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Background: In quantum mechanics entanglement is the most striking phenomenon which has no counterpart in classical systems. Although, different approaches have already been developed to study correlations in the case of indistinguishable particles, the exploration of the so-called mode-entanglement is still in its initial stage in nuclear physics.

Purpose: Study of mode-entanglement in the seniority model, derivation of analytic formulas for the one-body reduced density matrix of states with seniority $\nu = 0,\ 1,\ 2,$ and $\nu = 3$, and also determination of the particle number dependence of the one-body reduced density matrix for arbitrary seniority. In addition, comparison of the predictions of the seniority model with the results of the shell model to gain insight into the structure and correlations of the ground and lowest yrast states.

Methods: In the seniority model the analytic results are calculated using the quasi-spin formalism. The numerical shell model calculations are carried out in the standard shell model framework using an inert core. The applied realistic effective interactions are derived earlier using the G-matrix formalism. The density matrix renormalization group method is also applied in order to directly calculate the mode entropies.

Results: In the seniority model simple analytical expressions are given for the mode entropies. The peculiar behavior of the half-filled shells and the seniority-zero states are revealed. Numerical results are presented for the lightest stable calcium isotopes and for ^{94}Ru nucleus.

Conclusions: For ^{94}Ru, the seniority model accounts for the $0g_{9/2}$ mode entropies, but seniority mixing is important for certain yrast states. Interaction induced quantum fluctuations decrease the occupation of the $0f_{5/2}$, $1p_{3/2}$ and $1p_{1/2}$ shells, and amount in non-negligible mode entropies on these shells, too, clearly outside the scope of the simple $(0g_{9/2})^4$ seniority model. The $0f_{7/2}$ shell based seniority model is more accurate for the Ca isotopes, but seniority mixing is substantial for some ^{44}Ca yrast states, too. Mode and one-body entanglement entropies are useful tools to investigate the structure of quantum correlations in nuclei.

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 [6–13], the algebraic approach based on the correlation between observables [14–21], descriptions relying on quantum correlations of particles [22–25] and some 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 mode entropy [9, 11]. The 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 (SEN) model [33] in nuclear physics, and by comparing its predictions for entanglement with detailed model calculations.

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Entanglement investigations are often performed in atomic physics [34, 35], quantum chemistry [31], and condensed matter physics [4] 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. Some studies are carried out in the traditional nuclear shell model framework [38–44] and in an *ab initio* no-core shell model [45].

In this paper, we study few nucleon states within the SEN model. This investigation can be considered as an extension of our previous study on the entanglement of angular-momentum coupled two-nucleon states [44] to relatively simple many-nucleon states. Mode entanglement and two-orbital correlations in wave functions restricted to seniority-zero electron pair states have also been studied in Ref. [46] 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.

The physical motivation behind the SEN model is the pairing phenomenon [33]. The SEN model can be considered as a first step to describe pairing correlations in nuclei and the notion of collective pairs is generalized in more sophisticated models such as the generalized seniority model (see, e.g., Refs. [47–49]). The SEN model is a classification of good angular momentum states of a single-j shell, with the seniority quantum number ν naturally interpreted as the number of unpaired particles.

From a mathematical viewpoint, the SEN model is an exactly solvable model describing n particles interacting via seniority conserving interaction, and possessing a dynamically broken SU(2) quasi-spin symmetry [50]. 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 SEN 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 quantum number-based classification is still quite often applied [51–55]. Therefore, proceeding along these lines, we compute in this work mode entropies within the SEN model, and compare its predictions with the results of density matrix renormalization group (DMRG) [56] and configuration interaction (CI) computations, performed for the lightest stable calcium isotopes and for ^{94}Ru. Both belong to the family of semi-magic nuclei. In the case of Ca, the proton shell is closed and relevant neutrons dominantly occupy the valence $0f_{7/2}$ shell, while in ^{94}Ru the neutron shell is closed, and the relevant $0g_{9/2}$ (open) proton shell hosts four protons. Low-lying excited states with even angular momentum can be interpreted in both cases as seniority $\nu = 2$ pair breaking states with an admixture of seniority $\nu = 4$ states.

It is important to mention that in the SEN model based on the $g_{9/2}$-shell there are two particular seniority $\nu = 4$ states [57–61] with total angular momentum four and six, which can be shown to be eigenstates of *any* two-body interaction restricted to the $g_{9/2}$-shell. These states play an essential role in the explanation of the seniority isomerism and electromagnetic transitions [62–66] and, as we shall see, they are also important from the perspective of entanglement.

The paper is organized as follows. We review the concept of mode-entanglement in Section II. The basic concepts of the SEN 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 stable calcium isotopes and ^{94}Ru nucleus are investigated by means of the CI method and a nuclear shell version of the DMRG method [41, 67], using realistic effective interactions. Results obtained by the CI and DMRG methods are compared with the predictions of the 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, $\mathcal{A}_A$ and $\mathcal{A}_B$, spanned by operators composed from the sets A and B, respectively. A pure fermionic state is separable with respect to this bipartition if and only if it is of the form [18]

$$\mathcal{P}(\{c_{i\in A}^\dagger\})\,\mathcal{Q}(\{c_{j\in B}^\dagger\})|0\rangle, \tag{1}$$

with $\mathcal{P}$ 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, Ψ.

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

$$\rho_k \equiv \begin{pmatrix} \langle c_k^\dagger c_k\rangle & 0 \\ 0 & 1-\langle c_k^\dagger c_k\rangle \end{pmatrix}, \tag{2}$$

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 mode entropy,

$$\mathcal{S}_k \equiv -\mathrm{Tr}(\rho_k \ln(\rho_k)) = h(\langle c_k^\dagger c_k\rangle), \tag{3}$$

with the function h defined as

$$h(x) \equiv -x\ln(x) - (1-x)\ln(1-x)\,.$$

The total correlation introduced as

$$\mathcal{S}_c = \sum_{k=1}^{d} \mathcal{S}_k \tag{4}$$

yields then a global characterization of the entanglement of the state Ψ [10], which depends, however, on the choice of sp basis, $\{c\}$. A basis independent measure, the one-body entanglement entropy is defined as [11, 27, 28]

$$\mathcal{S}_{\rm 1B} = \min_{\{c\}} \mathcal{S}_c \ . \tag{5}$$

By the measure $\mathcal{S}_{1B}$, all fermion states that can be described by a single Slater determinant are classified as non-entangled, while other pure states are entangled [11, 22, 24].

