{fermionic}} a_1^\dagger a_0^\dagger |0\rangle\langle 0| a_1 = -\mathrm{Tr}_1^{\text{fermionic}} a_0^\dagger a_1^\dagger |0\rangle\langle 0| a_1 = -a_0^\dagger |0\rangle\langle 0| = -|1\rangle\langle 0|_0.$$

Finally, the definition of the fermionic partial trace is extended to superpositions of basis states by linearity.

We have used this definition of the partial trace when computing reduced density matrices. The impact of this choice is discussed briefly in appendix B.

Appendix F. discusses the structure of reduced density matrices in fermionic systems, and the importance of the particle number *parity superselection rule*.

1.8 Mutual information

Finally, *mutual information* is a useful measure of correlation across a bipartition of a quantum state. For example, the mutual information between nuclear orbitals was used in [15] to characterize the entanglement structure of the ground state of various nuclei. Given a bipartition (A, B) of a quantum state ρ_{AB}, the mutual information $I(A;B)$ is given by:

$$I(A;B) = H(\rho_A) + H(\rho_B) - H(\rho_{AB}), \tag{1.11}$$

where ρ_A, ρ_B are the reduced density matrices of the subsystems A, B respectively. Since ρ_{AB} is not constrained to be a pure state, the mutual information may be used quantify correlation between two given orbitals simply by first tracing out every other orbital.

For our purposes, mutual information has the disadvantage that it does not sufficiently distinguish classical from quantum correlations:

- when $1 < I_{\alpha\beta} \leq 2$, the orbitals must be entangled, but
- for $0 < I_{\alpha\beta} \leq 1$ they might be purely classically-correlated. [6]

That said, it's important to also note that in this context *all* classical correlations ultimately arise from entanglement, since the ground state is pure.

In this work we sometimes compute both mutual information (1.11) and entanglement of formation (1.4), since the two quantities give slightly different information.

[6] Note that in [15], the mutual information between orbitals was bounded above by one, and so we can't say for sure that pairs of orbitals were themselves entangled. We can nevertheless say that these correlations arose from the entanglement structure of the whole ground state.

Chapter 2 || The single-j nuclear model

The *nuclear shell model* assumes that nucleons are independent fermions moving within a static potential well generated by their own mean positions. Thus, the interaction between nucleons is approximated by an interaction between each nucleon and the mean field created by its fellows. Energy levels within the potential are determined by the shape of the potential—which is often taken to be of Woods-Saxon form—and by spin-orbit coupling splitting the energies of the $\ell \pm \frac{1}{2}$ subshells. The shell model, reviewed in [16], successfully reproduces a number of interesting features of atomic nuclei, most importantly, the organization of subshells labelled by level n, orbital angular momentum ℓ, and coupled angular momentum j—often written in the form $n\ell_j$—into shells separated by large energy gaps.

The existence of these energy gaps allows us to incorporate interactions between nucleons without blowing out the computational complexity of the problem by considering interactions only between "valence" nucleons located in the outermost shell or *valence space*.

A simple and popular nuclear interaction potential is the *pairing plus quadrupole* model. The pairing interaction was proposed in [17] by analogy with the BCS theory of superconductivity to explain an energy gap in the excitation spectrum of even-even nuclei. It's sometimes considered the dominant short-range interaction. Evidence for nucleon pairing is discussed in [18]. Meanwhile, the quadrupole interaction is simply the leading-order term in a multipole expansion of the long-range part of the nuclear potential.

The single-j model, introduced by [19], is a relatively simplistic model Hamiltonian implementing the pairing plus quadrupole model, with:

- valence nucleons of just one flavor, that is, all protons, or all neutrons,
- belonging to a valence space with just a single subshell of given angular momentum j.

The model incorporates neither isospin, nor proton-neutron interactions. The shell model itself fades into the background here, since the energy of the j subshell contributes a constant which depends only on the number of nucleons.

2.1 The single-j Hamiltonian

We work in a basis where single-particle states $|j, m\rangle$ are states of good total angular momentum j, labeled by vertical projection m, arising from spin-orbit coupling.[1] These single-particle states are often called *orbitals*.

The single-j Hamiltonian H is given by:

$$H = H_N + H_{P^2} + H_{Q^2}, \tag{2.1}$$

where the terms representing the energy of single-particle states, H_N, nucleon pairing, H_{P^2}, and quadrupole deformation, H_{Q^2}, are, respectively:

$$H_N = \epsilon N, \qquad H_{P^2} = -\frac{G}{2} P^\dagger P, \qquad H_{Q^2} = -\frac{\chi}{2} \sum\nolimits_\mu (-1)^\mu Q_\mu Q_{-\mu}, \tag{2.2}$$

[1] Thus, j and m always take half-integral values, $j = \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, m = \frac{1}{2}, \frac{3}{2}$, etc.

and $\epsilon(j)$ is the energy of single-particle states in the j-shell, G the strength of the pairing interaction, χ the strength of the quadrupole interaction.

For the many-body system, the *number operator* N is simply:

$$N = \sum_m n_m = \sum_m a_m^\dagger a_m, \tag{2.3}$$

where $a_m^\dagger$ creates a nucleon in the state $|j, m\rangle$. Since we will always take the number of valence nucleons to be fixed, N has a constant definite value, and so the H_N term contributes only an uninteresting constant shift to the energy.

The *pairing operator* P and its Hermitian conjugate $P^\dagger$ are given by:

$$P = \sum_m (-1)^{j-m}\, a_{-m} a_m, \qquad\qquad P^\dagger = \sum_m (-1)^{j-m}\, a_m^\dagger a_{-m}^\dagger, \tag{2.4}$$

where $(-1)^{j-m}\, a_{-m}^\dagger$ creates a nucleon in the time-reversed state $|\bar{m}\rangle \equiv (-1)^{j-m}\, |j, -m\rangle$ corresponding to $|j, m\rangle$. That is, $P^\dagger$ is a pair-creation operator.

The *quadrupole operator* Q_μ is a rank-2 spherical tensor operator[2] with index $\mu = -2, -1, 0, 1, 2$ and, making use of the Wigner-Eckart theorem [20] at the second inequality, may be expressed in terms of Clebsch-Gordan coefficients:

$$Q_\mu = \sum_{mn} \langle j, m|Q_\mu|j, n\rangle\, a_m^\dagger a_n = \sum_{mn} \langle j, n; 2, \mu|j, m\rangle\ \langle j||Q||j\rangle\, a_m^\dagger a_n. \tag{2.5}$$

The reduced matrix element $\langle j||Q||j\rangle$ depends only on j, and so, by defining $X(j) \equiv \chi \langle j||Q||j\rangle$, we may absorb it into the coefficient specifying the strength of the quadrupole interaction.

Finally, the Hamiltonian may be written as:

$$H = \underbrace{\epsilon N}_{\text{Constant}} \underbrace{- \frac{G}{2} \sum_{mn} (-1)^{2j-m-n} a_m^\dagger a_{-m}^\dagger a_{-n} a_n}_{\text{Pairing}} \underbrace{- \frac{X}{2} \sum_\mu (-1)^\mu \sum_{mnpq} \langle j, n; 2, \mu|j, m\rangle\, \langle j, q; 2, -\mu|j, p\rangle\, a_m^\dagger a_n a_p^\dagger a_q}_{\text{Quadrupole deformation}}. \tag{2.6}$$

With N fixed, the eigenstates of H do not depend on ϵ, and so the eigenstates are functions of the ratio X/G.

The pairing force favors the occupation of "Cooper pairs" with zero coupled vertical angular momentum projection M_{pair}[3], while the quadrupole force—non-obviously—acts to favor configurations with certain definite values of total angular momentum J^2. For $j < \frac{9}{2}$, H_{P^2} commutes with H_{Q^2} and the two terms may be simultaneously diagonalized. For $j \geq \frac{9}{2}$, the terms do not commute, and we'll see that the resulting competition between them leads to disruption of the Cooper pairs. Derivations of the pairing and quadrupole terms may be found in [18].

2.2 Symmetries of the single-j Hamiltonian

The Hamiltonian above commutes with N, the particle number operator, and with rotations, the generators of angular momentum. Therefore, particle number and angular momentum are conserved quantities.

In particular, eigenstates of the Hamiltonian have definite particle number, and states with a given particle number form a subspace of the full Hilbert space. Thus, particle number conservation allows us to diagonalize H within a subspace of fixed particle number, significantly reducing computational complexity.

[2] That is, it transforms like the spherical harmonic Y_2^μ.

[3] Since we work in a fermionic many-body basis, the Cooper pairs are antisymmetric under particle exchange. However, since $j > \frac{1}{2}$, a Cooper pair is *not* a state with definite coupled angular momentum $J^2_{\text{pair}} = 0$. This would tend to make the term "Cooper pair" seem inappropriate, but this language is fairly standard in nuclear physics.

Rotational symmetry means that states of the many-body-system with definite energy must also have definite total angular momentum J^2 arising from coupling the angular momenta of the individual particles. [4] [5] Furthermore, any such state with $J^2 > 0$ arises from spontaneously breaking the rotational symmetry and is expected to have degeneracy $2J + 1$. Only a state with $J^2 = 0$ is permitted to be non-degenerate. Later, we will see how this usually allows us to determine the angular momentum of an excited state, just by looking at its degeneracy. On the other hand, such degeneracies also lead to challenges.

In particular, every state with an odd number of particles has at least one unpaired spin-$\frac{1}{2}$ nucleon, and so the ground state for such a system—that is, the lowest-energy eigenstate belonging to a subspace with odd particle number—is always a degenerate state with spontaneously-broken rotational symmetry.

