Cluster properties of nuclear states in the modern shell model approach

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Abstract.   In this presentation we summarize our progress in the study of α-clustering in the shell model configuration interaction approach. We put forward Cluster-Nucleon Configuration Interaction Model where the study of clustering is facilitated by the SU(3) symmetry of the cluster channels and by Orthogonality Condition Model. Pioneering methods and results concerning α spectroscopic factors in sd-shell nuclei and in ^{16}O treated in p-sd shell are presented. Comparison with experimental data is in favor of the approach.

1. Introduction

Numerous theoretical techniques have been developed for addressing clustering phenomena in nuclei, and the present proceedings volume offers an exhaustive overview. However, many of these techniques focus on the structure of highly clustered nuclear states, often connecting them to experimental results using observables that are not directly related to clustering such as nuclear moments of inertia, quadrupole moments, gamma-transitions, etc. At the same time, a large body of experimental information concerning clustering, primarily α, is accumulated from measurements of spontaneous radioactivity, elastic scattering of composite particles, transfer and knock-out nuclear reactions. Recent results and rich prospects offered by the new thick ^{4}He target inverse kinematics elastic scattering techniques provide comprehensive experimental data on distribution of clustering strength in light nuclei; see Refs. [1–5] for example. This data shows both strongly and weakly clustered states, therefore a quantitative theoretical description of physics involving both nucleonic and cluster degrees of freedom is required.

   Magic- and light-cluster channels are distinguished by a specific – "elongated" – Elliott's SU(3) irreducible representations of the type $(n, 0)$. A symmetry-based approach to clustering is discussed in Ref. [6]. Weakly clustered states and single-nucleon dynamics, however, are better accessible in the microscopic shell model approach, where clustering questions have been pursued, Ref. [7–14]. In our contribution we put forward a technique that combines approaches in both directions: it is based on the shell model technique, and at the same time, takes into account the symmetry properties of cluster configurations. We implement large scale modern configuration interaction shell model with realistic effective Hamiltonians. It is a well established microscopic approach, where within the same formalism, a high quality description and good predictive power is achieved for numerous single-particle as well as collective nuclear properties [15-18]. In the nuclear shell model cluster degrees of freedom are not introduced explicitly. Thus, the emergence of clustering and interplay of cluster and single nucleon degrees of freedom can be

studied. Recent advances in computational techniques and exponential growth of computational power [15, 19, 20] facilitate work in this direction.

2. Formalism
Shell model configuration interaction approach and SU(3)-symmetric structures
In the shell model approach each many-nucleon state is built from the single-particle basis states as a linear combination of Slater determinants

$$|\Psi\rangle \equiv \Psi^\dagger|0\rangle = \sum_{\{1,2,3,\ldots A\}} \langle 1,2\ldots A|\Psi\rangle \, a_1^\dagger a_2^\dagger \ldots a_A^\dagger |0\rangle. \tag{1}$$

Here index $1 \equiv \{n,l,j,m\}$ denotes the single-particle j-scheme basis state built from the radial harmonic oscillator wave function (WF) $\varphi_{n_1,l_1}(r) \equiv \langle r|1\rangle \equiv \langle r|a_1^\dagger|0\rangle$; the operator $a_1^\dagger$ is the corresponding fermion creation operator in the second quantization; $\langle 1,2\ldots A|\Psi\rangle$ is the numeric coefficient determining the weight of each Slater determinant in the linear superposition (1).

In order to address clustering, multi-nucleon substructures related to a certain irreducible representation of the SU(3) group are constructed. In the present paper we discuss α-clustering. In the following, $\{\mathfrak{n}_i^{\alpha_i}\}$ denotes configuration where α_i is the number of particles in the major oscillator shell $\mathfrak{n}_i$; L, S, and T are orbital, spin, and isospin quantum numbers; (λ,μ) is the SU(3) Elliott's symbol; and the Young frame $[f]$ classifies the permutation symmetry. The four-nucleon states

$$|\Psi_{(n,0):L}\rangle \equiv \Psi_{(n,0):L}^\dagger|0\rangle \equiv |\{\mathfrak{n}_i^{\alpha_i}\}[f] = [4](n,0) : L, S = 0, T = 0\rangle \tag{2}$$

are constructed by diagonalization of some linear combination of the SU(3) Casimir operator of the second rank, L^2, T^2, S^2, and other operators as needed in the basis of four-nucleon shell-model states. The states (2) are normalized as $\langle\Psi_{(n,0):L}|\Psi_{(n,0):L}\rangle = 1$.