The quantity $S_{\rm 1B}$ is closely related to the eigenvalues of the one-body reduced density matrix (1B-RDM), defined as [77]

$$\rho_{i,j} = \langle \Psi | c_j^\dagger c_i | \Psi \rangle, \tag{6}$$

and normalized as Tr $\rho = n$, where n is the particle number. The basis where $\mathcal{S}_c$ reaches its minimum (*i.e.*, $\mathcal{S}_c = S_{\rm 1B}$) corresponds to the so-called natural orbitals, and there the 1B-RDM is diagonal, $\rho = {\rm diag}\{n_1, n_2, \ldots, n_d\}$ [11, 28]. There $\mathcal{S}_{\rm 1B}$ reads

$$\mathcal{S}_{\rm 1B} = \sum_{i=1}^{d} h(n_i), \tag{7}$$

where the n_i denote the occupation numbers of the natural orbitals.

III. SENIORITY MODEL: BASIC DEFINITIONS

In the SEN model [33], we assume that n identical nucleons occupy a single j shell, corresponding to a shell configuration j^n. For the sp states, we use the notation $|a, m\rangle = |n_a l_a j_a m\rangle$. In the SEN model, nucleons reside on a single multiplet, a. We can therefore suppress the label a and use the compact notations, $a^\dagger_{am} \to a^\dagger_m$ and $a_{am} \to a_m$ for the corresponding creation and annihilation operators.

The pair creation and annihilation operators, $S_\pm$, defined as

$$S_+ = \sum_{m>0} (-1)^{j-m} a^\dagger_m a^\dagger_{-m} \quad \text{and} \quad S_- = S_+^\dagger \tag{8}$$

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

$$S_0 = \frac{1}{2}\Big(\sum_m a^\dagger_m a_m - \frac{2j+1}{2} \Big) \ , \tag{9}$$

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

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

$$\psi_{JM}(j^n\, \nu\, \eta) = \mathcal{N}_{n,\nu}\, S_+^{(n-\nu)/2}\, \psi_{JM}(j^\nu\, \nu\, \eta) \tag{10}$$

has the same quasi-spin as $\psi_{JM}(j^\nu\, \nu\, \eta)$, but is an eigenstate of S_z with eigenvalue $-(j + \frac{1}{2} - n)/2$. The prefactor $\mathcal{N}_{n,\nu}$ here just ensures proper normalization. Clearly, instead of the quantum numbers n and ν, 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 $\Psi_{JMSS_z}(j\, \eta)$.

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

$$\Psi_{00}(j^n 0) = \mathcal{N}_{n,0}\, S_+^{n/2} |0\rangle. \tag{11}$$

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

$$\Psi_{jM}(j^n 1) = \mathcal{N}_{n,1}\, S_+^{(n-1)/2} a^+_M |0\rangle. \tag{12}$$

Seniority-two states have the form

$$\Psi_{JM}(j^n 2) = \mathcal{N}_{n,2}\, S_+^{(n-2)/2} \frac{1}{\sqrt{2}}\Big(\sum_m C^{J,M}_{j,m,\,j,M-m}\, a^\dagger_m a^\dagger_{M-m} \Big) |0\rangle, \tag{13}$$

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 [68, 69].

IV. ONE-BODY REDUCED DENSITY MATRIX

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

$$\rho^{a,a'}_{m,m'}(JM) = \langle \Psi_{JM} | a^\dagger_{a'm'} a_{am} | \Psi_{JM} \rangle \ . \tag{14}$$

Conservation of the z component of the angular momentum implies that all $m \neq m'$ off-diagonal elements of $\rho^{a,a'}_{m,m'}(JM)$ vanish. In the special case, $J = 0$, moreover,

simple group theoretical arguments imply $j_a = j_{a'}$ for non-zero matrix elements, and the non-zero elements of the 1B-RDM are independent from m

$$\rho^{a,a'}_{m,m'}(00) = \delta_{m',m}\delta_{j_{a'},j_a}\,\hat{\rho}^{aa'}(00)\ . \tag{15}$$

This immediately implies that in any $J = 0$ state the mode entropies do not depend on the magnetic quantum number m of the sp modes, as also observed numerically in Ref. [41] and proved in [44] for two-body problems.

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

$$\left[a^\dagger_{a'} \otimes \tilde{a}_a\right]^K_k = \sum_m C^{K,\,k}_{j_{a'},m,\,j_a,\,k-m}\, a^\dagger_{a',m}\tilde{a}_{a,k-m}\ ,$$

and express the 1B-RDM as

$$\rho^{a,a'}_{m,m'}(JM) = \delta_{m',m}\,(-1)^{j_a-m} \sum_K C^{K,0}_{j_{a'},m,\,j_a,-m}\langle\Psi_{JM}|\left[a^\dagger_{a'} \otimes \tilde{a}_a\right]^K_0|\Psi_{JM}\rangle. \tag{16}$$

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, $\rho_{m,m'}(JM, j^n\nu\,\eta)$, associated with the state $\Psi_{JM}(j^n\nu\,\eta)$ within the SEN model. We shall do that using the quasi-spin formalism [70], where we introduce a quasi-spin tensor of rank $\frac{1}{2}$ as

$$R^{\frac{1}{2}}_{\mu;m} = \begin{cases} a^\dagger_m & \text{if}\ \ \mu = 1/2\ , \\ -\tilde{a}_m & \text{if}\ \ \mu = -1/2\ . \end{cases} \tag{17}$$

From these we define quasi-spin tensors of rank $K = 0$ and $K = 1$ as [70]

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

The nucleon number dependence of the matrix element of the operator $a^\dagger_{m'}a_m$ can be determined by using the identity

$$a^\dagger_{m'}a_m = \frac{(-1)^{j+m}}{\sqrt{2}}\left(R^0_{0\,;\,m',-m} + R^1_{0\,;\,m',-m}\right)\ , \tag{19}$$

