Entanglement and seniority

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We study mode-entanglement in the seniority model, derive analytic formulas for the one-body reduced density matrix of states with seniority ν = 0, 1, 2, and ν = 3, and also determine the particle number dependence of the one-body reduced density matrix for arbitrary seniority. We carry out numerical calculations for the lightest calcium isotopes and for 94Ru nucleus, and investigate the structure of their ground and low energy yrast states. We investigate the fulfillment of several predictions of the seniority model regarding the behavior of one-mode entropies, which we compare with the results of configuration interaction (CI) and density matrix renormalization group (DMRG) computations. For 94Ru, the seniority model accounts for the 0f5/2 mode entropies, but seniority mixing is important for certain yrast states. Interaction induced quantum fluctuations decrease the occupation of the 0f5/2, 1p1/2 and 1p1/2 shells, and amount in finite mode entropies on these shells, too, clearly outside the scope of the simple (0f5/2)4 seniority model. The 0f5/2 shell based seniority model is more accurate for the light Ca isotopes, but seniority mixing is substantial for some 44Ca yrast states, too.

I. INTRODUCTION

In recent decades, considerable effort has been devoted to entanglement in many areas of physics. Besides investigations motivated by the application of entanglement as a resource [1], more and more attention is devoted to the structure and role of entanglement in many-body problems [2–4]. While entanglement is an early concept of quantum theory and has been the subject of intense investigations [5], in systems of indistinguishable particles, such studies do not have a long history. In the latter case, the definition of subsystems is a more subtle question, since decomposition based on the tensor product of Hilbert spaces does not lead to physically meaningful subsystems. Different approaches are introduced to overcome this problem: the mode entanglement method [9–13], the algebraic approach based on the correlation between observables [14–21], descriptions relying on quantum correlations of particles [22–25] and concepts generalized to quasi-particles [11, 26].

In this paper, we follow the formalism based on algebraic partitions of bounded operators generated by the fermionic creation and annihilation operators, and we apply the entanglement measure called one-mode entropy [9, 11]. The one-mode entropy being, however, basis dependent [9, 11], we also utilize the notion of basis independent one-body entanglement entropy, introduced in Refs. [11, 27, 28] to characterize entanglement.

Entanglement and correlations are somewhat related concepts. Correlations play an unavoidable role in non-perturbative many-body problems [29, 32] and, – similar to entanglement, – characterize the connections or independence of certain quantities or subsystems. There is therefore a natural demand to investigate concrete correlated quantum mechanical models from the viewpoint of entanglement. This paper aims to contribute to this line of investigations by the study of the seniority model [33] in nuclear physics, and by comparing its predictions for entanglement with detailed model calculations.

Entanglement investigations are often performed in atomic physics [34, 35], quantum chemistry [31], and condensed matter physics [41] to date. Although investigations of the Lipkin-model [36, 37] and fermionic superconducting systems [26], do have some relevance for nuclear physics, exploration of this research area in the context of nuclear physics is, however, still in its initial stage. Apart from studies carried out in the traditional nuclear shell model framework [38, 39] and an investigation performed in an ab initio no-core shell model [44], we are not aware of other works pursuing this research direction.

In this paper, we study few nucleon states within the seniority model. This investigation can be considered as an extension of our previous study on the entanglement of angular-momentum coupled two-nucleon states [43] to relatively simple many-nucleon states. One-mode entanglement and two-orbital correlations in wave functions restricted to seniority zero electron pair states have also been studied in Ref. [45] in a quantum chemistry context. There, however, a general framework is used, without exploiting the conservation of total angular momentum, an almost mandatory constraint in nuclear physics.

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The physical motivation behind the seniority model is the pairing phenomenon [33]. The seniority model can be considered as a first step to describe short-range correlations in nuclei, but can also be used as an essential building block for more sophisticated models such as the generalized seniority model (see, e.g., Refs. [46–48]). The seniority model is a \(jj\)-coupling classification of nucleons residing on a single-\(j\) shell, with the seniority quantum number \(\nu\) naturally interpreted as the number of unpaired particles.

From a mathematical viewpoint, the seniority model is an exactly solvable model describing \(n\) particles interacting via seniority conserving interaction, and possessing a dynamically broken SU(2) quasi-spin symmetry [49]. Even though realistic interactions with seniority mixing do not possess this dynamical symmetry, the classification of states based on seniority quantum numbers often proves very useful for interpretation. Although the seniority model and its generalization to multi-\(j\) shells appeared early in nuclear physics, they provide a valid and quite accurate description for many nuclei, and a seniority number-based classification is still quite important from the perspective of entanglement.

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The paper is organized as follows. We review the concept of mode entanglement in Section II. The basic concepts of the seniority model are presented in Section III. States with seniority \(\nu = 0\), \(\nu = 1\), and \(\nu = 2\) are analyzed from the perspective of mode-entanglement in Section IV. Section V discusses our analytical results, while numerical results are presented in Section VI where the lightest calcium isotops and \(^{94}\text{Ru}\) nuclei are investigated by means of the configuration interaction (CI) method and a nuclear shell version of the density matrix renormalization group (DMRG) method [40, 65], using realistic effective interactions. Results obtained by the CI and DMRG methods are compared with the predictions of the seniority (SEN) model. Finally, Section VII concludes and summarizes the results.