A given such degenerate state need not be perfectly representative of the properties of all states within the degenerate subspace, making it difficult to characterize the properties of the whole subspace. In particular, quantum information metrics such as entanglement entropy and mutual information are not quantum observables, being basis-dependent quantities. Such metrics are thus not well-defined on a degenerate subspace. In this work, we therefore restrict our attention to systems with even particle number N. For such systems, the ground state has zero total angular momentum, is rotationally symmetric, and non-degenerate.

To be more specific, we focus mainly on the case of $N = 4$ nucleons, that is, on systems with two occupied Cooper pairs. This case enables us to investigate and quantify the effects of interactions within and between Cooper pairs, without introducing unnecessary extra complexity or computational cost.

Finally, the unitary operator:

$$U \equiv \prod_{m=-j}^{j} \Big(a_m + a_m^\dagger\Big), \tag{2.7}$$

which is defined in [21] commutes with H_{Q^2} and with $N - \frac{1}{2}P^\dagger P$. Moreover:

$$\begin{aligned} U^\dagger N U &= U^\dagger \left(\sum_m a_m^\dagger a_m\right) U \\ &= \sum_m \Big(U^\dagger a_m^\dagger\Big)\Big(a_m U\Big) \\ &= \sum_m \Big(-a_m U^\dagger\Big)\Big(-U a_m^\dagger\Big) \\ &= \sum_m a_m a_m^\dagger \\ &= \sum_m \Big(1 - a_m^\dagger a_m\Big) \\ &= 2j + 1 - N, \end{aligned} \tag{2.8}$$

where $2j + 1$ is the available number of states, and so U trades particle for holes.

Therefore, when $\epsilon = G$, the full Hamiltonian H commutes with U and has a particle-hole symmetry. Even after restricting to a subspace with fixed N, this results in a degenerate ground state for the case of a half-filled subshell with $2j + 1 = 2N$. But since there's no reason at all for ϵ and G to be numerically equal, we set them to different values, and do not further consider this problematic special case.

Even though the particle-hole symmetry is broken when $\epsilon \neq G$, we nevertheless find that ground state solutions for $\bar{N} = 2j + 1 - N$ are qualitatively similar to solutions for N.

[4] The total angular momentum J^2 of an energy eigenstate of the many-body system must not be confused the total angular momentum j we use to label the shell itself—j is the angular momentum of an orbital, a single-particle state.

[5] An exception to this occurs when states with distinct J^2 are degenerate in energy—but even in this case we may choose a basis for the degenerate subspace so that the basis states are organized into multiplets with definite J^2.

Chapter 3 || Exact solution

The ground and excited states of the single-j model were computed numerically, using brute-force diagonalization of the Hamiltonian, while varying j, N, and X/G. Here we summarize the qualitative results obtained.

3.1 Ground state

Generically, the ground state of the single-j model may be characterized as:

- nondegenerate and rotationally symmetric,
- having zero total angular momentum, $J = M = 0$, and
- having no quadrupolar deformation, in the sense defined below in 3.5.

For $j < \frac{9}{2}$, the ground state is an equal superposition of states with $N/2$ occupied Cooper pairs, which, therefore, each have total $M = 0$. Ground states for various j and N are written out explicitly in table 3.1 below.

j	N	Ground state
$\frac{3}{2}$	2	$\frac{1}{\sqrt{2}}\|1001\rangle - \frac{1}{\sqrt{2}}\|0110\rangle$
$\frac{3}{2}$	4	$\|1111\rangle$
$\frac{5}{2}$	2	$\frac{1}{\sqrt{3}}\|001100\rangle - \frac{1}{\sqrt{3}}\|010010\rangle + \frac{1}{\sqrt{3}}\|100001\rangle$
$\frac{5}{2}$	4	$\frac{1}{\sqrt{3}}\|011110\rangle - \frac{1}{\sqrt{3}}\|101101\rangle + \frac{1}{\sqrt{3}}\|110011\rangle$
$\frac{7}{2}$	2	$\frac{1}{2}\Big(\|00011000\rangle - \|00100100\rangle + \|01000010\rangle - \|10000001\rangle\Big)$
$\frac{7}{2}$	4	$\frac{1}{\sqrt{6}}\Big(-\|00111100\rangle + \|01011010\rangle - \|01100110\rangle - \|10011001\rangle + \|10100101\rangle + \|11000011\rangle\Big)$

Table 3.1: Ground state for various N, j

With a nod to the caveat noted above in section 1.3, we observe that for $j = \frac{3}{2}, N = 2$, the ground state can be interpreted as a Bell state involving occupation of the two available Cooper pairs. [1]

Similarly, for $j = \frac{5}{2}$, the ground state is extremely similar in nature to a W state. Thus, it may be understood as a state involving bipartite entanglement between each pair of Cooper pairs, with no residual 3-tangle.

For $j \leq \frac{7}{2}$ the ground state is completely unaffected by the strength of the quadrupole interaction, since in this regime H_{P^2} commutes with H_{Q^2}. But this insensitivity to X/G does not continue to larger j. For a shell with $j = \frac{9}{2}$ and $N = 4$ particles:

- with $X = 0$, the ground state is an equal superposition of the $\binom{5}{2} = 10$ states with two occupied pairs, but
- for $X > 0$, the ground state superposition also includes eight states with non-zero total angular momentum $J, M > 0$ and containing no occupied pair with zero angular momentum.

[1] The state $|1001\rangle$ represents occupation of the pair with $m = \pm\frac{3}{2}$, and the state $|0110\rangle$ represents occupation of the pair with $m = \pm\frac{1}{2}$.

This behavior is characteristic of the behavior for shells with larger j, and leads to a dependence of quantum correlations on the strength of X/G, as discussed below in section 3.3.

3.2 Excited states and degeneracy

The structure of excited states depends on the value of X.

- When $X = 0$, there are a small number of highly-degenerate excited states.
- The degeneracy is partially broken when $X > 0$, and the states are organized into multiplets.

For $X > 0$ we found that each degenerate multiplet has a basis whose states may be labeled by well-defined M. The total M takes consecutive integral values within the subspace. For example:

- the first-excited 5-plet common to all solutions has a basis with states labeled $M = -2, -1, 0, 1, 2$, and
- similarly, the second-excited 9-plet has a basis with states labeled $M = -4, -3, -2, -1, 0, 1, 2, 3, 4$.

Notice that each of these degenerate subspaces looks much like a subspace with some angular momentum ℓ where $\ell = 0$ for the ground state, $\ell = 2$ for the first-excited state, $\ell = 4$ for the second-excited state, and so on. We have identified this angular momentum as the total angular momentum of the many-body system $\ell \equiv J$, resulting from coupling the angular momenta of the N individual particles. [2]

That is, the ground and excited states are states of good total angular momentum, as befits a system with spherical symmetry, according to the discussion above in 2.2. The ground state is a singlet state with zero total angular momentum $J = 0$, and each excited state spontaneously breaks rotational symmetry by acquiring a definite nonzero total angular momentum $J > 0$. The effect of the quadrupole coupling in the Hamiltonian is simply to split the energy levels of states with distinct total J.

The multiplets for various j, N are listed in the following table 3.2.

j	N	Multiplets
$\frac{3}{2}$	2	$J = 0, 2$ (1 ground states, 5 excited states)
$\frac{5}{2}$	2	$J = 0, 2, 4$ (1 ground state, 5 first-excited, 9 second-excited)
$\frac{5}{2}$	4	$J = 0, 2, 4$ (1 ground state, 5 first-excited, 9 second-excited)
$\frac{7}{2}$	2	$J = 0, 2, 4, 6$
$\frac{7}{2}$	4	$J = 0, 2, 4, 6, 4, 5, 2, 8$
$\frac{9}{2}$	2	$J = 0, 2, 4, 8, 6$
$\frac{9}{2}$	4	$J = 0, 2, 4, 6, 6, 4, 8, 2, 7, 5, 10, 3, 8, 4, 6, 9, 0, 12$
$\frac{15}{2}$	2	$J = 0, 2, 4, 6, 14, 8, 12, 10$

Table 3.2: Excited state multiplets for various N, j

The ordering of multiplets shown in this table is indicative of their energy levels at large values of X/G. With variation in X/G, the energy levels of distinct multiplets can cross, with the multiplets becoming degenerate at the crossing point.

The table exhibits two uninterpreted features: a repeated pattern $0, 2, 4$ for the lowest-energy multiplets; and multiplets with repeated J, including, for example, multiple $J = 6$ multiplets, and a second higher-energy $J = 0$ singlet for $j = \frac{9}{2}, N = 4$.

[2] We have verified this by explicitly calculating total angular momentum J only for the easiest case of $N = 2$ particles, according to the formulas derived in appendix A. But it must also be true in general based on the symmetry arguments given above in 2.2.

Furthermore, we notice that for $N = 2$ every multiplet has even J. This feature results from the mechanics of angular momentum coupling for fermions, and is explained in appendix A.

Figure 3.1 shows how the energy of each multiplet varies with X/G, for various values of j, showing explicitly the partial breaking of the degeneracy of excited states.