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

$$\langle\Psi_{JMSS_z}(j\,\eta)|a^\dagger_{m'}a_m|\Psi_{JMSS_z}(j\,\eta)\rangle = \delta_{m',m}\frac{(-1)^{j+m}}{\sqrt{2}} \Big\{C^{S,S_z}_{S,S_z,0,0}\langle\Psi_{JMS}(j\,\eta)\,\|\!\|\,R^0_{m,-m}\,\|\!\|\,\Psi_{JMS}(j\,\eta)\rangle + C^{S,S_z}_{S,S_z,1,0}\langle\Psi_{JMS}(j\,\eta)\,\|\!\|\,R^1_{m,-m}\,\|\!\|\,\Psi_{JMS}(j\,\eta)\rangle\Big\},$$

where $\|\!\|$ indicates the reduced matrix element in quasi-spin space. By using the explicit values of the Clebsch-Gordan coefficients and the relations between S, S_z, n, and ν, we obtain for $n > \nu$

$$\rho_{m,m'}(JM, j^n\nu\,\eta) = \delta_{m,m'}\tfrac{(-1)^{j+m}}{\sqrt{2}}\left[\langle\Psi_{JM}(j^\nu\nu\,\eta)|R^0_{0;\,m,-m}|\Psi_{JM}(j^\nu\nu\,\eta)\rangle + \tfrac{2(j-n)+1}{2(j-\nu)+1}\langle\Psi_{JM}(j^\nu\nu\,\eta)|R^1_{0;\,m,-m}|\Psi_{JM}(j^\nu\nu\,\eta)\rangle\right]\ . \tag{20}$$

This formula allows us to relate the 1B-RDM of a system of $n > \nu$ particles to that of a system of ν particles, both in states with seniority ν. Such a recurrence relation for matrix elements of operators is usual in the SEN model [33].

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 in 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)),

$$\rho_{m,m'}(00, j^n0) = \delta_{m',m}\ \frac{n}{2j+1}\ . \tag{21}$$

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,

$$\rho_{m,m'}(jM, j^n1) = \delta_{m',m}\begin{cases} 1 & \text{if}\quad m = M\ , \\ 0 & \text{if}\quad m = -M\ , \\ \frac{n-1}{2j-1} & \text{if}\quad |m| \neq |M|\ . \end{cases} \tag{22}$$

For seniority-two wave functions with $n > 2$, the 1B-RDM has the form

$$\rho_{m,m'}(JM, j^n2) = \delta_{m',m}\Big\{\left(C^{J,M}_{j,m,j,M-m}\right)^2 - \left(C^{J,M}_{j,-m,j,M+m}\right)^2 + \tfrac{1}{2} + \tfrac{2(j-n)+1}{2j-3}\Big[\left(C^{J,M}_{j,m,j,M-m}\right)^2 + \left(C^{J,M}_{j,-m,j,M+m}\right)^2 - \tfrac{1}{2}\Big]\Big\}, \tag{23}$$

where the total angular momentum is even and ranges from $J = 2$ to $J = 2j - 1$. In the case of $n = \nu = 2$ the formula is given in (A5) and (A9).

The complicated analytical form of the 1B-RDM is given in Appendix A for seniority-three states (see Eqs. (A3), (A5) and (A15)) .

V. ANALYTICAL RESULTS

We now discuss the consequences of the previous results from the perspectives of the mode and one-body entanglement entropies. Having constructed the 1B-RDM, we obtain the mode entropies by Eq. (3) as

$$\mathcal{S}^a_m(JM) = h\left(\rho^{a,a}_{m,m}(JM)\right). \tag{24}$$

A mode m of a multiplet a is therefore non-entangled if and only if $\rho^{a,a}_{m,m}(JM) = 0$ or $\rho^{a,a}_{m,m}(JM) = 1$, 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 the mode entropies of the state $\Psi_{J\,M}$ are related to those of the state $\Psi_{J\,-M}$ as $\mathcal{S}^a_m(J\,-M) = \mathcal{S}^a_{-m}(J\,M)$.

For states with $J = 0$ and fixed total parity, the one particle density matrix is diagonal in π, j, and m. Therefore, $S_c = \mathcal{S}_{1\mathrm{B}}$ if all involved multiplets have different parities or angular momenta.

States in the SEN model related by particle-hole transformation have identical one-body entanglement entropies. Particle-hole conjugation, is represented by a linear unitary operator, Γ, having the properties [70]

$$\Gamma\,\Psi_{JM}(j^n\nu\,\eta) = (-1)^{\frac{n-\nu}{2}}\,\Psi_{JM}(j^{2j+1-n}\nu\,\eta), \tag{25}$$

and

$$\Gamma^\dagger a^\dagger_m \Gamma = -\tilde{a}_m\ , \quad \Gamma^\dagger \tilde{a}_m \Gamma = a^\dagger_m\ . \tag{26}$$

From these relations one immediately obtains the relation $\rho_{\tilde{m},\tilde{m}}(JM, j^{2j+1-n}\nu\,\eta) = 1 - \rho_{m,m}(JM, j^n\nu\,\eta)$, with $\tilde{m} = -m$ referring to the time-reversed orbital. Since $h(1-x) = h(x)$, this immediately implies $\mathcal{S}_{-m}(JM, j^{2j+1-n}\nu\,\eta) = \mathcal{S}_m(JM, j^n\nu\,\eta)$, and the relation

$$\mathcal{S}_{1\mathrm{B}}(JM, j^{2j+1-n}\nu\,\eta) = \mathcal{S}_{1\mathrm{B}}(JM, j^n\nu\,\eta)\,, \tag{27}$$

where we introduced the notations $\mathcal{S}_m(JM, j^n\nu\,\eta)$ and $\mathcal{S}_{1\mathrm{B}}(JM, j^n\nu\,\eta)$ for mode and one-body entanglement entropies within the SEN model. Thus n-particle and n-hole states have the same one-body entanglement entropy.