II. MODE ENTANGLEMENT

In this work, we apply the second quantized formalism to determine mode-entanglement in a many-body framework. The primary objects for a fermionic system of \(d\) modes are the creation and destruction operators, \(c_i^\dagger\) and \(c_i\), \(i \in \{1,2,\ldots,d\}\), satisfying canonical anti-commutation relations. The single-particle (sp) states \(c_i^\dagger|0\rangle\) span the single particle Hilbert space of dimension \(d\), with \(|0\rangle\) referring to the vacuum. Considering a bipartition of the \(d\) modes to subsets \(A\) and \(B\), we get two algebras, \(A_A\), and \(A_B\), spanned by operators composed from the sets \(A\) and \(B\), respectively. A purely fermionic state is separable with respect to this bipartition if and only if it is of the form

\[
P(\{c_i^\dagger \}_{i \in A})\mathcal{Q}(\{c_j^\dagger \}_{j \in B})|0\rangle,
\]

with \(P\) and \(\mathcal{Q}\) denoting polynomials of the creation operators. In this work, we restrict ourself to the case, where \(A\) refers to a single mode, \(k\), while \(B\) contains all other \(i \neq k\) modes, and the whole system is in a pure state, \(\Psi\).

To characterize this type of bipartition, one introduces the one-mode reduced density matrix,

\[
\rho_k \equiv \begin{pmatrix} \langle c_k^\dagger c_k \rangle & 0 \\ 0 & 1 - \langle c_k^\dagger c_k \rangle \end{pmatrix},
\]

with \(\langle c_k^\dagger c_k \rangle = \langle \Psi | c_k^\dagger c_k | \Psi \rangle\). The entanglement measure of this simple bipartition is the one-mode entropy,

\[
S_k \equiv -\text{Tr}(\rho_k \ln(\rho_k)) = h(\langle c_k^\dagger c_k \rangle),
\]

with the function \(h\) defined as

\[
h(x) \equiv -x \ln(x) - (1 - x) \ln(1 - x).
\]

The total correlation introduced as

\[
S_c = \sum_{k=1}^d S(\rho_k).
\]

yields then a global characterization of the entanglement of the state \(\Psi\), which depends, however, on the choice of sp basis, \(\{c\}\). A basis independent one-body entanglement entropy can then be defined as

\[
S_{1B} = \min_{\{c\}} S_c.
\]

By the measure \(S_{1B}\), all fermion states described by a single Slater determinant are classified as non-entangled, while other pure states are entangled [11, 22, 24].

The quantity \(S_{1B}\) is closely related to the eigenvalues of the one-body reduced density matrix (1B-RDM), defined as

\[
\rho_{ij} = \langle \Psi | c_j^\dagger c_i | \Psi \rangle,
\]
and normalized as Tr ρ = n, with n the particle number. The basis where \( S(\alpha) \) reaches its minimum (i.e., \( S(\alpha) = S_{1B} \)) corresponds to the so-called natural orbitals, and there the 1B-RDM is diagonal, \( \rho = \text{diag}\{n_1, n_2, \ldots, n_d\} \). There \( S_{1B} \) reads

\[
S_{1B} = \sum_{i=1}^{d} h(n_i),
\]

(7)

where the \( n_i \) denote the occupation numbers of the natural orbitals.

### III. SENIORITY MODEL: BASIC DEFINITIONS

In the seniority model, we assume that \( n \) nucleons occupy a single \( j \) shell, corresponding to a shell configuration \( j^n \). For the \( s, p \) states, we use the notation \( |a, m\rangle = |n_a a_j k_j m\rangle \). In the seniority model, nucleons reside on a single multiplet, \( a \). We can therefore suppress the label \( a \) and use the compact notations, \( a_{am}^\dagger \rightarrow a_{m}^\dagger \) and \( a_{am} \rightarrow a_m \) for the corresponding creation and annihilation operators.

The pair creation and annihilation operators, \( S_{\pm} \), defined as

\[
S_+ = \sum_{m>0} (-1)^{-m} a_{m}^\dagger a_{-m} \quad \text{and} \quad S_- = S_+^\dagger
\]

(8)

create/destroy a zero angular momentum pair of particles. Together with

\[
S_0 = \frac{1}{2} \left( \sum m a_m^\dagger a_m - \frac{2j+1}{2} \right)
\]

(9)

the \( S_{\pm} \) obey standard SU(2) angular momentum commutation relations, and the operators \( S_z = (S_+ + S_-)/2 \), \( S_y = (S_+ - S_-)/2i \), and \( S_x = S_0 \) form components of the so-called quasi-spin operator, \( S \).

In the seniority model, a state of angular momentum \( J \) and projection \( J_z = M \) is denoted by \( \Psi_{JM}(j^n \nu \eta) \), where \( \eta \) stands for an angular momentum multiplicity label. If the state is multiplicity-free, the index \( \eta \) can (and will) be suppressed. In the seniority model, we start from unpaired \( \nu \)-particle states, which do not contain paired particles, \( \Psi_{JM}(j^n \nu \eta) = 0 \), and are quasi-spin eigenstates of spin \( S = (j+\frac{1}{2} - \nu)/2 \) and \( S_z = -S \). The quantum number \( \nu \) defines the seniority of this and all descendent states. From the properties of the quasi-spin operators it follows that the \( n \)-particle state

\[
\psi_{JM}(j^n \nu \eta) = N_{n,\nu} S^{(n-\nu)/2} \psi_{JM}(j^n \nu \eta)
\]

(10)

has the same quasi-spin as \( \psi_{JM}(j^n \nu \eta) \), but is an eigenstate of \( S_z \) with eigenvalue \(-\nu - (j + \frac{1}{2} - n)/2 \). The prefactor \( N_{n,\nu} \) here just ensures proper normalization. Clearly, instead of the quantum numbers \( n \) and \( \nu \), we can thus use the values of the quasi-spin \( S \) and its third component \( S_z \) as quantum numbers, and denote the state \( \psi_{JM}(j^n \nu \eta) \) as \( \Psi_{JMSS, (j, \eta)} \).