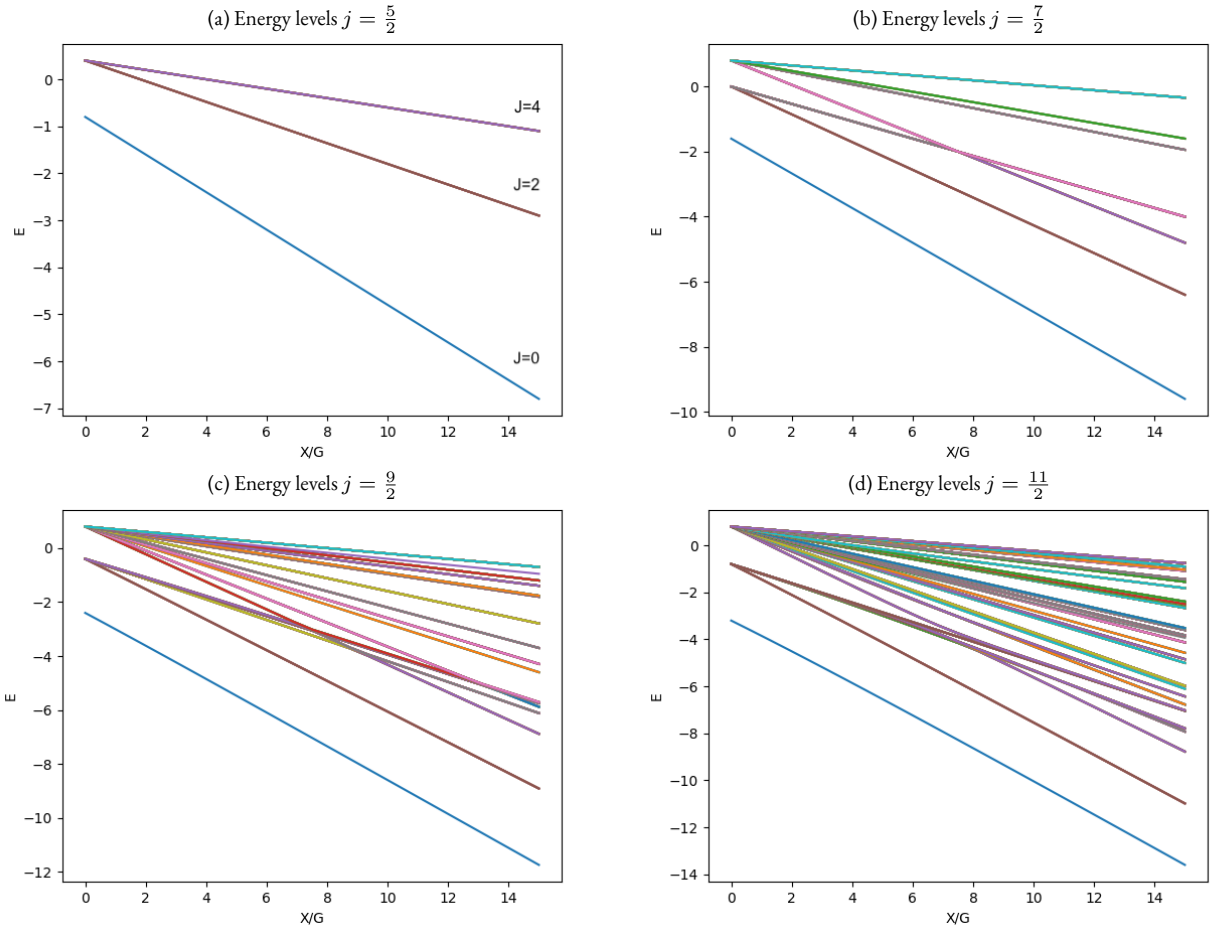


Figure 3.1: Dependence of energy levels on X/G for $N = 4$, various j

To visualize the multiplicity of the degenerate states, we may add a small constant magnetic field directed in the vertical direction to the Hamiltonian, which breaks the degeneracy completely, by splitting states with distinct M. This visualization is shown in figure 3.2.

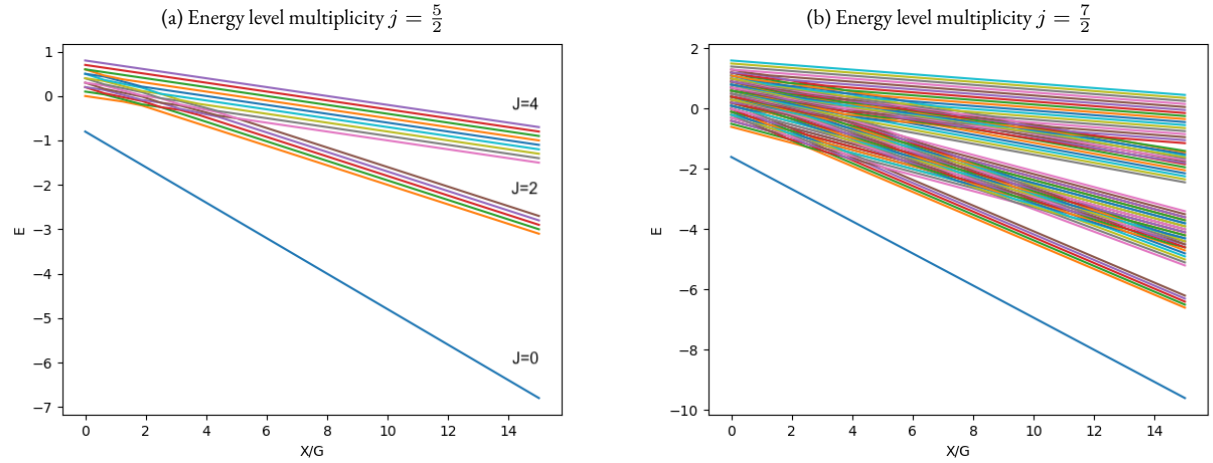


Figure 3.2: Multiplicity of degenerate states for $N = 4$, visualized by adding magnetic field

Interestingly, the one-body density matrix (1.6), along with the one- and two-orbital reduced density matrices are also diagonal for excited states—the $|j, m\rangle$ basis of single-particle states is their natural basis.

3.3 Correlations and entanglement in the ground state

In the ground state, the one-body density matrix (1.6), along with all one- and two-orbital reduced density matrices, are always diagonal, as befits a many-body quantum state expressed in its natural single-particle basis.[3] The two-orbital reduced density matrix for a paired orbital represents a perfectly classically-correlated state, except as noted below. Even three-orbital reduced density matrices are diagonal. Entanglement is observed in *four*-orbital reduced density matrices.

From the results of our numerical computations we were able to infer a set of general formulae for the reduced density matrices.[4] We define the average occupation p of a single-particle state by $p = \frac{N}{2j+1}$. When $N = 2$, when $j < \frac{9}{2}$, or when $X = 0$, every single-orbital reduced density matrix takes the form:

$$(1-p)\,|0\rangle\langle 0| + p\,|1\rangle\langle 1|\,, \tag{3.1}$$

and, furthermore, every two-orbital reduced density matrix for Cooper-paired states has the similar form:

$$(1-p)\,|00\rangle\langle 00| + p\,|11\rangle\langle 11|\,. \tag{3.2}$$

Four-orbital reduced density matrices for a choice of orbitals containing two Cooper pairs are always entangled states. When $N = 2$, when $j < \frac{9}{2}$, or when $X = 0$, they are of form:

$$\frac{d-a-b}{d}\underbrace{|0000\rangle\langle 0000|}_{\text{both pairs unoccupied}} + \frac{a}{d}\underbrace{|1111\rangle\langle 1111|}_{\text{both pairs occupied}} + \frac{b}{d}\underbrace{\tfrac{1}{2}\Big(|1001\rangle \pm |0110\rangle\Big)\Big(\langle 1001| \pm \langle 0110|\Big)}_{\text{exactly one pair occupied}}, \tag{3.3}$$

where:

$$d = \binom{j+\frac{1}{2}}{2}, \qquad a = \begin{cases} 0 & \text{for } N = 2 \\ 1 & \text{for } N = 4 \end{cases}, \qquad b = \begin{cases} j - \frac{1}{2} & \text{for } N = 2 \\ 2j - 3 & \text{for } N = 4 \end{cases}.$$

We might choose think of this as resulting from some sort of entangling interaction "between" Cooper pairs, but it's important to remember that we only need $N = 2$ particles to observe such entanglement in the occupation of paired states. Indeed, this way of thinking isn't strictly-speaking correct, since the pairing term H_{P^2} represents an interaction between two particles, not between two Cooper pairs.

For $j \geq \frac{9}{2}$, $N = 4$, and $X > 0$, the deforming force disrupts the correlation of zero-angular momentum Cooper pairs, as shown in figure 3.3.