For seniority $\nu = 0$ wave functions the 1B-RDM is diagonal (see Eq. (21)), and the mode entropy is mode independent, $\mathcal{S}_m = h(n/(2j+1))$. The one-body entanglement entropy is therefore

$$\mathcal{S}_{1\mathrm{B}}(00, j^n 0) = (2j+1)\,h\left(\tfrac{n}{2j+1}\right). \tag{28}$$

For seniority-zero states the largest $\mathcal{S}_{1B}$ therefore corresponds to a half-filled shell, $n = j + \frac{1}{2}$.

One may ask, which state is having the largest one-body entanglement entropy from all possible wave functions of a configuration j^n? It has been shown that the total correlation has its minimum value in the natural basis [11, 28], and the upper limit of the one-body entanglement entropy is reached when the 1B-RDM is proportional to the unit matrix, $\rho^{\max}_{m,m'} = \frac{n}{2j+1}\,\delta_{m',m}$ [44]. This criterion is satisfied by seniority-zero wave functions as well as by any $J = 0$ wave function, which are therefore *maximally entangled* states with respect to one-body entanglement.

Seniority $\nu = 1$ states must contain a broken pair, and are less entangled. Indeed, in the state $\Psi_{jM}(j^n 1)$ ($j > 1/2$), the modes with $m = \pm M$ are occupied or empty with probability one (see Eq. (22)), and are therefore non-entangled. All other $m \neq \pm M$ modes, – hosting the remaining $(n-1)/2$ pairs of particles, – have mode entropies $h((n-1)/(2j-1))$. We thus obtain the following one-body entanglement entropy for seniority $\nu = 1$ states,

$$\mathcal{S}_{1B}(jM, j^n 1) = (2j-1)\,h\Big(\tfrac{n-1}{2j-1}\Big)\,. \tag{29}$$

Thus for $\nu = 1$, too, the largest one-body entanglement entropy corresponds to a half-filled shell, just as for states with $\nu = 0$. Notice that $\mathcal{S}_{1B}(jM, j^n 1)$ is independent of M.

The one-body entanglement entropy for seniority $\nu = 2$ states is more complicated, in general. An interesting situation arises, however, if $j + \frac{1}{2}$ is an even number, $M = 0$, and we consider a half-filled shell, $n = j + \frac{1}{2}$. Then each mode is maximally entangled, $\mathcal{S}_m(J0, j^{j+1/2}\,2) = \ln 2$ since $\rho_{m,m}(J\,0, j^{j+1/2}\,2) = 1/2$, and $\mathcal{S}_{1\mathrm{B}}(J\,0, j^{j+1/2}\,2) = (2j+1)\,\ln 2$. We thus conclude that maximally one-body entangled states exist even with broken pairs, $\nu \neq 0$ and $J \neq 0$.

Typically, all modes are entangled to some degree in seniority-two states. Non-entangled modes can be observed, however, when the angular momentum has its maximal value, $J = 2j-1$, and $M = 2j-1$ or $M = 2j-2$. In the case $M = 2j-1$, the modes $m = j$ and $m = j-1$ and their time-reversed pairs, $m = -j$ and $m = 1-j$, are non-entangled, while for $M = 2j-2$ the modes $m = j$ and $m = j-2$ and their pairs, $m = -j$ and $m = 2-j$ become non-entangled. These statements can be directly verified for $n > 2$ by using the expression (23), but a physical explanation can also be given. In the two-particle wave function $\Psi_{2j-1,2j-1}(j^2\,2)$, e.g., the states $m = j$ and $m = j-1$ are occupied, while all other states are empty. Applying the operator $S_+^{(n-2)/2}$ 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_+ can populate time reversed pairs $\{\pm m\}$ only simultaneously. As a consequence, the four modes $m \in \{\pm j, \pm(j-1)\}$ have vanishing mode entropy [78]. This corollary is demonstrated later in Figs. 2 and 6 for

the $J = J_z = 6$ state of ^{44}Ca and for the $J = J_z = 8$ state of ^{94}Ru. Similar arguments carry over to the modes $m \in \{\pm j, \pm(j-2)\}$ in the state $\Psi_{2j-1,2j-2}(j^n 2)$.

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 quasi-spin 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 successfully applied to calcium isotopes [33, 71] and $N = 50$ isotones [33], where the main prediction of the SEN 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 SEN model. We always focus on states with maximal J_z i.e. $J_z = J$.

Numerical computations were carried out using the BIGSTICK code [72] and the nuclear shell module of the Budapest DMRG code [73]. The BIGSTICK code determines the reduced matrix elements

$$\frac{1}{\sqrt{2K+1}}\langle \Psi_J || \left[c_a^\dagger \otimes \tilde{c}_{a'}\right]^K || \Psi_J\rangle, \tag{30}$$

from which we can construct the 1B-RDM and from those the mode entropies using Eq. (16).

In the numerical calculations harmonic oscillator sp basis is used. In our shell model calculations there is an inert core and a few subshells above it and we do not enforce any restrictions on the occupancy numbers of the sp orbits, thus our model can be called as complete-active-space method or full CI calculation for short.

The DMRG method provides solution on a cleverly selected truncated Hilbert space based on Schmidt decomposition, where the truncation on the Schmidt spectrum, so-called bond dimension, determines the accuracy of the calculation [41, 56]. In case if the full spectrum is used, i.e., no truncation is applied, the DMRG leads to the exact (full-CI) solution of the problem. In the corresponding figures the untruncated DMRG data are shown which is equivalent to the full CI solution. On the other hand, the advantage of the DMRG in the considered cases is that quantum information entropies can be easily calculated using the DMRG code since these quantities are directly accessible in the DMRG formalism.

A. Calcium isotopes

Seniority can be viewed as a quantum number that differentiates between states with the same total angular momentum in the configuration j^n. The simplest example is the configuration $(0f_{7/2})^4$, where there are two $J = 2$ and two $J = 4$ states with different seniorities

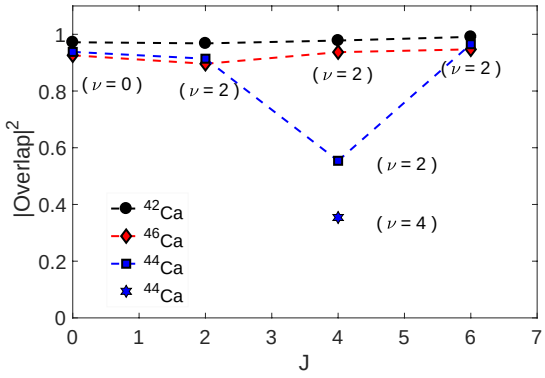

FIG. 1: Squared overlap of the CI and SEN model wave functions, as a function of the total angular momentum for ^{42}Ca, ^{44}Ca, and ^{46}Ca nuclei. Full CI calculations were performed with the GXPF1 interaction. The ground states and the yrast states are very well captured by $\nu = 0$ seniority and $\nu = 2$ seniority states, respectively, excepting the $J = 4$ state of ^{44}Ca, where a mixing with seniority $\nu = 4$ excitations is apparent.