The advantage of the second quantization formalism implemented in the modern polymorphic configuration interaction techniques is the full correspondence between states $|\Psi\rangle$ and the creation and annihilation operators $\Psi^\dagger$ and Ψ. Thus, many-body overlap integrals needed to evaluate fractional parentage coefficients (FPCs)

$$\mathcal{F}_{nl} \equiv \langle\Psi_P|\hat{\mathcal{A}}\{\Psi_{(n,0):l}\,\Psi_D\}\rangle \equiv \langle 0|\Psi_P\{\Psi_{(n,0):l}\Psi_D\}^\dagger|0\rangle \tag{3}$$

can be readily computed between arbitrary states $|\Psi_P\rangle$ and $|\Psi_D\rangle$ of the type described in Eq. (1). Here $\hat{\mathcal{A}}$ is the antisymmetrization operator. Some examples of FPCs and channel norms for selected states with SU(3) symmetry are shown in Tab. 1. In the last column the channel norms are shown, which can be seen as a measure of bosonic enhancement. Indeed, if four-nucleon $L = 0$ operators $\Psi^\dagger$ and Ψ are thought of as boson creation and annihilation operators, then $\Psi\Psi^\dagger = 1 + N_b$, where N_b is the boson number operator. The numbers in the last column in Tab. 1 are less than 2, showing that four-nucleon configurations (2) are not true bosons. However, since larger shells can accommodate more "bosons" the non-bosonic effects are reduced and the norm gets closer to 2.

Cluster form factors and spectroscopic factors
The basic measure of clustering – cluster form factor (CFF), also commonly referred to as the spectroscopic amplitude – is defined as:

$$\phi_l(\rho') = \langle\Psi'_P|\hat{\mathcal{A}}\{\Psi'_D \frac{\delta(\rho - \rho')}{\rho^2} Y_{lm}(\Omega_\rho)\Psi'_\alpha\}\rangle, \tag{4}$$

where Ψ'_P, Ψ'_D, and Ψ'_α are internal, translationally invariant, free of the center of mass (c.m.) coordinate WFs of the parent (P) nucleus, the daughter (D) nucleus, and the α-cluster,

$\mathfrak{n}$	Ψ_P	Ψ	$\left| \langle \Psi_P | \Psi^\dagger | \Psi \rangle \right|^2$	$\langle \Psi | \Psi \Psi^\dagger | \Psi \rangle$
1	$(p)^8\,(0,4)$	$(p)^4\,(4,0)$	$1.42222^\star$	1.42222
2	$(sd)^8\,(8,4)$	$(sd)^4\,(8,0)$	0.487903	1.20213
3	$(fp)^8\,(16,4)$	$(fp)^4\,(12,0)$	0.292411	1.41503
4	$(sdg)^8\,(24,4)$	$(sdg)^4\,(16,0)$	0.209525	1.5278

Table 1. Fractional parentage coefficients and channel norms for selected SU(3) states. All WF and operators are $L = 0$. *For p-shell this result agrees with the value of $64/45 = 1.42222$ found in the literature [21].

respectively. Here and below we use primed notation to distinguish these WFs from those of the shell model type (1) that implicitly depend on the c.m. motion. The coordinate ρ is the Jacobi radial coordinate of the relative cluster-daughter motion; a proper coupling to a relative angular momentum l is established.