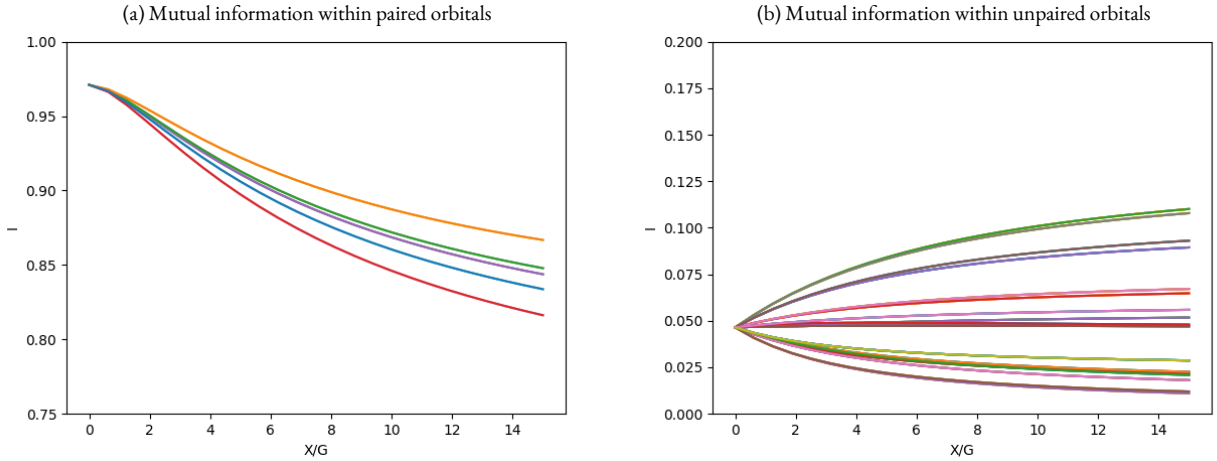


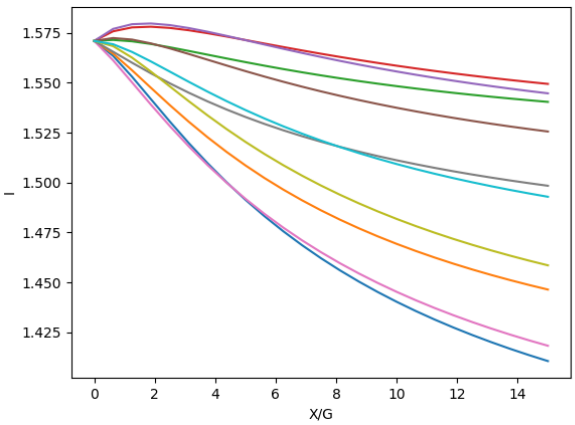
Figure 3.3: Mutual information (a) within Cooper pairs and (b) between unpaired orbitals for $j = \frac{9}{2}$, $N = 4$

Interestingly, the deforming force increases entanglement between some pairs, and decreases entanglement between others, while reducing classical correlations, as shown in figure 3.4.

[3] See section 1.5 and appendix F.

[4] Armed with these formulae, it's straightforward to calculate quantities like mutual information and entanglement entropy by hand. Note that it would also be possible, if tedious, to derive these formulae algebraically from the known form of the ground state given in 3.1.

(a) Mutual information between pairs of paired orbitals



(b) Entanglement of formation between pairs of paired orbitals

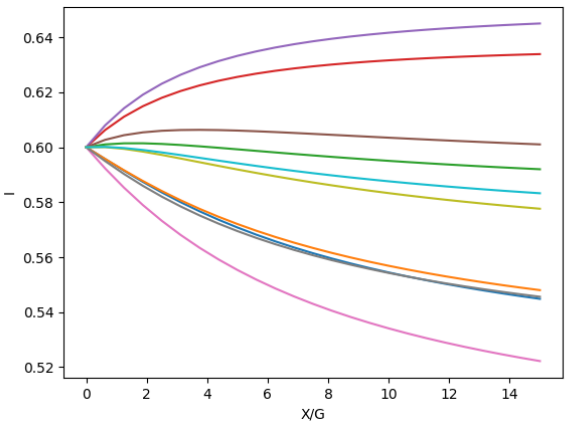
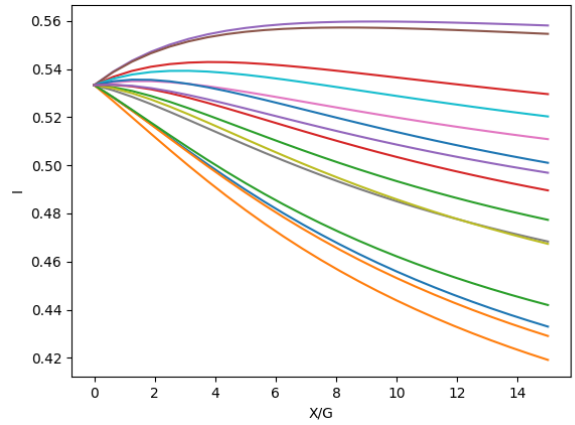


Figure 3.4: Mutual information and entanglement of formation between Cooper pairs for $j = \frac{9}{2}, N = 4$

This qualitative behavior is generic for shells with higher values of j. For example, figure 3.5 shows entanglement between Cooper pairs with $j = \frac{11}{2}$.

(a) Entanglement between pairs of paired orbitals $N = 4$



(b) Entanglement between pairs of paired orbitals $N = 6$

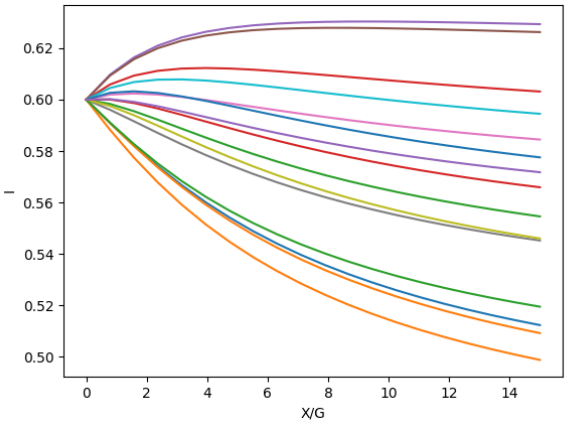
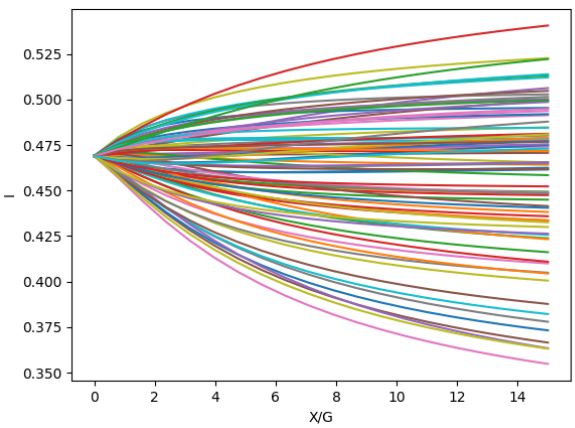


Figure 3.5: Entanglement of formation between (a) two and (b) three Cooper pairs for $j = \frac{11}{2}$

Furthermore, for $X > 0$, entanglement arises in the four-orbital reduced density matrices which were previously diagonal, as can be seen in figures 3.6 and 3.7. That is, the quadrupole interaction leads to bipartite entanglement in certain selections of four orbitals, even when the orbitals were not previously quantumly-correlated.

(a) Mutual information within pairs of unpaired orbitals



(b) Entanglement between pairs of unpaired orbitals

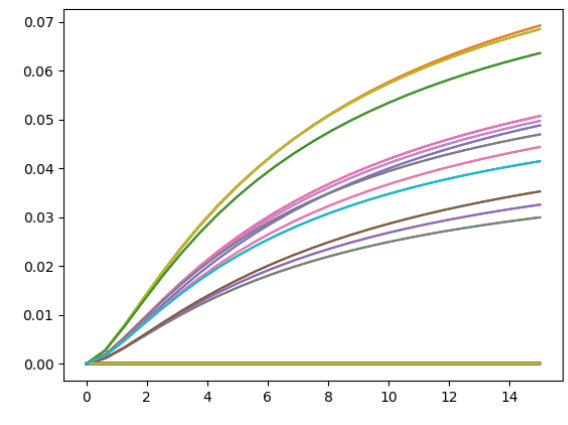
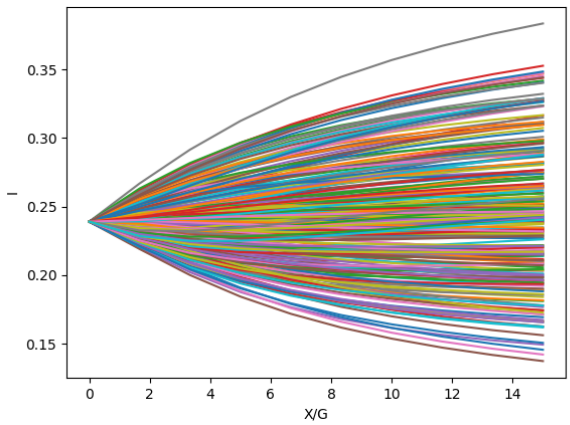


Figure 3.6: Mutual information and entanglement of formation, groups of four mutually-unpaired orbitals, $j = \frac{9}{2}, N = 4$

We note that this is a very subtle effect—the amount of entanglement is tiny. Correlations within these four-orbital reduced density matrices remain almost entirely classical.

(a) Mutual information within pairs of unpaired orbitals



(b) Entanglement between pairs of unpaired orbitals

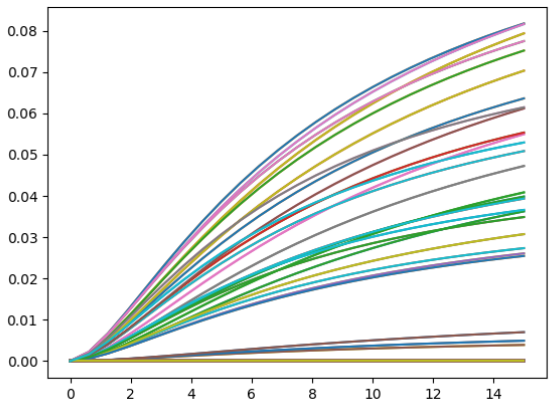


Figure 3.7: Mutual information and entanglement of formation, groups of four mutually-unpaired orbitals, $j = \frac{11}{2}$, $N = 4$

3.4 Total entanglement of the ground state

To characterize the *total* entanglement of the ground state, following [11, 22], we may consider the sum S of single-orbital entanglement entropies, as defined by (1.5). We find that S generally increases with j, unsurprisingly, since we're summing over a greater number of orbitals.