If all nucleons are paired, the \( n \)-particle seniority-zero wave function reads

\[
\psi_{00}(j^n0) = N_{n,0} S^n_+^{n/2} |0\rangle.
\]

(11)

For an odd number of particles, there is only one unpaired particle in the ground state, and the corresponding seniority-one eigenfunction is

\[
\psi_{JM}(j^n1) = N_{n,1} S^{(n-1)/2}_{+} a^\dagger_M|0\rangle.
\]

(12)

Seniority-two states have the form

\[
\psi_{JM}(j^n2) = N_{n,2} S^{(n-2)/2}_+ \left( \sum_m c_{j,M}\frac{M}{m} a_{m}^\dagger a_{M-m}^\dagger \right) |0\rangle,
\]

(13)

where \( J = 2j - 1, 2j - 3, \ldots, 2 \). In the cases of \( \nu = 0 \), \( \nu = 1 \) and \( \nu = 2 \) the states are multiplicity free. The form of higher seniority states is much more complicated, and analytical forms are only known for \( \nu = 3, 4 \) and 5 [66, 67].

### IV. ONE-BODY REDUCED DENSITY MATRIX

To determine the 1B-RDM, we consider first a general, model-independent state, \( \Psi_{JM} \), with angular momentum, \( J \), and \( J_z = M \). The 1B-RDM is then given by

\[
\rho_{m'm}^{a'a}(JM) = \langle \Psi_{JM} | a_{a'}^\dagger m' a_{am} | \Psi_{JM} \rangle.
\]

(14)

Conservation of the \( z \) component of the angular momentum implies that all \( m \neq m' \) off-diagonal elements of \( \rho_{m'm}^{a'a}(JM) \) vanish. In the special case, \( J = 0 \), moreover, simple group theoretical arguments imply \( j_a = j_a' \), and that all diagonal matrix elements are equal

\[
\rho_{m'm}^{a'a}(00) = \delta_{m'm} \delta_{j_a j_a} \rho_{a'a}(00).
\]

(15)

This immediately implies that in any \( J = 0 \) state the one-mode entropies do not depend on the magnetic quantum number \( m \) of the \( s, p \) modes, as also observed numerically in Ref. [40] and proved in [43] for two-body problems.

To compute the matrix elements of the operators \( a_{a'm'}^\dagger a_{am} \) for \( J \neq 0 \), we express these in terms of spherical tensor operators. The operators \( a_{am}^\dagger \) and \( a_{am} \), with \( m = (-1)^{j_a + m} a_{a-m} \) are both tensor operators of rank (spin) \( j_a \). We can define from these spherical tensor operators of rank \( K \) using the usual SU(2) addition rules as

\[
\sum_{K} c_{j_a, m, j_a, -m}^K \langle \psi_{JM} | a_{a'}^\dagger \otimes a_{a'} \rangle^K_0 | \psi_{JM} \rangle.
\]

(16)
Clearly, for $J = 0$ only the $K = 0$ term remains, and the expression simplifies to Eq. (15).

Our goal is to calculate the 1B-RDM, $\rho_{m,m'}(J M, j^n \nu \eta)$, associated with the state $\Psi_{J M}(j^n \nu \eta)$ within the seniority model. We shall do that using the quasi-spin formalism [68], where we introduce a quasi-spin tensor of rank $\frac{1}{2}$ as

$$ R_{\mu;m}^\frac{1}{2} = \begin{cases} a_m^\dagger & \text{if } \mu = 1/2, \\ -a_m & \text{if } \mu = -1/2. \end{cases} \quad (17) $$

From these we define quasi-spin tensors of rank $K = 0$ and $K = 1$ as [68]

$$ R^K_{\kappa;m',m} = \sum_{\mu,\mu'} C^{K,\kappa}_{\frac{1}{2},\mu,\mu'} R_{\mu;m,m'}^\frac{1}{2} R_{\mu';m'}^\frac{1}{2}. \quad (18) $$

The nucleon number dependence of the matrix element of the operator $a_m^\dagger a_m$ can be determined by using the identity

$$ a_{m'}^\dagger a_m = \frac{(-1)^{j+m}}{\sqrt{2}} \left( R_{0;m',-m}^0 + R_{0;m',-m}^1 \right), \quad (19) $$

and by applying the Wigner-Eckart theorem in the quasi-spin space, yielding

$$ \langle \Psi_{J M S_z}(j \eta) | a_{m'}^\dagger a_m | \Psi_{J M S_z}(j \eta) \rangle = \delta_{m'-m} \langle (-1)^{j+m} \sqrt{2} \left( R_{0;m',-m}^0 + R_{0;m',-m}^1 \right) \rangle. \quad (20) $$

This formula allows us to relate the 1B-RDM of a system of $n$ particles to that of a system of $\nu$ particles, both in states with seniority $\nu$.

We now proceed and give the analytical expression for the 1B-RDM for wave functions with seniority $\nu = 0, 1,$ and $\nu = 2$. Details of the derivations are to Appendix A.