$(\nu = 2, 4)$. According to Ref. [74], the ground and $J = 2$ yrast states of the nuclei ^{42}Ca, ^{44}Ca, ^{46}Ca are almost pure $(0f_{7/2})^n$ configurations, and the occupations of the other sp orbitals are negligible. In this subsection we study the mode-entanglement properties of the lightest stable calcium isotopes.

We first determined the occupations (subshells' particle numbers) $\sum_m \langle \Psi_{JJ}|c_{am}^\dagger c_{am}|\Psi_{JJ}\rangle$ of ^{44}Ca for the yrast states $J = 0, 2$, and 4 by using the interaction GXPF1 [75] 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.

More detailed information can be gained regarding correlations through the mode entropies of the sp orbitals or from the overlap of the CI wave functions with the SEN model states. Fig. 1 shows that all many-body eigenstates are essentially $\nu = 0$ or $\nu = 2$ states, with the sole exception of the $J = 4$ state of ^{44}Ca. In the case 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 square of 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 the SEN models' mode

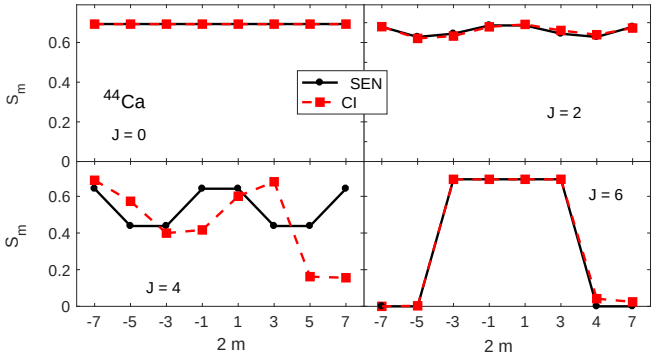

FIG. 2: Mode entropies of the sp orbital $0f_{7/2}$ for ^{44}Ca ground and yrast states. The results of CI and DMRG calculations performed with the GXPF1 interaction are compared with predictions of the SEN model (ground state $\nu = 0$, yrast states $\nu = 2$) .

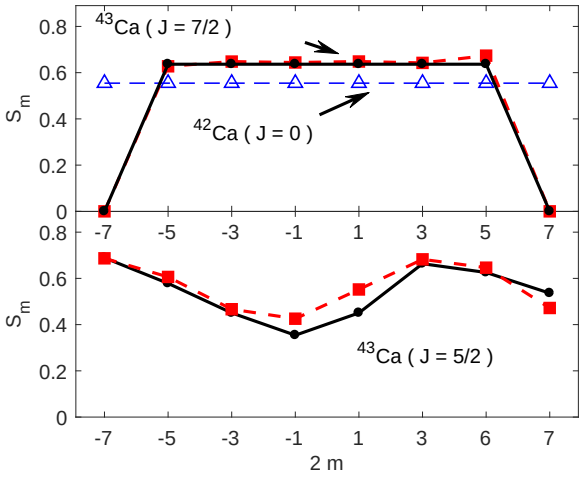

FIG. 3: Mode entropies of the sp orbital $0f_{7/2}$ in the $J = 7/2$ ground state of ^{43}Ca, and in its $J = 5/2$ yrast state, as determined by CI/DMRG calculations (red squares) and predicted by the SEN model (black continuous lines). As a reference, we also display the ground state entropies of ^{42}Ca (empty triangles).

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 V, the mode entropies are supposed to reach their maximal value $\ln 2 \approx 0.6931$ 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, may be 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 CI/DMRG 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 $\mathcal{S}_m$. We mention that no seniority $\nu = 4$ states exist for ^{42}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 SEN 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 mode entropies as the SEN model predicts (see Fig. 3). The ground state of ^{43}Ca has angular momentum $J = 7/2$. According to Section V, in the $M = 7/2$ seniority $\nu = 1$ state, only the modes $m = -7/2$ and $m = 7/2$ have $\mathcal{S}_m = 0$, while the occupation and entropy of the other modes slightly increases. The mode entropies of the excited $J^\pi = (5/2)^-$ state are also well captured by the $\nu = 3$ SEN model state. From Figs. 2 and 3 we thus conclude that mode entropy can be used as a sensitive tool to characterize the seniority structure of the ground state and low lying excitations.

We close this subsection by presenting the total correlations and the basis independent one-body entanglement entropies for the ground and yrast states of ^{42}Ca, ^{44}Ca, and ^{46}Ca in Fig. 4. The one-body entanglement entropy is obtained after diagonalizing the 1B-RDM, and using the natural orbitals as a basis. The total correlation computed using the original orbitals provides a very good estimate for $\mathcal{S}_{1B}$, indicating that mixing with other orbitals is rather small. This is only slightly lowered if we use the basis of natural orbitals, where the total correlation $\mathcal{S}_c$ coincides with $\mathcal{S}_{1B}$. If natural orbitals are used for ^{42}Ca, the $J = J_z = 6$ state is described by one Slater determinant, and so $S_{1B} = 0$.