Alternatively, instead of summing over orbitals, we may consider the entanglement entropy for a single given orbital $|j, m\rangle$. We find that this quantity is identical for every orbital in the j shell, that is, that it's a constant not depending on m, and so:

$$S = (2j + 1) \cdot H(\rho_{|j,m\rangle}). \tag{3.4}$$

We then find that the entanglement entropy $H(\rho_{|j,m\rangle})$ takes its maximum value $H = 1$ for the case of half-filling, since in this case each orbital has probability $\frac{1}{2}$ of being occupied. Away from the half-filled case, the entanglement entropy is smaller since the occupation probability increases with N. Indeed, we may infer the following simple formula for the total entanglement:

$$S = (2j + 1) \cdot h\left(\frac{N}{2j + 1}\right), \qquad h(p) \equiv -p \log_2 p - (1 - p) \log_2(1 - p), \tag{3.5}$$

which agrees perfectly with results obtained numerically, and with [7].

Significantly, the single-orbital entanglement entropies—and thus also the total entanglement S—are constant for a given choice of j and N, and do not depend on the strength X/G of the quadrupole term. This leads us to view the effect of varying X/G as simply a *redistribution* of entanglement between pairs of *paired* orbitals to entanglement between pairs of previously *unpaired* orbitals.

In appendix E. we consider another quantity of interest: the entanglement entropy for the bipartition of the ground state with the largest Schmidt rank, which is given by:

$$T_{AB} = \log_2 \binom{j + \frac{1}{2}}{N/2}, \tag{3.6}$$

where the partition is by the sign of m, that is, A includes orbitals $|j, m\rangle$ with $m < 0$ and B orbitals with $m > 0$.

3.5 Quadrupole deformation

The total quadrupole deformation of a nuclear state may be quantified using the *quadrupole deformation parameter*:

$$\beta^2 = \sum_{\mu} |\langle Q_\mu \rangle|^2, \tag{3.7}$$

which involves the expectation value of a non-Hermitian operator.

Excited states of the single-j model in general feature nonzero quadrupole deformation $\beta^2 > 0$, leading to spontaneously broken rotational symmetry, and are therefore degenerate states. There is an exception for the case of a half-filled shell, where every excited state has no average deformation and $\beta^2 = 0$. The relationship between deformation and half-filling is shown below in table 3.3.

j	N	Filling	Deformation
$\frac{3}{2}$	2	half-filled	$\beta^2 = 0$
$\frac{5}{2}$	2		$\beta^2 > 0$
$\frac{5}{2}$	4		$\beta^2 > 0$
$\frac{7}{2}$	2		$\beta^2 > 0$
$\frac{7}{2}$	4	half-filled	$\beta^2 = 0$
$\frac{9}{2}$	2		$\beta^2 > 0$
$\frac{9}{2}$	4		$\beta^2 > 0$

Table 3.3: Excited state deformation for various N, j

Note that the quadrupole deforming force H_{Q^2} couples to eigenstates of the operator $\sum_\mu (-1)^\mu Q_\mu Q_{-\mu}$ which are *not* eigenstates of Q_μ. Therefore, the value of β^2 for an energy eigenstate is in general an average over superimposed states with inhomogeneous deformation, even when the pairing force is turned off. Furthermore, energy eigenstates belonging to a degenerate subspace—for example, the subspace of first excited states—do not share a constant value of β^2. We cannot, therefore, characterize such a degenerate subspace by its deformation.

3.6 Comparison with mean-field solutions

In this work we're interested in characterizing the properties of the true ground state and excited states of the single-j model with fixed particle number, which we obtain simply by brute-force diagonalization of the Hamiltonian within a subspace of fixed N.

The ground state of the single-j model for even N was previously investigated in [7] by restoring the spontaneously-broken (rotational and particle number) symmetries of a mean-field Hartree-Fock-Bogoliubov solution. The exact solutions we obtain for the ground state differ significantly in character from those reported for the mean field solution, showing better agreement with the reported symmetry-restored states.[5]

First, mean-field solutions were found to undergo a phase transition for large enough X, where deformation spontaneously breaks rotational symmetry of the ground state. We observed no such phase transition, and the exact ground state never featured deformation or broken rotational symmetry.

Second, in the mean-field solution, two-particle states involving paired orbitals are always pure due to the nature of the Hartree-Fock-Bogoliubov ansatz, with correlations between paired orbitals represented as entanglement. Since both the two-particle states and the entire mean-field ground state are pure, there may be no correlations, classical nor quantum, between pairs of paired states. In our exact solution, we find the exact opposite: pairing results in perfectly classically-correlated two-particle states, with no entanglement—that is, the two-orbital reduced density matrix is always diagonal. On the other hand, we find entanglement at the level of four-body reduced density matrices, which may be interpreted as entanglement between Cooper pairs. This result agrees qualitatively with [7], which found that symmetry restoration trades entanglement of two-particle states for correlations between pairs.

[5] Note that exact ground state solutions were not reported in [7].

Chapter 4 || Comparison with a realistic nuclear Hamiltonian

The single-j model is a toy we've used to gain an intuitive picture of the effects of the pairing and quadrupole interactions on a nucleus with just one flavor of nucleon in its valence shell. We would now like to compare this picture with results obtained using a more realistic nuclear Hamiltonian.

Such a family of realistic phenomenological Hamiltonians is discussed in [23] and was used in [15] to study the entanglement structure of ground states of various nuclei. For ease of comparison with results obtained above using the single-j model, we selected a member of this family with two protons occupying the pf shell.

The lowest-energy subshell of the pf shell is $0f_{7/2}$, so we will compare its ground state with our results for the single-j model with $j = \frac{7}{2}$. However, the pf shell also includes the higher-energy subshells $0f_{5/2}$, $1p_{1/2}$, and $1p_{3/2}$, as shown in figure 4.1, and so this is not therefore a single-j model. Nor is the Hamiltonian a simple direct sum of single-j models—interactions between nucleons result in nonzero Hamiltonian elements connecting orbitals with distinct j. Thus, we may expect such interactions to produce non-zero occupation of states in the higher-energy subshells.

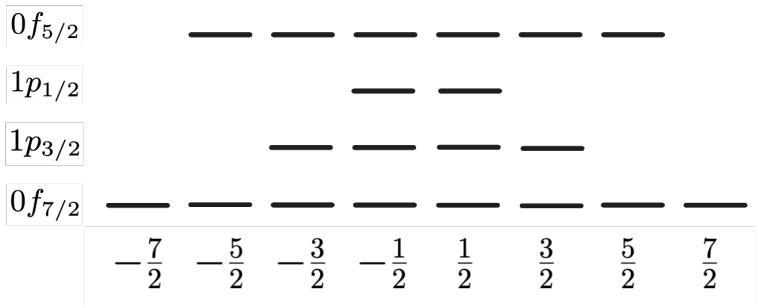


Figure 4.1: Valence space of nuclear pf shell, showing subshells vertically and orbitals horizontally

An important caveat is that this Hamiltonian is expressed in an incomplete basis comprising only many-body states with $M = 0$. So, while the full many-body basis has $\binom{8+4+2+6}{2} = 190$ states, here we consider a basis with only 30 such Cooper pairs. This restriction helps control the computational complexity of the problem.

The Hamiltonian was again diagonalized exactly by brute force.

4.1 Ground state and entanglement

In table 3.1 we reported that the ground state of the single-j model with $N = 2$ and $j = \frac{7}{2}$ is:

$$\frac{1}{2}\Big(|00011000\rangle - |00100100\rangle + |01000010\rangle - |10000001\rangle\Big), \tag{4.1}$$

which is just an equal superposition of the four states with one occupied Cooper pair.

For our realistic Hamiltonian, this state is the main contribution to the ground state, but, as anticipated above, the higher-energy subshells are also partially-occupied. The full expression for the ground state of the pf shell is:

$$\begin{aligned}
&0.4804\Big(|00011000\rangle - |00100100\rangle + |01000010\rangle - |10000001\rangle\Big)_{0f_{7/2}} \\
&+ 0.1249\Big(|0110\rangle - |1001\rangle\Big)_{1p_{3/2}} \\
&+ 0.1110\Big(-|001100\rangle + |010010\rangle - |100001\rangle\Big)_{0f_{5/2}} \\
&+ 0.0941\Big(-|11\rangle\Big)_{1p_{1/2}}.
\end{aligned} \tag{4.2}$$

Notice, furthermore, that the occupation of orbitals belonging to the higher-energy subshells also agrees with what we expect from our experience with the single-j model. Indeed, this state is simply a superposition of the ground states for the single-j models with $j = \frac{7}{2}$, $j = \frac{3}{2}$, $j = \frac{1}{2}$, and $j = \frac{5}{2}$.

The ground state has total angular momentum $J = 0$, also in agreement with the single-j model.

Thus, it's no surprise that figure 4.2 shows that the ground state correlates single-particle states within subshells, with negligible correlations between subshells.