In the simplest case, $\nu = 0$, the total angular momentum vanishes, $J = 0$, and therefore $\rho_{m,m'}$ is proportional to the unit matrix (see also Eq. 15),

$$ \rho_{m,m} (00, j^n 0) = \delta_{m',m} \frac{n}{2j + 1}. \quad (21) $$

For $\nu = 1$, only the sp orbitals $m = \pm M$ behave differently from the rest. In this case, the $m = M$ orbital is occupied, while $m = -M$ is empty, and the remaining $n-1$ particles reside on the other $2j-1$ orbitals with uniform probability,

$$ \rho_{m,m} (j M, j^n 1) = \delta_{m',m} \begin{cases} 1 & \text{if } m = M, \\ 0 & \text{if } m = -M, \quad (22) \\ \frac{n-1}{2j-1} & \text{if } m \neq |M|. \end{cases} $$

For seniority-two wave functions, the 1B-RDM has the form

$$ \rho_{m,m}(J M, j^n 2) = \delta_{m',m} \left\{ \left( C_{J,j,m,j,M-m}^{J,M} \right)^2 - \left( C_{j,-m,j,M+m}^{J,M} \right)^2 + \frac{1}{2} \right\} \left\{ \left( C_{J,j,m,j,M-m}^{J,M} \right)^2 + \left( C_{j,-m,j,M+m}^{J,M} \right)^2 - \frac{1}{2} \right\}, \quad (23) $$

where the total angular momentum is even and ranges from $J = 2$ to $J = 2j - 1$. The complicated analytical form of the 1B-RDM is given in the Appendix for seniority-three states.

V. ANALYTICAL RESULTS

We now discuss the consequences of the previous results from the perspectives of the mode- and one-body entropies. Having constructed the 1B-RDM, we obtain

$$ S^n_m (J M) = h \left( \rho_{m,m}^a (J M) \right). \quad (24) $$

A mode $m$ of a multiplet $a$ is therefore non-entangled if and only if $\rho_{m,m}^a (J M) = 0$ or $\rho_{m,m}^a (J M) = 1$, i.e., if it is completely empty (the mode is not in the wave function) or completely occupied (each term of the CI expansion contains the mode). From Eq. (16) it follows that for any state of total angular momentum $J$ and projection $M = 0$, the modes $m$ and $-m$ of a multiplet $a$ have identical mode entropies, $S^n_m (J 0) = S^n_{-m} (J 0)$. A further
one-body entropy for seniority

entropies

h

entropy corresponds to a half-filled shell, just as for states

\( \nu \)

m

entangled. All other

modes with

m

are non-entangled. These statements can be directly veri-

fied by using the expression (23), but a physical explana-

tion can also be given. In the two-particle wave function

\( \Psi_{2j-1,2j}(j^2) \), e.g., the states

\( m = j \) and

\( m = j-1 \)

are occupied, while all other states are empty. Applying the

operator

\( \hat{S}_{1B}(n-2)^2 \) on this state leaves the states

\( m = j \)

and

\( m = j-1 \) occupied and their time reversed pairs,

\( m = -j \)

and

\( m = -j-1 \) empty, since

\( S_{n} \)

can populate time reversed pairs \( \{ \pm m \} \) only simultane-

ously [70]. As a consequence, the four modes

\( m \in \{ \pm j, \pm (j-1) \} \)

have vanishing one mode entropy. Similar arguments carry over to the modes

\( m \in \{ \pm j, \pm (j-2) \} \) in the state

\( \Psi_{2j-1,2j-2}(j^n) \).

VI. NUMERICAL RESULTS

The concept of seniority has proven useful for semi-

magic nuclei, where only one type of nucleon is active, and the seniority (i.e., the pseudospin \( S \)) turns out to be conserved with good accuracy. The seniority scheme of the 0f\(_{7/2}\) and 0g\(_{9/2}\) subshells, in particular, can be success-

fully applied to calcium isotopes [59, 63] and \( N = 50 \) isotopes [53], where the main prediction of the seniority model, namely that excitation energies are approximately independent of the particle number is fulfilled. As we now show, entanglement measures detect delicate structures in these correlated quantum states, which we can access through CI and DMRG calculations, and compare with the predictions of the seniority (SEN) model.

Numerical computations were carried out using the BIGSTICK code [70] and the nuclear shell module of the Budapest DMRG code [71]. The BIGSTICK code determines the reduced matrix elements

\[
\frac{1}{\sqrt{2K+1}} \langle \Psi_j | c_{v}^{\dagger} \otimes \tilde{c}_{w}^{\dagger} (K) | \Psi_j \rangle,
\]

from which we can construct the 1B-RDM and from those the mode entropies using Eq. (16). The DMRG code
Clearly, the four valence shell neutrons reside almost exclusively on the $\nu = 0$, $\nu = 0.02$, $\nu = 0.006$, and $(3.89, 0.07, 0.04, 0.005)$, respectively. The average occupation numbers take similar values for the $J = 2$ and $J = 4$ states of $^{44}$Ca, where a mixing with seniority $\nu = 4$ excitations is apparent.

We first determined the occupations $\sum_{m} \langle \Psi_{J} | c^\dagger_{am} c_{am} | \Psi_{J} \rangle$ of $^{44}$Ca for the yrast states $J = 0, 2$, and $4$ by using the interaction GXPF1 within a full CI approach. For the orbitals $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$, and $1p_{1/2}$ we obtain the ground state occupation numbers $(3.89, 0.06, 0.05, 0.01)$, while the occupation numbers of the $J = 2$ and $J = 4$ states read $(3.89, 0.08, 0.02, 0.006)$ and $(3.89, 0.07, 0.04, 0.005)$, respectively. Clearly, the four valence shell neutrons reside almost exclusively on the $0f_{7/2}$ shell, and occupy the other three shells with very small probabilities. Interestingly, the average occupation numbers take similar values for the ground state and the $J = 2$ and $J = 4$ yrast states.