The CFFs are computed using the shell model approach. In our calculations the parent and daughter states are computed implementing Glockner-Lawson procedure [22] leading the c.m. motion being in the lowest oscillator state $\varphi_{00}(R)$. The oscillator frequency parameter in the WF depends, in the usual way, on the mass number. Of the WF $|\Psi_{(n,0):l}\rangle$, we are interested in the component where the c.m. of the α-particle is in the oscillator state $\varphi_{nl}(R_\alpha)$. We assume that the α-particle's WF is represented by the lowest four-nucleon oscillator function written through the Jacobi coordinates

$$|\Psi'_\alpha\rangle \equiv |(0s)^4[f] = [4](\lambda,\mu) = (0,0) : L = 0, S = 0, T = 0\rangle. \tag{5}$$

Then the component of interest, referred to as the cluster coefficient, is known analytically [8, 9, 23],

$$X_{nl}^{(\lambda 0)} \equiv \langle \Psi_{(\lambda,0):l} | \varphi_{nl}(R_\alpha)\,\Psi'_\alpha \rangle = \sqrt{\frac{1}{4^n} \frac{n!}{\prod_i (\mathfrak{n}_i!)^{\alpha_i}} \frac{4!}{\prod_i \alpha_i!}}. \tag{6}$$

By expanding the parent state using FPC (3) and by decoupling intrinsic and c.m. variables, the CFF in Eq. (4) is expanded in oscillator states as [7, 8, 9, 11]

$$\phi_l(\rho) = \sum_n \mathcal{C}_{nl}\,\varphi_{nl}(\rho), \quad \mathcal{C}_{nl} = X_{nl}\,\mathcal{F}_{nl}\,\mathcal{R}_n \quad \text{where} \quad \mathcal{R}_n = (-1)^n [(m_d + m_\alpha)/m_d]^{n/2}, \tag{7}$$

is a recoil factor that comes from recoupling the c.m. variables R_α and R_D into their relative coordinate ρ and the parent c.m. coordinate R_P.

Identifying the CFF in Eq. (7) with the observable spectroscopic factors (SFs) $\mathcal{S}_l = \sum_n |\mathcal{C}_{nl}|^2$ has been common in the literature. However, it was argued in Refs. [24, 25] that the matching of $\phi_l(\rho)$ with the two-body cluster-nucleus solution is not appropriate. Instead, one should use the channel WF in the form of Resonating Group Model or, for easier reduction to a two-body problem, in the form of Orthogonality Condition Model (OCM) [26]. Therefore, the CFF should be redefined as

$$f_l(\rho) \equiv \hat{\mathcal{N}}_l^{-1/2}\phi_l(\rho), \quad \text{where the norm operator} \quad \hat{\mathcal{N}}_l\phi_l(\rho) \equiv \int \mathcal{N}_l(\rho',\rho)\phi_l(\rho)\rho^2 d\rho \tag{8}$$

contains an overlap norm kernel

$$\mathcal{N}_l(\rho',\rho'') = \langle \hat{\mathcal{A}}\{\Psi'_D \frac{\delta(\rho - \rho')}{\rho^2} Y_{lm}(\Omega_\rho)\Psi'_\alpha\} | \hat{\mathcal{A}}\{\Psi'_D \frac{\delta(\rho - \rho'')}{\rho^2} Y_{lm}(\Omega_\rho)\Psi'_\alpha\}\rangle \tag{9}$$

The validity and importance of this new definition are discussed in details in Refs. [27, 28]. We construct and diagonalize the norm kernel operator as a matrix in the oscillator basis,

$$\langle \varphi_{n'l} | \hat{\mathcal{N}}_l | \varphi_{nl} \rangle = \mathcal{R}_{n'} \mathcal{R}_n X_{n'l} X_{nl} \langle \hat{\mathcal{A}} \{ \Psi_{(n',0):l} \, \Psi_D \} | \hat{\mathcal{A}} \{ \Psi_{(n,0):l} \, \Psi_D \} \rangle. \tag{10}$$