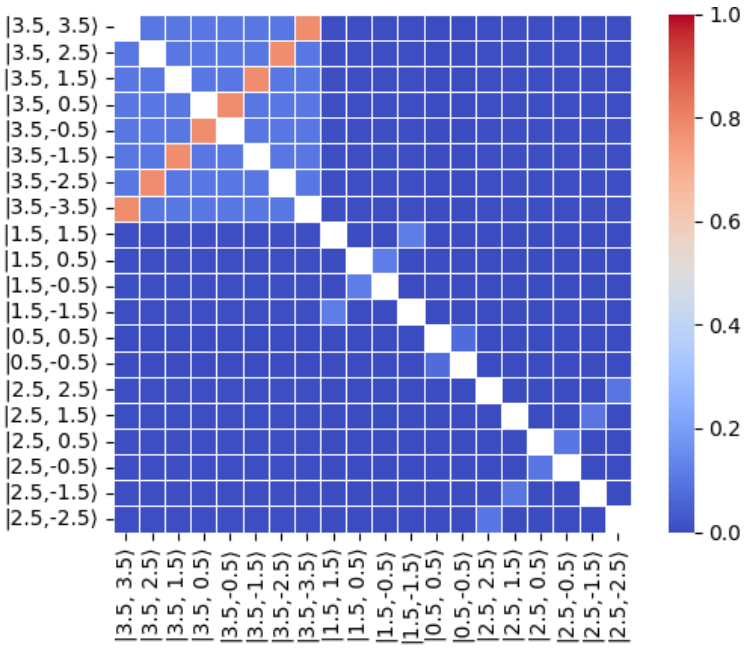


Figure 4.2: Two-orbital mutual information matrix for pf shell, $N = 2$ protons

In 3.3 we considered the single-orbital reduced density matrices, along with the two-orbital and four-orbital reduced density matrices for paired orbitals in the ground state of the single-j model. For $j = \frac{7}{2}$, $N = 2$, expressions (3.1), (3.2), and (3.3) respectively take the form:

$$\begin{aligned}
&\tfrac{3}{4}\,|0\rangle\langle 0| + \tfrac{1}{4}\,|1\rangle\langle 1|\,, \qquad \tfrac{3}{4}\,|00\rangle\langle 00| + \tfrac{1}{4}\,|11\rangle\langle 11|\,, \\
&\tfrac{1}{2}\,|0000\rangle\langle 0000| + \tfrac{1}{4}\Big(|1001\rangle \pm |0110\rangle\Big)\Big(\langle 1001| \pm \langle 0110|\Big).
\end{aligned} \tag{4.3}$$

In the ground state of our realistic Hamiltonian, these density matrices retain their form:

$$\begin{aligned}
&0.769\,|0\rangle\langle 0| + 0.231\,|1\rangle\langle 1|\,, \qquad 0.769\,|00\rangle\langle 00| + 0.231\,|11\rangle\langle 11|\,, \\
&0.538\,|0000\rangle\langle 0000| + 0.230\Big(|1001\rangle \pm |0110\rangle\Big)\Big(\langle 1001| \pm \langle 0110|\Big).
\end{aligned} \tag{4.4}$$

and the small numerical differences are explained by the partial occupation of the higher-energy subshells.

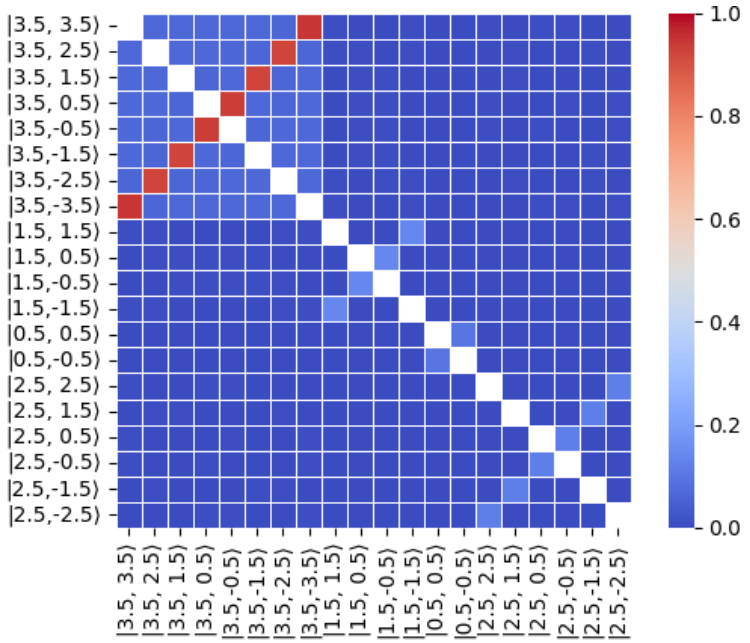


Figure 4.3: Two-orbital mutual information matrix for pf shell, $N = 4$ protons

If we now turn our attention to a case with $N = 4$ protons, the ground state is now *much* more complicated—too complicated to write down—since there are $\binom{30}{2} = 435$ different ways to occupy 30 Cooper pairs, but the overall structure of correlations is similar, as shown by figure 4.3.

Correlations in the lowest-energy $0f_{7/2}$ subshell are numerically stronger with $N = 4$, but this is expected since the subshell is half-filled, which maximizes the von Neumann entropy as we mentioned above in 3.4. Correlations between subshells remain negligible, and we notice no new features that aren't already familiar from our discussion of the single-j model.

4.2 Excited states in the restricted basis

In 3.2 we saw that the 27 excited states of the single-j model with $N = 2$ and $j = \frac{7}{2}$ were organized into degenerate multiplets with good $J = 2, 4, 6$, and that this organization could be explained as a consequence of rotational symmetry.

But at first glance, the excited states obtained with our realistic Hamiltonian are completely different. The states all have $M = 0$ and are non-degenerate with, starting from the ground state:

$$J = 0, 2, 4, 6, 2, 4, 3, 5, 0, 2, 4, 3, 2, 6, 1, 2, 1, 4, 3, 5, 1, 4, 0, 3, 2, 2, 3, 0, 2, 4. \tag{4.5}$$

A straightforward explanation for this discrepancy may be found in the restricted set of basis states: we cannot build a state with $M \neq 0$ using only basis states with $M = 0$. So it might appear that the realistic Hamiltonian, restricted to this basis, is unable to correctly reproduce the spectrum of excitations we would expect to see in a real nucleus.

But this is something we can also test with the single-j model, by similarly restricting the basis to states with $M = 0$. What we find is that diagonalizing the Hamiltonian in this restricted basis correctly reproduces the energy levels, but not the degeneracy, of the excited states of the full Hamiltonian. This is because each degenerate multiplet includes a "representative" state with definite total $M = 0$, and this state *can* be represented in the restricted basis.

Thus, we may simply infer that each state listed in (4.5) is the $M = 0$ representative of a degenerate $(2J+1)$-plet.

The single-j model seems to take us no further in understanding these excited states. In particular, the spectrum of J-plets of a direct sum of single-j Hamiltonians with $j = \frac{7}{2}, j = \frac{3}{2}, j = \frac{1}{2}, j = \frac{5}{2}$ does not predict the above listed values of J for the energy levels of our realistic Hamiltonian—at least not beyond the familiar $0, 2, 4, 6$ pattern for the four lowest levels.

Chapter 5 || Summary and conclusions

The single-j model provides a simple framework for exploring the effects of a pairing plus quadrupole interaction. We have seen that the effect of the pairing interaction is to produce classical correlations between Cooper-paired orbitals, that is, between orbitals with angular momentum projection $M = 0$. These classical correlations within Cooper pairs arise from entangled states involving at least four orbitals.

For an odd number N of nucleons, the ground state of the single-j model is degenerate, and thus quite difficult to properly characterize. But for an even number of nucleons, the ground state is a non-degenerate, rotationally symmetric state with no deformation and zero total angular momentum. When only the pairing interaction is present, the ground state is simply a superposition of states with $N/2$ occupied Cooper pairs. For $j < \frac{9}{2}$, the quadrupole term commutes with the pairing term, and the addition of the quadrupole interaction does not change the ground state. The picture changes for a subshell with $j \geq \frac{9}{2}$ and $N = 4$ particles, in the presence of the quadrupole interaction. In this regime, the quadrupole interaction partially disrupts the Cooper pairing and produces entanglement between orbitals which were not entangled in its absence. The total entanglement S does not depend on the strength of the quadrupole term, and so we feel comfortable in characterizing this effect as a redistribution of correlations.

We speculate that an appropriate change of basis of single-particle states would reveal that the correlations are simply redistributed from Cooper-paired orbitals in the $|j, m\rangle$ basis to some set of paired orbitals in this new basis. It would be very interesting to show that such a basis does—or does not—exist.

When only the pairing interaction is present, excited states are highly degenerate. The effect of the quadrupole interaction is to partially-break this degeneracy, splitting the energy levels of excited states into degenerate multiplets with good total angular momentum. This structure of excited states should be understood as a natural consequence of the rotational symmetry of the Hamiltonian. Excited states are deformed states, except in the case of a half-filled subshell.

One would be perfectly entitled to doubt that such a simple model could reproduce the characteristics of a real nucleus. We have answered this skepticism by showing that for a much more realistic nuclear Hamiltonian, the ground state may be viewed as a superposition of the ground states of several independent single-j subshells. The single-j model cannot, of course, account for interactions between subshells, and so does not predict the occupation of higher-energy subshells. Indeed, a Hamiltonian formed as the direct sum of single-j Hamiltonians would predict zero occupation for all but the lowest-energy subshell. But, on the other hand, we've also seen that correlations between orbitals in different subshells are extremely weak, and so, quite surprisingly, the single-j model doesn't actually appear to be missing any interesting entanglement structure here.

Finally, the single-j model features only one flavor of nucleon. Previous work has found that correlations between protons and neutrons are much weaker than correlations between just protons, or between just neutrons. On the other hand, based on some initial exploration, we noticed that incorporation of isospin into the realistic nuclear Hamiltonian introduces certain effects which are not present in the single-j model. It would be interesting to understand any such differences, perhaps by treating the realistic Hamiltonian as a perturbation of the direct sum of single-j Hamiltonians.