The CI / DMRG one-mode entropies of the $J = 4$ state of $^{44}$Ca can not be reproduced with a simple seniority $\nu = 2$ state and, similar to the $J = 4$ state of $^{94}$Ru, discussed later, a mixing of the $\nu = 2$ and $\nu = 4$ seniority states is needed to reproduce the observed pattern of $S_m$. We mention that no seniority $\nu = 4$ states exist for $^{45}$Ca and $^{46}$Ca, where the CI / DMRG results agree well with the SEN model predictions with $\nu = 0$ and $\nu = 2$ states only.

The seniority model predictions also agree well with the CI / DMRG results for odd calcium nuclei. To demonstrate this, let us consider the ground ($\nu = 1$) and first excited states ($\nu = 3$) of $^{43}$Ca. Increasing the neutron number from 22 to 23 modifies the ground state one-mode entropies as the seniority model predicts (see Fig. 5). The ground state of $^{43}$Ca has angular momentum $J = 7/2$. According to Section 4, in the $M = 7/2$ state of $^{44}$Ca, it is known that there is strong seniority mixing $^{33}$. We can determine the amplitudes of the seniority $\nu = 2$ and $\nu = 4$ components by maximizing the overlap between the CI and the mixed seniority state. By mixing seniority $\nu = 2$ and $\nu = 4$ states appropriately, we can increase the overlap with the $J = 4$ $^{44}$Ca state to 0.953.

The precise seniority content of the states and seniority mixing can be further verified by investigating the mode entropies, displayed in Fig. 2 for $^{44}$Ca. Clearly, comparison of the CI / DMRG and SEN one-mode entropies confirms that the ground and $J = 2, 6$ states of $^{44}$Ca are seniority-zero and seniority-two states, respectively. As discussed in Section 5, the mode entropies are supposed to reach their maximal value $\ln 2$ in the seniority-zero $J = 0$ state of a half-filled shell. This prediction is indeed very well satisfied according our full CI / DMRG calculations in the ground state of $^{44}$Ca. Mode entropies are, however, reduced by pair breaking. In particular, in the $J = 6$ yrast state, the pair-broken neutrons occupy the $m = 7/2$ and $m = 5/2$ states, and the mode entropy of the states $m = \pm 7/2$ and $m = \pm 5/2$ is indeed close to zero.
The ground state and yrast states of \( \nu = 4 \) states of the configuration \( \{ 9/2 \} \) are special seniority \( \pi = 2 \) shell SEN wave function has a particle-hole symmetry – a characteristic property of the single shell SEN model – is just approximate.

B. Entanglement in \( ^{94}\text{Ru} \) nucleus

As a next example, we consider the nucleus \( ^{94}\text{Ru} \) among the \( N = 50 \) isotones. In case of \( N = 50 \) isotones, coupling within the \( 0g_{9/2} \) proton subshell is expected to dominate, but contribution from nearby orbitals may also play a role. In a \( 0g_{9/2} \) shell-based seniority model, the seniority quantum number is not enough to uniquely distinguish between states with identical total angular momentum. In particular, seniority \( \nu = 4 \) states with angular momenta and parity \( J^\pi = 4^+ \) and \( 6^+ \) are not uniquely defined since they both span two-dimensional subspaces \([49]\). As noticed in \([56, 58]\), there are special seniority \( \nu = 4 \) states with quantum numbers \( J^\pi = 4^+ \) and \( 6^+ \), which have ‘good seniority’ for any interaction, i.e. states, which are eigenvectors of both seniority conserving and seniority mixing Hamiltonians, when restricted to the \( 0g_{9/2} \) shell. These states are called solvable \([62]\) or \( \alpha \) states \([61]\), and they do not mix directly (i.e., in first order) with other seniority \( \nu = 2 \) or seniority \( \nu = 4 \) states of the configuration \((9/2)^4\).

In the CI / DMRG description, we used the \( 0f_{5/2}, 1p_{3/2}, 1p_{1/2}, \) and \( 0g_{9/2} \) sp orbitals to span the shell model’s active space, and a \( ^{56}\text{Ni} \) nucleus as a core. The one mode entropies were computed for the ground state, \( J^\pi = 0^+ \), and the yrast states \( J^\pi = 2^+, 4^+, 6^+, \) and \( 8^+ \). For the nucleon-nucleon interaction we used the so-called jun45 force \([74]\), and the lisp interaction \([75]\).

The CI wave functions contain sixteen protons, whereas the single \( j = 9/2 \) shell SEN wave function has only four. To compare these two wave functions, we extend the SEN model by simply building on the top of closed \( 1p_{1/2}, 1p_{3/2}, \) and \( 0f_{5/2} \) shells as

\[
\Phi_{g9/2}|p_{1/2}^4 p_{3/2}^4 f_{5/2}^6 \rangle ,
\]

\[ (31) \]
with the operator $\hat{\Psi}_{g_9/2}$ creating a four-particle state $\Psi_{g_9/2}$ within the $0g_{9/2}$ shell. We refer to seniority states of this form as CI-SEN states or "seniority-like" shell model configurations in the following. Clearly, the one mode entropies associated with the filled $1p_{3/2}$, $1p_{1/2}$, and $0f_{5/2}$ shells vanish, while the mode entropies of the $0g_{9/2}$ orbitals in a CI-SEN state are identical to those of the corresponding four-particle $j = 9/2$ SEN state.