For a given isotope, the ground state has the largest

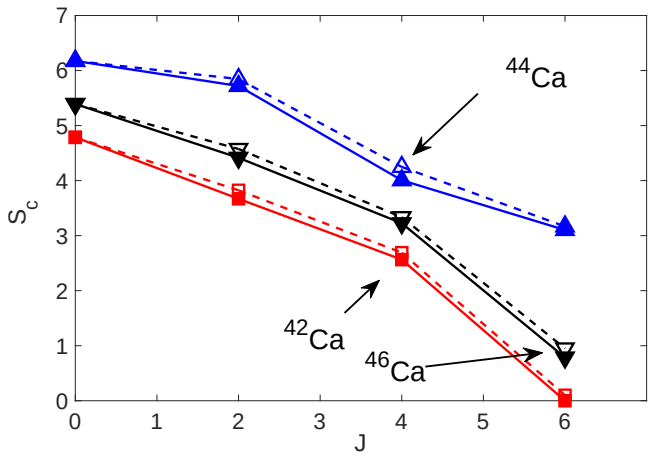

FIG. 4: Total correlations (dashed lines, empty symbols) and one-body entanglement entropies (continuous lines, filled symbols) as a function of total angular momentum for ground and yrast states of the nuclei ^{42}Ca, ^{44}Ca, and ^{46}Ca. Full CI/DMRG calculations were carried out with the GXPF1 interaction.

one-body entanglement entropy. Excited states contain broken Cooper-pairs, and are less and less entangled with increasing J. This latter trend follows from the general entanglement structure of spin states: two coupled spins tend to be most entangled in the smallest, 'antiferromagnetic' spin state, while they are completely unentangled in the largest, 'ferromagnetic' spin state. In the $J = 0$ ground states, $\mathcal{S}_{1B}$ and $\mathcal{S}_c$ agree with each other. Also, for a fixed J, the one-body entanglement entropy is maximal for a half-filled shell , i.e. for ^{44}Ca. This is predicted by the SEN model for seniority-zero and one states. The one-body entanglement entropies of ^{42}Ca and ^{46}Ca follow very similar lines, but they are not identical, as particle-hole symmetry would imply. This deviation from the prediction of the SEN model signals again that particle-hole symmetry – a characteristic property of the single shell SEN model – is just approximate.

B. Entanglement in ^{94}Ru nucleus

As a next example, we consider the nucleus ^{94}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 SEN 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 [50]. As noticed in [57, 59], there are special seniority $\nu = 4$ states with quantum numbers $J^\pi = 4^+$ and 6^+, which are eigenvectors of both seniority conserving and seniority mixing Hamiltonians, when restricted to the $0g_{9/2}$ shell. These states are called solvable [63] or α states [62], 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}Ni nucleus as a core. The 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 [76].

The CI wave functions contain sixteen protons, whereas the single $j = 9/2$ shell SEN wave functions have only four. To compare these two types of wave functions, we extend the SEN model by simply building on the top of closed $1p_{1/2}^2$, $1p_{3/2}^4$, and $0f_{5/2}^6$ shells as

$$\hat{\Psi}_{JM}(j^4\nu\eta)|p_{1/2}^2\, p_{3/2}^4\, f_{5/2}^6\rangle\ , \qquad (31)$$

with the operator $\hat{\Psi}_{JM}(j^4\nu\eta)$ creating a four-particle SEN state $\Psi_{JM}(j^4\nu\eta)$ 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 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.

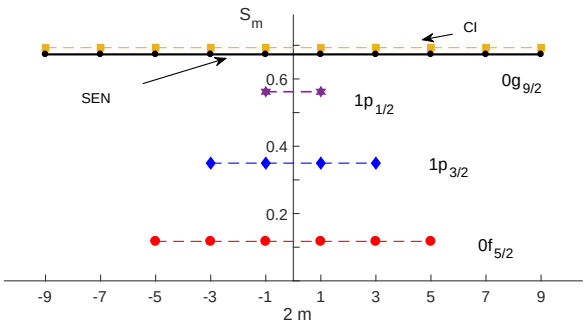

FIG. 5: Ground state mode entropies of ^{94}Ru sp orbitals obtained by CI/DMRG (symbols, dashed lines), compared with the SEN model prediction (black continuous line).

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 square of the modulus of the overlaps with the aforementioned solvable or α states and with the β states. The $\Psi_{JM}(j^4 4\,\beta)$ 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

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

In most cases, similar to the Ca isotopes, the seniority $\nu = 0$ and $\nu = 2$ states dominate, and the contribution

J^π	model	P
0^+	$\Psi_{00}(j^4 0)$	0.517
	$\Psi_{00}(j^4 4)$	2.1×10^{-4}
2^+	$\Psi_{22}(j^4 2)$	0.633
	$\Psi_{22}(j^4 4)$	9.4×10^{-5}
4^+	$\Psi_{44}(j^4 2)$	0.416
	$\Psi_{44}(j^4 4\,\alpha)$	0.277
	$\Psi_{44}(j^4 4\,\beta)$	5.5×10^{-4}
	mix	0.692
6^+	$\Psi_{66}(j^4 2)$	0.646
	$\Psi_{66}(j^4 4\,\alpha)$	2.2×10^{-4}
	$\Psi_{66}(j^4 4\,\beta)$	6.1×10^{-4}
8^+	$\Psi_{88}(j^4 2)$	0.657
	$\Psi_{88}(j^4 4)$	4.0×10^{-5}

TABLE I: Square of the modulus of the overlap of different CI-SEN states with the CI wave functions ($P = |\langle\Psi_{CI}|\Psi_{CI-SEN}\rangle|^2$).

of seniority $\nu = 4$ states is negligible. An exception is the state with $J^\pi = 4^+$, where the contribution of the seniority-four α state is significant. Since the overlap with the β state turns out to be very small, mixing calculations for states of the form (32), presented in Table I, have been restricted to the solvable (α) state only.

In the 4^+ state, the 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 when the square of the amplitudes are $|v_2|^2 = 0.593$, $|v_{4,\alpha}|^2 = 0.407$. This observation agrees with the results of Ref. [62], where it was shown that these properties of the wave function calculated by the jun45 interaction can explain the observed E2 transition probabilities of ^{94}Ru.

We emphasize that the mixing of the states $\hat{\Psi}_{JM}(j^4 2)|0\rangle$ and $\hat{\Psi}_{JM}(j^4 4\alpha)|0\rangle$ is not possible if interactions are strictly restricted to the $j = 9/2$ shell. Interactions can, however, mix the seniority-two and seniority-four components due to the presence of other shells [62].