Ultimately, it's clear that the single-j model can act as a useful reference point in ongoing work to understand the entanglement and deformation of medium-to-heavy nuclei.

Appendices

A. Angular momentum coupling for fermions

For systems of distinguishable particles, addition of angular momentum is performed with the help of the Clebsch-Gordan coefficients defined by:

$$\langle j_1, m_1; j_2, m_2 | J, M \rangle \equiv \left(\langle j_1, m_1 | \otimes \langle j_1, m_1 | \right) | J, M, j_1, j_2 \rangle \,,$$

where J is the total angular momentum and $M = m_1 + m_2$ its vertical projection in the coupled basis. We will use the notation:

$$|j_1, m_1; j_2, m_2\rangle_{\text{distinguishable}} \equiv |j_1, m_1\rangle \otimes |j_2, m_2\rangle \,.$$

Then we may expand such a tensor product state in the coupled basis:

$$\begin{aligned} |j_1, m_1; j_2, m_2\rangle_{\text{distinguishable}} &= \sum_J |J, M, j_1, j_2\rangle\langle J, M, j_1, j_2 | \, |j_1, m_1; j_2, m_2\rangle \\ &= \sum_J \langle J, M, j_1, j_2 | j_1, m_1; j_2, m_2\rangle \, |J, M, j_1, j_2\rangle \\ &= \sum_J \langle j_1, m_1; j_2, m_2 | J, M\rangle \, |J, M, j_1, j_2\rangle \,, \end{aligned}$$

where the last step is legal since the coefficients are real-valued.

For indistinguishable fermions we must work with antisymmetric basis states, and we will use the notation:

$$|j_1, m_1; j_2, m_2\rangle_{\text{fermions}} \equiv \tfrac{1}{\sqrt{2}} \, |j_1, m_1\rangle \otimes |j_2, m_2\rangle - \tfrac{1}{\sqrt{2}} \, |j_2, m_2\rangle \otimes |j_1, m_1\rangle \,.$$

Then for $N = 2$ fermions we have:

$$|j_1, m_1; j_2, m_2\rangle_{\text{fermions}} = \tfrac{1}{\sqrt{2}} \sum_J \langle j_1, m_1; j_2, m_2 | J, M\rangle \, |J, M, j_1, j_2\rangle - \langle j_2, m_2; j_1, m_1 | J, M\rangle \, |J, M, j_2, j_1\rangle \,, \tag{A.1}$$

where in general $\langle J, M, j_1, j_2 | J, M, j_2, j_1\rangle = \delta_{j_1 j_2}$.

In the single-j model, we have $j_1 = j_2 = j$, and so this formula simplifies to:

$$\begin{aligned} |j_1, m_1; j_2, m_2\rangle_{\text{fermions}} &= \tfrac{1}{\sqrt{2}} \sum_J \Big(\langle j, m_1; j, m_2 | J, M\rangle - \langle j, m_2; j, m_1 | J, M\rangle \Big) \, |J, M, j, j\rangle \\ &= \tfrac{1}{\sqrt{2}} \sum_J \Big(1 - (-1)^{2j-J} \Big) \, \langle j, m_1; j, m_2 | J, M\rangle \, |J, M, j, j\rangle \\ &= \tfrac{1}{\sqrt{2}} \sum_J \Big(1 + (-1)^{J} \Big) \, \langle j, m_1; j, m_2 | J, M\rangle \, |J, M, j, j\rangle \\ &= \tfrac{2}{\sqrt{2}} \sum_{J \text{even}} \langle j, m_1; j, m_2 | J, m_1{+}m_2\rangle \, |J, m_1{+}m_2, j, j\rangle \,, \end{aligned} \tag{A.2}$$

where we used that $2j$ is always odd. Notice that this is a sum of states with even J. We must employ this formula when computing the expectation value of total angular momentum for an arbitrary state with $N = 2$ fermions.

B. Impact of fermionic partial trace

In 1.7 we introduced the fermionic partial trace and argued that it should be used to compute information-related quantities in the qubit space isomorphic to a fermion system under the Jordan-Wigner mapping. For the single-j model, the impact of using the fermionic partial trace instead of the regular partial trace is not profound.

For example, the following figure shows little difference in the two-orbital mutual information matrices calculated using the competing definitions of the partial trace:

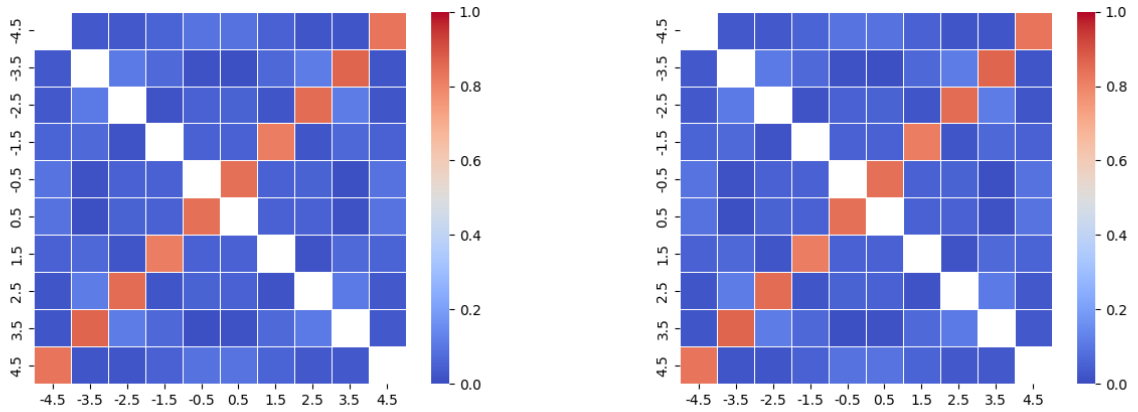


Figure B.1: Mutual information with (L) and without (R) the fermionic partial trace, $j = \frac{9}{2}, N = 4, X/G = 15$

On the other hand, there are subtle effects in certain cases, as shown by these plots of entanglement of formation for unpaired orbitals:

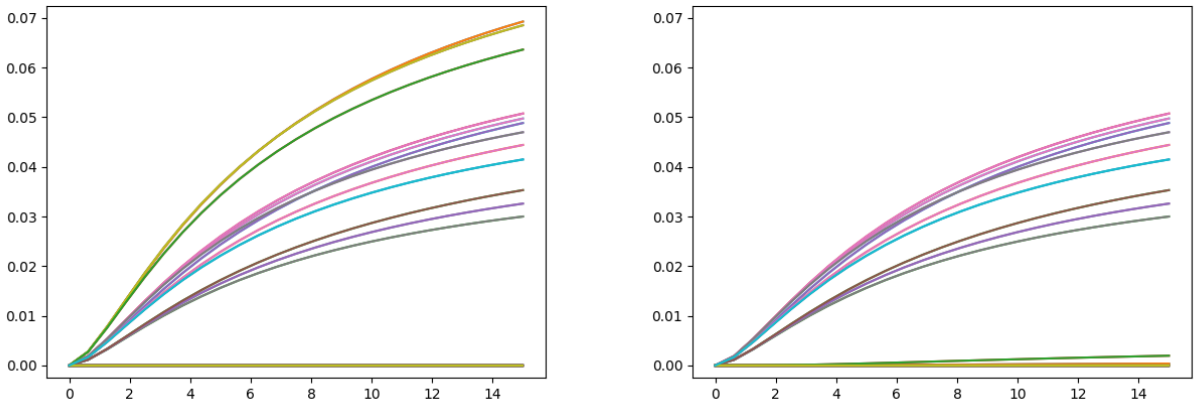


Figure B.2: Entanglement of formation calculated with (L) and without (R) the fermionic partial trace

C. The tangle

The n-tangle, introduced in [24], is an *entanglement monotone*, that is, a quantity which:

- vanishes for separable states,
- cannot increase under the action of local operators, and
- takes its maximum value for a maximally entangled state.

Unlike the entanglement entropy or entanglement of formation defined in 1.4, the tangle is not a quantity which has a direct operational interpretation in information processing. However, for pure two-qubit states, the bipartite tangle τ is just the square of the concurrence, and is thus directly related to the entanglement entropy T by the following formula given in [6]:

$$T_{AB}(|\psi\rangle) = h\left(\tfrac{1}{2}\left(1 + \sqrt{1 - \tau_{AB}(|\psi\rangle)}\right)\right). \tag{C.3}$$

For a pure state $|\psi\rangle$ of a finite-dimensional system, [25] gives the following formula for the bipartite tangle:

$$\tau_{AB}(|\psi\rangle) = 2\left(1 - \mathrm{Tr}_A\left(\mathrm{Tr}_B\,|\psi\rangle\langle\psi|\right)^2\right), \tag{C.4}$$

and extends the definition to mixed states ρ by taking the convex roof:

$$\tau_{AB}(\rho) = \min_{\rho=\sum_i p_i\,|\psi^{(i)}\rangle\langle\psi^{(i)}|} \sum_i p_i\,\tau_{AB}\left(\left|\psi^{(i)}\right\rangle\right). \tag{C.5}$$

For general mixed states, the n-tangle is difficult to calculate, involving a minimization over ensembles. But for the four-body states we encounter in the ground state of the single-j model, the minimization is trivial— just as it was for entanglement of formation—and the tangle is therefore easy to compute. We have not presented calculations of the bipartite tangle in this work, because exactly the same information is already available in the entanglement of formation. However, the 4-tangle is a quantity of interest in future investigation.