To quantify the seniority content of a CI wave function, we calculate the square of the modulus of the overlap of the CI wave function and a given CI-SEN state, i.e., the overlap probabilities. Results are listed in Table I. For $J^\pi = 4^+$ and $J^\pi = 6^+$, Table I includes overlaps with the aforementioned solvable or $\alpha$ states and with the $\beta$ states. The $\Psi_{JM}(J^4 \beta)$ states are four-particle seniority-four states with $J = 4, 6$ such that they are orthogonal to the corresponding solvable states. In all cases, seniority-four states are slightly mixed in, and the optimal overlap is reached with a state

$$|\Psi_{\text{mixed}}\rangle = \sum_{\nu,\eta} v_{\nu\eta} \hat{\Psi}_{JM}(J^4 \nu\eta) |p_{1/2}^4 p_{3/2}^4 f_{5/2}^6\rangle.$$  \hspace{1cm} (32)

In most cases, similar to the Ca isotopes, the seniority $\nu = 0$ and $\nu = 2$ states dominate, and the contribution of seniority $\nu = 4$ states is negligible. An exception is the state with $J^\pi = 4^+$ computed by using the jun45 interaction, where the contribution of the seniority-four $\alpha$ state is significant. Since the overlap with the $\beta$ state turns out to be very small, mixing calculations for states of the form (32) presented in Table I have been restricted to solvable (\alpha) states only.

In the $4^+$ state, the jun45 interaction generates strong seniority mixing, and the square of the modulus of the overlap of the CI wave function and the seniority mixed CI-SEN state is maximal for the amplitudes $|\nu_2|^2 = 0.593$, $|\nu_{4a}|^2 = 0.407$. This observation agrees with the results of Ref. [61], where it was shown that these properties of the jun45 wave function can explain the observed $E2$ transition probabilities of $^{94}$Ru.

We emphasize that the mixing of the states $\hat{\Psi}_{JM}(J^4 \beta)$ of the seniority mixed CI-SEN state is maximal for the amplitudes $|\nu_2|^2 = 0.593$, $|\nu_{4a}|^2 = 0.407$. This observation agrees with the results of Ref. [61], where it was shown that these properties of the jun45 wave function can explain the observed $E2$ transition probabilities of $^{94}$Ru.

![FIG. 5: Ground state mode entropies of $^{94}$Ru sp orbitals obtained by CI / DMRG with the jun45 interaction (symbols, dashed lines), compared with the SEN model prediction (black continuous line).](image1)

![FIG. 6: Mode entropies of the sp orbital $0g_{9/2}$ in the yrast excited states of $^{94}$Ru, constructed using full CI and DMRG with the jun45 interaction (red squares), and compared with seniority $\nu = 2$ states of the SEN model (black continuous lines).](image2)
tions can, however, mix the seniority-two and seniority-four components due to the presence of other shells [61].

As we have seen, the CI wave functions are reasonably well described in terms of mixed CI-SEN states. Particle number fluctuations on the $1p_{3/2}$, $1p_{1/2}$, and $0f_{5/2}$ shells are, however, non-negligible, and these shells are thus not completely filled. This is clearly shown by the ground state mode entropies, displayed in Fig. 5. Since the ground state has quantum numbers $J^\pi = 0^+$, mode entropies are independent of the magnetic quantum number $m$ in this case within any shell. The CI / DMRG mode entropies in the $0g_{9/2}$ shell are almost identical to those of the CI-SEN model. However, the mode entropies of the $1p_{3/2}$, $1p_{1/2}$, and $0f_{5/2}$ shells are relatively large in the CI / DMRG calculations, implying that these shells have substantial proton number fluctuations, induced by nucleon-nucleon interactions. Indeed, the mode entropies are directly related to the occupation probabilities of these modes, numerically computed as $P_{m,3/2} = 0.8884$, $P_{m,5/2} = 0.9749$, and $P_{m,1/2} = 0.7502$ by using the jun45 interaction.

Mode entropies of the yrast states obtained using the jun45 interaction are shown in Fig. 6 and compared with the predictions of the SEN model using seniority $\nu = 2$ states only (no seniority mixing). We display only mode entropies for the sp state, $0g_{9/2}$. The two models give similar patterns for the one-mode entropies, and the quantitative agreement is also satisfactory except for the $4^+$ state, where the non-mixing SEN model has a somewhat larger deviation with respect to CI and DMRG computations.

As shown in Fig. 7, neither the seniority-two SEN model, nor the seniority-four solvable state can explain the shape of the one mode entropies of the CI and DMRG computations. One must use the seniority mixed CI-SEN wave function to obtain a better agreement, and indeed, the optimal mixing amplitude $|v_2|^2 = 0.723$, $|v_4,\alpha|^2 = 0.277$ produces a quite satisfactory agreement. The remaining relatively small discrepancies between the two calculations can be attributed to the fact that the full CI / DMRG wave states contain, of course, excitations and configurations beyond the CI-SEN components.

VII. SUMMARY

In this work, we analyzed the entanglement structure of the open shells of certain semi-magic nuclei, and compared the observed structures with the predictions of a single-$j$ shell seniority (SEN) model.

We first derived analytical expressions for the one-body reduced density matrix within the SEN model for states with seniority zero, one, two, and three. We determined the particle number dependence of the one-body reduced density matrix for arbitrary seniority, and we have shown that, within the $j^n$ configuration space, wave functions of angular momentum $J = 0$ have maximal one-body entanglement entropy, irrespective of the seniority. Breaking Cooper-pairs, and aligning the angular momenta of the pair-broken nuclei reduces the one-body entropy, and the one-body entropy is found to decrease with increasing $J$ for a given nucleus.

The seniority model predicts peculiar properties for half-filled shells, also manifest in entanglement measures. For seniority-zero and seniority one states, the one-body entanglement entropy is maximal for a half-filled shell, $n = (2j + 1)/2$. Also, in the seniority model, the entropy displays particle-hole symmetry: $n$-particle and $n$-hole $(2j + 1 - n)$ particle states are predicted to have identical one-body entanglement entropies.