As we have seen, the CI wave functions are reasonably well described in terms of mixed CI-SEN states. Subshell particle number fluctuations on the $1p_{3/2}$, $1p_{1/2}$, and $0f_{5/2}$ subshells are, however, non-negligible, and these subshells 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. The slightly increased value of the CI result is due to proton excitations to the $0g_{9/2}$ shell from the lower ones. However, the mode entropies of the $1p_{3/2}$, $1p_{1/2}$, and $0f_{5/2}$ subshells are relatively large in the CI/DMRG calculations, implying that these subshells have considerable subshell 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 $P_{m,9/2} = 0.5096$, $P_{m,3/2} = 0.8884$, $P_{m,5/2} = 0.9749$, and $P_{m,1/2} = 0.7502$.

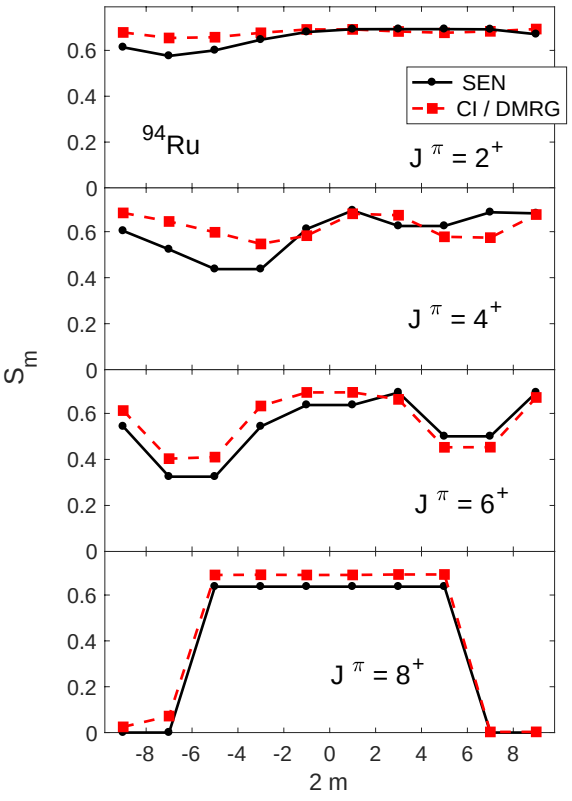

FIG. 6: Mode entropies of the sp orbital $0g_{\frac{9}{2}}$ in the yrast excited states of ^{94}Ru, constructed using full CI and DMRG (red squares), and compared with seniority $\nu = 2$ states of the SEN model (black continuous lines).

Mode entropies of the yrast states 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 orbital $0g_{9/2}$. The two models give similar patterns for the 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 state, nor the seniority-four solvable state can explain the shape of the 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 squares of the optimal mixing amplitudes $|v_2|^2 = 0.723$, $|v_{4,\alpha}|^2 = 0.277$ produce 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 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 generally reduces the one-body entanglement entropy, and the one-body entanglement entropy is found to decrease with increasing J for a given nucleus.

The SEN model predicts peculiar properties for half-filled shells, also manifest in entanglement measures. For

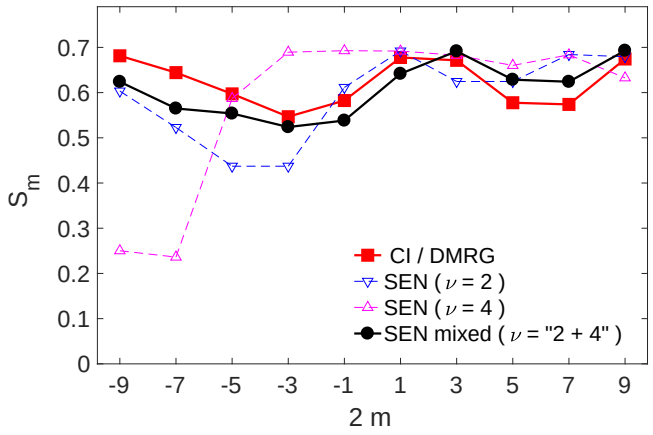

FIG. 7: Mode entropies of the ^{94}Ru sp orbital $0g_{9/2}$, calculated for the yrast state $J^\pi = 4^+$ using full CI/DMRG computations, and compared with the $0g_{9/2}$ shell SEN model. Mixing with the so-called α seniority-four state accounts for the observed structures, and is needed to yield satisfactory agreement.

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 SEN 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 numerical calculations by full CI and DMRG methods for ^{42}Ca, ^{43}Ca, ^{44}Ca, and ^{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 SEN 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 SEN model for Ca isotopes. For all even isotopes (^{42}Ca, ^{44}Ca, and ^{46}Ca), the one-body entanglement is maximal in the $J = 0$ ground state, takes a value very close to the one predicted by the SEN model, and decreases with increasing J. As predicted by the SEN model, for $\nu = 0, 1$, one-body entanglement is maximal for a half-filled shell (^{44}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 the subshells' neutron-number fluctuations; subshells have fractional occupations and, correspondingly, exhibit non-negligible mode entropies.

The full CI/DMRG wave functions of the ground and yrast states have large overlaps with seniority $(0f_{7/2})^4$ 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 turns out to be essential to explain the fine structures of mode-entanglement.

For ^{94}Ru, 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 $J^\pi = 0^+$) or $\nu = 2$ (for $J^\pi = 2^+$, $J^\pi = 6^+$, and $J^\pi = 8^+$). However, seniority mixing pattern is also observed in ^{94}Ru. Similarly to ^{44}Ca, the 4^+ yrast state of ^{94}Ru displays strong seniority mixing with the so-called solvable seniority $\nu = 4$ state (or α state). The $1p_{1/2}$, $1p_{3/2}$, and $0f_{5/2}$ proton shells exhibit sizable mode entropies, and display corresponding fractional occupations. Our findings are in line with earlier observations [62] that mixing with the solvable seniority $\nu = 4$ state may be significant due to the presence of other configurations, and is essential to explain the B(E2) transition probabilities of ^{94}Ru.

Mode and one-body entanglement 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 SEN model provides an appropriate analytical framework and reference point. Extending our approach to study quantum fluctuations and quantum correlations in generic, open shell nuclei represents exciting perspectives for future research.