D. Anticommutation relations in the Jordan-Wigner isomorphism

It's straightforward to verify that the Jordan-Wigner mapping introduced in section 1.6 preserves the standard fermionic anticommutation relations between annihilation and creation operators. For example, the anticommutator $\left\{a_n, a_n^\dagger\right\} = 1$ may be verified as follows:

$$\begin{aligned}\left\{\left(\bigotimes_{i=0}^{n-1} Z_i\right)\otimes|1\rangle\langle 0|_n, \left(\bigotimes_{j=0}^{n-1} Z_j\right)\otimes|0\rangle\langle 1|_n\right\} &= \left(\bigotimes_{i=0}^{n-1} Z_iZ_i\right)\otimes|1\rangle\langle 0|_n\,|0\rangle\langle 1|_n + \left(\bigotimes_{i=0}^{n-1} Z_iZ_i\right)\otimes|0\rangle\langle 1|_n\,|1\rangle\langle 0|_n \\ &= \left(\bigotimes_{i=0}^{n-1}\mathbb{1}_i\right)\otimes\mathbb{1}_n = \mathbb{1}.\end{aligned}$$

Similarly, for the anticommutator $\{a_n, a_n\} = 0$ we have:

$$\begin{aligned}\left\{\left(\bigotimes_{i=0}^{n-1} Z_i\right)\otimes|1\rangle\langle 0|_n, \left(\bigotimes_{j=0}^{n-1} Z_j\right)\otimes|1\rangle\langle 0|_n\right\} &= \left(\bigotimes_{i=0}^{n-1} Z_iZ_i\right)\otimes|1\rangle\langle 0|_n\,|1\rangle\langle 0|_n + \left(\bigotimes_{i=0}^{n-1} Z_iZ_i\right)\otimes|1\rangle\langle 0|_n\,|1\rangle\langle 0|_n \\ &= 0.\end{aligned}$$

The remaining anticommutators are similarly straightforward.

E. An interesting Schmidt decomposition of the ground state

It's natural to consider a bipartition (A, B) of the ground state of the single-j model into orbitals A with $m < 0$ and orbitals B with $m > 0$. This is intuitively the bipartition with the largest Schmidt rank, and so we would like to know its Schmidt decomposition. Ignoring for now the fermionic nature of our Fock space, what we notice almost immediately is that the ground states given above in 3.1 are already written in a Schmidt basis for this bipartition. For example, the ground state for $j = \frac{5}{2}, N = 4$ is already just:

$$\tfrac{1}{\sqrt{3}}\,|011\rangle_A\otimes|110\rangle_B - \tfrac{1}{\sqrt{3}}\,|101\rangle_A\otimes|101\rangle_B + \tfrac{1}{\sqrt{3}}\,|110\rangle_A\otimes|011\rangle_B\,.$$

For general j, the Schmidt rank is:

$$r_{S,AB} = \binom{j+\frac{1}{2}}{N/2}, \tag{E.6}$$

which is the number of ways that N particles can occupy the available Cooper paired orbitals, and so the entanglement entropy associated with the bipartition is:

$$T_{AB} = \log_2\binom{j+\frac{1}{2}}{N/2}. \tag{E.7}$$

F. The structure of reduced density matrices

Completely generically, a single-orbital reduced density matrix takes the form:

$$\rho_\alpha = b\,|0\rangle\langle 0| + a\,|1\rangle\langle 1| + c\,|0\rangle\langle 1| + d\,|1\rangle\langle 0|\,. \tag{F.8}$$

For a state of indistinguishable fermions expressed in terms of occupation numbers, a term like $c\,|x\rangle\langle y|$ which survived the process of tracing out every orbital except the orbital α must have resulted from a corresponding term of form $c\,|xabc\ldots\rangle\langle yabc\ldots|$ in the original density matrix ρ, where, for notational convenience, and without loss of generality, we've ordered the single-particle states so that α is the first orbital. If the full state ρ is pure, then it must have nonzero contributions from the basis states $|xabc\ldots\rangle$ and $|yabc\ldots\rangle$.

On the other hand, if the Hamiltonian conserves *particle number parity*, then its eigenstates cannot superimpose states with an odd number of occupied orbitals with states with an even number of occupied orbitals. Therefore, ρ cannot have contributions from both $|0abc\ldots\rangle$ and $|1abc\ldots\rangle$, and the single-orbital reduced density matrix ρ_α must be diagonal:

$$\rho_\alpha = \begin{bmatrix} 1-p & \\ & p \end{bmatrix}, \tag{F.9}$$

where p is the average occupation of the orbital α.

In fact, [26] shows that Lorentz symmetry—via the spin-statistics theorem—leads to a *parity superselection rule*, since a state with an odd number of fermions change sign under a rotation by 2π, whereas a state with an even number of fermions does not. And this superselection rule is also a requirement for entanglement entropy to be well-defined in a fermionic system. Dropping the superselection rule leads to violation of the important equality:

$$\mathrm{Tr}_A^{\text{fermionic}}\,\rho_{AB} = \mathrm{Tr}_B^{\text{fermionic}}\,\rho_{AB}.$$

Therefore, any sensible many-body Hamiltonian must have eigenstates with diagonal single-orbital reduced density matrices.

But we may now take this reasoning a step further. An element like $c\,|xy\rangle\langle zw|$ of a *two*-orbital reduced density matrix $\rho_{\alpha\beta}$ must have arisen from a superposition of states of form $|xyabc\ldots\rangle$, $|zwabc\ldots\rangle$ in the full pure state ρ, and so now the parity superselection rule leads to *two*-orbital reduced density matrices of form:

$$\rho_{\alpha\beta} = \begin{bmatrix} * & & & * \\ & ** & & \\ & ** & & \\ * & & & * \end{bmatrix}. \tag{F.10}$$

If, in addition, particle number is conserved, instead of only its parity, a further simplification results:

$$\rho_{\alpha\beta} = \begin{bmatrix} * & & & \\ & ** & & \\ & ** & & \\ & & & * \end{bmatrix}. \tag{F.11}$$

We've mentioned above in 1.5 that [7] argues that the remaining off-diagonal elements also vanish in the natural basis.

We may even play this game with larger matrices. With particle number conservation, the reduced three-orbital density matrix $\rho_{\alpha\beta\gamma}$ must take the form:

$$\rho_{\alpha\beta\gamma} = \begin{bmatrix} * & & & & & & & \\ & * & * & & * & & & \\ & * & * & & * & & & \\ & & & * & & * & * & \\ & * & * & & * & & & \\ & & & * & & * & * & \\ & & & * & & * & * & \\ & & & & & & & * \end{bmatrix}. \tag{F.12}$$

G. Entanglement of formation for X-shaped states

Consider the following mixed quantum state:

$$\rho = \begin{bmatrix} A & 0 & 0 & C \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ C & 0 & 0 & B \end{bmatrix}.$$

For simplicity we take its elements to be real.

If this were a pure state, then it would satisfy:

$$A + B = 1, \qquad AB = C^2, \tag{G.13}$$

and we could factorize the state as:

$$|\psi\rangle = \sqrt{q}\,|00\rangle + \sqrt{1-q}\,|11\rangle = \sqrt{A}\,|00\rangle + \sqrt{B}\,|11\rangle\,.$$

Then its entanglement entropy would be simply:

$$T_{AB}(|\psi\rangle) = h(q) = -q\log q - (1-q)\log(1-q). \tag{G.14}$$

Our mixed state need not satisfy these conditions, and its entanglement of formation, as defined in (1.4), is an optimization over decompositions of the state as convex combinations of pure states. But since the entanglement of formation must agree with the entanglement entropy in the special case where the state is pure, it suffices to minimize over the following family of decompositions of ρ, parameterized by probabilities p and q:

$$\begin{gathered} \rho = p\,|\phi(q)\rangle\langle\phi(q)| + (A - pq)\,|00\rangle\langle 00| + (B - p + pq)\,|11\rangle\langle 11|\,, \\ |\phi(q)\rangle = \sqrt{q}\,|00\rangle + \sqrt{1-q}\,|11\rangle\,, \end{gathered} \tag{G.15}$$

subject to the following constraints:

$$p\sqrt{q(1-q)} = C, \qquad pq \le A, \qquad p(1-q) \le B. \tag{G.16}$$

We may use the equality to eliminate p, and then minimize the entropy over q, subject to the inequalities.

The states $|00\rangle\langle 00|$ and $|11\rangle\langle 11|$ have zero entropy, and so the entropy of formation is given by:

$$T_{AB}(\rho) = \min_q p(q)\cdot h(q) = C \min_q \frac{h(q)}{\sqrt{q(1-q)}}. \tag{G.17}$$

This is a concave function of q, and so its minimum must occur at one endpoint of the range:

$$\frac{C^2}{C^2 + B^2} \le q \le \frac{A^2}{C^2 + A^2}, \tag{G.18}$$

which means our minimization requires only two evaluations of the function $h(q)/\sqrt{q(1-q)}$ in (G.17).

If we now take the state ρ to be pure once more, via equations (G.13) the range collapses to $q = A$, then (G.16) gives $p = 1$, and we recover (G.14) as expected.

We've derived this result for a 4×4 density matrix, but the logic we relied on is more general, and the resulting formulae may be used whenever a mixed state can be expressed as the convex combination of a diagonal state with an entangled "X"-shaped state. In particular, we used this approach in 3.3 to compute the entanglement of formation for four-orbital reduced density matrices in the single-j model.

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