We carried out full CI and numerical density matrix renormalization group (DMRG) calculations for $^{42}$Ca, ..., $^{46}$Ca, isotopes and for $^{94}$Ru, and compared the numerical results with the predictions of the corresponding $(0f_{7/2})$ and $(0g_{9/2})$ shell seniority models. Mode entropies show an overall good agreement for the ground and yrast states with a few exceptions, where clear signatures of seniority mixing are observed.

We first verified the predictions of the seniority model for Ca isotopes. For all even isotopes ($^{42}$Ca, $^{44}$Ca, and $^{46}$Ca), the one-body entanglement entropy is maximal in the $J = 0$ ground state, and decreases with increasing $J$. As predicted by the seniority model, for a given $J$, one-body entanglement is maximal for a half-filled shell ($^{42}$Ca), and an approximate particle-hole symmetry is observed between the $^{42}$Ca and $^{46}$Ca isotopes. The breaking of particle-hole symmetry can be attributed to neutron number fluctuations on deeper shells, which have fractional occupations and, correspondingly, exhibit sizable one-body entropies.

The full CI / DMRG wave functions of the ground
and yrast states have large overlaps with seniority-like $(0f_{7/2})^4$ configurations, with the dominant components having seniority $\nu = 0$ (for $J = 0^+$) and $\nu = 2$ (for $J = 2$ and $J = 6$). In case of the $J = 4$, yrast state of $^{44}$Ca, however, strong mixing is observed with the $\nu = 2$ and $\nu = 4$ states. This mixing, generated by neutron number fluctuations on other shells, turns out to be essential to explain the fine structures of mode entanglement.

A similar mixing pattern is observed in $^{94}$Ru, where the full CI wave functions of the ground and yrast states are found to have large overlaps with seniority-like $(0g_{9/2})^4$ configurations. The dominant components have also seniority $\nu = 0$ (for $J^z = 0^+$) or $\nu = 2$ (for $J^z = 2^+$ and $J^z = 6^+$). Similar to $^{44}$Ca, however, the $4^+$ yrast state of $^{94}$Ru displays strong seniority mixing with the so-called solvable seniority $\nu = 4$ state (or $\alpha$ state). Similar to the neutron shells of Ca, the $1p_{1/2}$, $1p_{3/2}$, and $0f_{5/2}$ proton shells exhibit sizable one-body entropies, and display corresponding fractional occupations. Our findings are in line with earlier observations\textsuperscript{[21]} that mixing with the solvable seniority $\nu = 4$ state may be significant due to the presence of other, non seniority-like configurations, and is essential to explain the BE(2) transition probabilities of $^{94}$Ru.

Mode and one-body entropies are thus extremely useful tools to investigate the structure of quantum correlations in nuclei. Here we restricted our discussions to simple semi-magic nuclei, where the seniority model provides an appropriate analytical framework and reference point. Extending our approach to study quantum fluctuations and quantum correlations in generic, open shell nuclei represent exciting perspectives for future research.

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### Appendix A: Matrix elements of the 1B-RDM

Here we analytically calculate the matrix elements of the quasi-spin tensor operators $R_{m,-m'}$ and $R_{m,-m'}$, which has to be used in the reduction formula\textsuperscript{[20]} for states with $\nu = 0, 1, 2$.

Equation \textsuperscript{(20)} shows that we have to calculate matrix elements of the following operators:

\[
R^0_{0,m,-m'} = \frac{1}{\sqrt{2}} \left[ (-1)^{j_1 + m'} a_{j,m} a_{j,-m} - (-1)^{j_1 - m} \left( \delta_{m,m'} a_{j,-m}^\dagger a_{j,-m} \right) \right]
\]

and

\[
R^1_{0,m,-m'} = \frac{1}{\sqrt{2}} \left[ (-1)^{j_1 + m'} a_{j,m} a_{j,m'} + (-1)^{j_1 - m} \left( \delta_{m,m'} a_{j,m}^\dagger a_{j,-m} \right) \right].
\]

In the case of $\nu = 0$ according to the reduction formula\textsuperscript{[20]}, we need only the following matrix elements

\[
\langle 0 | R^0_{0,m,-m'} | 0 \rangle = -\delta_{m,m'} \frac{(-1)^{j_1 - m}}{\sqrt{2}}
\]

and

\[
\langle 0 | R^1_{0,m,-m'} | 0 \rangle = \delta_{m,m'} \frac{(-1)^{j_1 - m}}{\sqrt{2}}.
\]

Substituting the last two expressions into \textsuperscript{(20)}, we get\textsuperscript{[21]}

When the seniority is one, the corresponding wave function that enters into the reduction formula\textsuperscript{[20]} is

\[
\Psi_{J M}(j^1 1) = a_{j M}^\dagger |0\rangle.
\]

Simple calculation gives

\[
\langle \Psi_{J M}(j^1 1) | R^0_{0,m,-m'} | \Psi_{J M}(j^1 1) \rangle = \delta_{m,m'} \frac{(-1)^{j_1 - m}}{\sqrt{2}} \left( 1 - \delta_{-m,-M} - \delta_{m,M} \right)
\]

and

\[
\langle \Psi_{J M}(j^1 1) | R^1_{0,m,-m'} | \Psi_{J M}(j^1 1) \rangle = \delta_{m,m'} \frac{(-1)^{j_1 - m}}{\sqrt{2}} \left( 1 - \delta_{-m,-M} - \delta_{m,M} \right).
\]

Using these last two expressions and\textsuperscript{[20]}, we can derive\textsuperscript{[22]}

In order to calculate the 1B-RDM in the case of seniority equals to two, we have to determine the matrix
elements of the operators \( R_{m,-m'00} \) and \( R_{m,-m';10} \) between two-particle wave functions. The normalised two-body wave function with total angular momentum \( J \) and projection \( M \) is

\[
\Psi_{J,M}(j^2) = \frac{1}{\sqrt{2}} \sum_m C_{j,m,j,M}^J a_m^I a_M^I |0\rangle,
\]

where \( J = 2, 4, \ldots, 2j - 1 \). The building blocks are the matrix elements

\[
\langle \Psi_{J,M}(j^2) | a_m^I a_m' | \Psi_{J,M}(j^2) \rangle = \delta_{m,m'} 2 \left( C_{j,m,j,M}^J \right)^2
\]

which can be obtained with the use of the Wick theorem.