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Appendix A: Matrix elements of the 1B-RDM in the seniority model

Here we calculate analytically the matrix elements of the quasi-spin tensor operators $R^0_{0;m',-m}$ and $R^1_{0;m',-m}$, used in the reduction formula (20) for states with $\nu = 0, 1, 2$, and $\nu = 3$.

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

$$R^0_{0;m',-m} = \frac{1}{\sqrt{2}}\left[(-1)^{j+m'}\left(\delta_{m',m} - a^\dagger_{-m}a_{-m'}\right) - (-1)^{j-m}a^\dagger_{m'}a_m\right] \tag{A1}$$

and

$$R^1_{0;m',-m} = -\frac{1}{\sqrt{2}}\left[(-1)^{j-m}a^\dagger_{m'}a_m + (-1)^{j+m'}\left(\delta_{m',m} - a^\dagger_{-m}a_{-m'}\right)\right]. \tag{A2}$$

In order to simplify the calculations, we rewrite first the general expression (20) with the help of (A1) and (A2) in the form

$$\rho_{m,m'}(JM, j^n\nu\eta) = \tfrac{1}{2}\delta_{m,m'}\left[1 - A^{\nu,\eta}_{-m,-m} + A^{\nu,\eta}_{m,m} + \tfrac{2(j-n)+1}{2(j-\nu)+1}\left(A^{\nu,\eta}_{m,m} + A^{\nu,\eta}_{-m,-m} - 1\right)\right], \tag{A3}$$

where $n > \nu$ and

$$A^{\nu,\eta}_{m,m} = \langle\Psi_{JM}(j^\nu\nu\eta)|a^\dagger_m a_m|\Psi_{JM}(j^\nu\nu\eta)\rangle. \tag{A4}$$

For $n = \nu$ we can write

$$\rho_{m,m'}(JM, j^\nu\nu\eta) = \delta_{m,m'}A^{\nu,\eta}_{m,m}. \tag{A5}$$

For seniority-zero states we need $\langle 0|a^\dagger_m a_m|0\rangle$ and so

$$A^0_{m,m} = 0. \tag{A6}$$

When the seniority is one, the wave function in (A4) is $\Psi_{jM}(j^1 1) = a^\dagger_{jM}|0\rangle$ and we have

$$A^1_{m,m} = \delta_{m,M}. \tag{A7}$$

The normalised two-body wave function with total angular momentum J and projection M is

$$\Psi_{JM}(j^2 2) = \frac{1}{\sqrt{2}}\sum_m C^{J,M}_{j,m,j,M-m}a^\dagger_m a^\dagger_{M-m}|0\rangle, \tag{A8}$$

where $J = 2, 4, \ldots, 2j-1$. Substituting (A8) into (A4) we get

$$A^2_{m,m} = 2\left(C^{J,M}_{j,m,j,M-m}\right)^2. \tag{A9}$$

If we use Eqs. (A6), (A7), and (A9) in (A3) and in (A5), we can recover the results in (21), (22), and (23).

The general form [22] of a pure three-particle state is

$$\Psi = \sum_{ijk} w_{ijk}c^\dagger_i c^\dagger_j c^\dagger_k|0\rangle, \tag{A10}$$

where the coefficients w_{ijk} are fully antisymmetric. Using the antisymmetric property of the coefficients w_{ijk} and the anticommutation relations of the fermionic operators, we can get the following expression

$$\langle\Psi|c^\dagger_x c_y|\Psi\rangle = 18\sum_{jk} w^*_{xjk}w_{yjk}. \tag{A11}$$

A seniority-three state can be turned into the form [68, 69]

$$\Psi_{JM}(j^3 3J_2) = \tfrac{1}{\mathcal{N}}\left(\left[a^\dagger\otimes\left[a^\dagger\otimes a^\dagger\right]^{J_2}\right]^J_M|0\rangle + A_3\left[\left[a^\dagger\otimes a^\dagger\right]^0\otimes a^\dagger\right]^J_M|0\rangle\right), \tag{A12}$$

where J_2 is even and positive and

$$\mathcal{N} = \left[2 + 4(2J_2+1)\begin{Bmatrix} j & j & J_2\\ j & J & J_2\end{Bmatrix} - \frac{8\delta_{j,J}(2J_2+1)}{(2j+1)(2j-1)}\right]^{\frac{1}{2}}, \tag{A13}$$

$$A_3 = \frac{2\sqrt{2J_2+1}}{2j-1}\delta_{j,J}. \tag{A14}$$

Now we apply the general expression (A11) and after a lengthy but straightforward calculation get

$$\begin{aligned} A^{3,J_2}_{m,m} &= \frac{2}{\mathcal{N}^2}\Bigg\{\sum_a\left(C^{J,M}_{j,M-m-a,J_2,m+a}C^{J_2,m+a}_{j,m,j,a} + C^{J,M}_{j,m,J_2,M-m}C^{J_2,M-m}_{j,a,j,M-m-a} + C^{J,M}_{j,a,J_2,M-a}C^{J_2,M-a}_{j,M-m-a,j,m}\right)^2 \\ &+ \frac{2A_3}{\sqrt{2j+1}}\Bigg[2(-1)^{j-m}\left(C^{J,M}_{j,M,J_2,0}C^{J_2,0}_{j,m,j,-m} + C^{J,M}_{j,m,J_2,M-m}C^{J_2,M-m}_{j,-m,j,M} + C^{J,M}_{j,-m,J_2,M+m}C^{J_2,M+m}_{j,M,j,m}\right) \\ &+ \delta_{m,M}\sum_a(-1)^{j-a}\left(C^{J,M}_{j,-a,J_2,m+a}C^{J_2,m+a}_{j,m,j,a} + C^{J,M}_{j,m,J_2,0}C^{J_2,0}_{j,a,j,-a} + C^{J,M}_{j,a,J_2,m-a}C^{J_2,m-a}_{j,-a,j,m}\right)\Bigg] \\ &+ \frac{A_3^2}{2j+1}\Bigg[2 + (2j-3)\delta_{m,M} - 2\delta_{m,-M}\Bigg]\Bigg\}. \end{aligned} \tag{A15}$$

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