Finally from (A1), (A2) and (A8) we derive

\[
\langle \Psi_{J,M}(j^2) | R_{0;m,-m'}^0 | \Psi_{J,M}(j^2) \rangle = \delta_{m,m'}(-1)^{j-m} \frac{1}{\sqrt{2}} \left[ -2 \left( C_{j,m,j,M-M}^J \right)^2 + 2 \left( C_{j,-m-j,M+m}^J \right)^2 - 1 \right]
\]

(A9)

and

\[
\langle \Psi_{J,M}(j^2) | R_{0;m,-m'}^1 | \Psi_{J,M}(j^2) \rangle = \delta_{m,m'}(-1)^{j-m} \frac{1}{\sqrt{2}} \left[ -2 \left( C_{j,m,j,M-M}^J \right)^2 - 2 \left( C_{j,-m-j,M+m}^J \right)^2 + 1 \right]
\]

(A10)

If we use the equation (A9) and (A10) the reduction formula (20) we get the 1B-RDM in the form (23).

In order to calculate the 1B-RDM for seniority-three states first we rewrite the general expression (20) in the form

\[
\rho_{m',m}(J M, j^\nu \rho) = -\delta_{m,m'} \frac{1}{2} \left[ -A_{m,m}^\nu + A_{m,-m}^\nu - 1 \right]
+ \frac{m + 1}{m - 1} \left( -A_{m,m}^\nu - A_{m,-m}^\nu + 1 \right),
\]

where

\[
A_{m,m}^\nu = \langle \Psi_{J,M}(j^\nu \rho) | c_m^I c_m^I | \Psi_{J,M}(j^\nu \rho) \rangle
\]

(A11)

A general pure three-particle state can be written in the form (22)

\[
\Psi = \sum_{ijk} w_{ijk} c_i^J c_j^J c_k^J |0\rangle,
\]

where the coefficients \( w_{ijk} \) of the superposition are fully antisymmetric. Using the antisymmetry property of the coefficients \( w_{ijk} \) and the commutation relations of the creation operators we can get the following expression

\[
\langle \Psi | c_{j}^I c_p^I | \Psi \rangle = 18 \sum_{jk} w_{xjk} w_{yjk}.
\]

(A14)

A seniority-three state can be turned into the form

\[
\Psi_{J,M}(j^3 J_2) = \frac{1}{N} \left[ \left[ a^I \otimes [a^I \otimes a^I]^{(J_2)} \right]_M |0\rangle
+ A_3 \left[ [a^I \otimes a^I]^{(0)} \otimes a^I \right]_M |0\rangle \right),
\]

(A15)

where \( J_2 \) is even and positive and

\[
N = \left[ 1 + 2(2J_2 + 1) \left\{ \begin{array}{ccc} j & j & J_2 \\ j & J & J_2 \end{array} \right\} - 4\delta_{J_2} (2J_2 + 1) \right]^{1/2},
\]

(A16)

\[
A_3 = \frac{2\sqrt{2J_2 + 1}}{2j - 1} \delta_{J_2}.
\]

(A17)

Now we apply the general expression (A14) and after a lengthy but straightforward calculation get
\begin{align}
\langle \Psi | a_m^\dagger a_m^\dagger | \Psi \rangle &= \frac{\delta_{m,-M}}{\sqrt{N}} \left\{ \sum_a \left( C_{j,M,j-M,m,a}^{J,M} C_{j,m,j,a}^{J,m,M} + C_{j,M,j-M,m,a}^{J,M} C_{j,m,j,a}^{J,m,M} + C_{j,M,j-M,m,a}^{J,m,M} C_{j,m,j,a}^{J,M} + C_{j,m,j,a}^{J,m,M} C_{j,M,j-M,m,a}^{J,M} \right) \right. \\
&+ \left. \frac{2A_3}{\sqrt{2j+1}} \left[ 2(-1)^j m \left( C_{j,m,j-2j,0}^{J,m,M} C_{j,M,j-M,m,a}^{J,M} + C_{j,M,j-M,m,a}^{J,M} C_{j,m,j,0}^{J,m,M} + C_{j,m,j-2j,0}^{J,m,M} C_{j,M,j-M,m,a}^{J,M} + C_{j,m,j,a}^{J,m,M} C_{j,M,j-M,m}^{J,M} \right) \right. \\
&+ \left. \delta_{m,M} \sum_a (-1)^j - a \left( C_{j,m,j-2j,0}^{J,m,M} C_{j,M,j-M,m,a}^{J,M} + C_{j,M,j-M,m,a}^{J,M} C_{j,m,j,0}^{J,m,M} + C_{j,m,j-2j,0}^{J,m,M} C_{j,M,j-M,m,a}^{J,M} + C_{j,m,j,a}^{J,m,M} C_{j,M,j-M,m}^{J,M} \right) \right. \\
&+ \left. \frac{A_3^2}{2j+1} \left[ 2 + (2j-3)\delta_{m,M} - 2\delta_{m,-M} \right] \right\}. \tag{A18}
\end{align}

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