This leads to a new definition of the SF:

$$S_l \equiv \int \rho^2 d\rho \, |f_l(\rho)|^2 = \sum_k \frac{1}{N_{kl}} \left| \sum_n \langle kl | \varphi_{nl} \rangle \mathcal{C}_{nl} \right|^2, \tag{11}$$

where $|kl\rangle$ is an eigenvector and N_{kl} is the associated eigenvalue of the norm kernel $\hat{\mathcal{N}}_l |kl\rangle = N_{kl} |kl\rangle$, both corresponding to angular momentum l. In this form the SFs are normalized; for any given parent nucleus the sum of all SF for a given partial wave l and to a particular daughter state equals to the number of channels (characterized by different values of n in four-nucleon functions $\Psi_{(n,0):l}$) involved. In the one-channel case (such examples are considered in the next section) using the completeness of the parent states, $\sum_i |\Psi_{P_i}\rangle\langle\Psi_{P_i}| \equiv 1$, the single diagonal matrix element for the norm (10) can be expressed as

$$N_{nl} = \mathcal{R}_n^2 X_{nl}^2 \sum_i (\mathcal{F}_{nl}^i)^2 = \sum_i \mathcal{S}_l^i, \quad \text{thus} \quad S_l^i = \mathcal{S}_l^i / \sum_{i'} \mathcal{S}_l^{i'} = (\mathcal{F}_{nl}^i)^2 / \sum_{i'} (\mathcal{F}_{nl}^{i'})^2. \tag{12}$$

In what follows we demonstrate this approach using some realistic examples. We refer to our approach as Cluster-Nucleon Configuration Interaction Model (CNCIM). Additional details and applications can be found in Refs. [5, 29].

3. Applications
Study of the ground state α-clustering in sd-shell nuclei
There is a large body of both theoretical [10, 12] and experimental [30–33] work exploring the α strength in low-lying states of *sd*-shell nuclei. We performed calculations of α-particle SFs for ground state to ground state transitions of even-even *sd*-shell nuclei. The USDB [34] Hamiltonian was used. Within this model only one four-nucleon operator with SU(3) quantum numbers (8,0) contributes. Thus, the relationship (12) holds.

Our results, when compared to the experimental data in Tab. 2, highlight the merits of the method. The long-standing problem that the values of the old SFs (third column in Tab. 2) are not only several times smaller than the ones extracted from various experiments (columns 4–6 in Tab. 2) but also rapidly decrease with the increasing nuclear mass appears to be resolved in our approach, as indicated by the new SFs in the second column. Furthermore, the measured SFs and their tendencies to drop down towards the middle of the *sd*-shell and to increase at the edges are well-reproduced. It is noteworthy that the values of the "old" spectroscopic factors obtained by us and the ones presented in Ref. [10] are close – the difference is not larger than 12 percent.
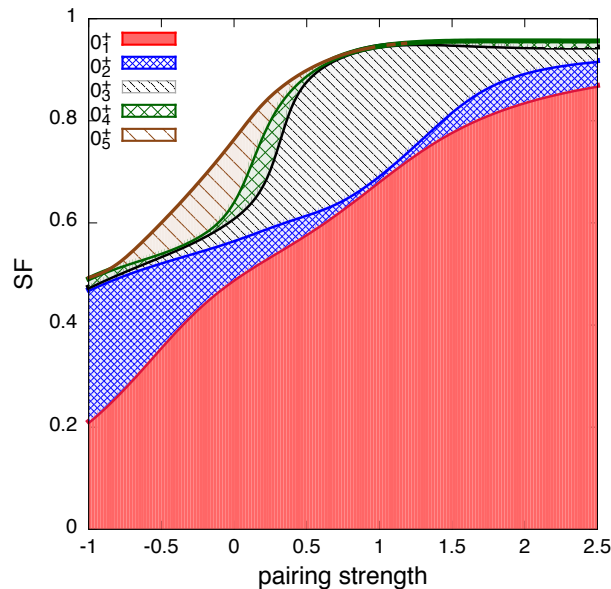
In Fig. 1 we explore the dependence of the new SFs on the pairing interaction. Here, all the isovector pairing ($T = 1$, $J = 0$) matrix elements are scaled, and the SFs are shown as a function of this scaling. The role of pairing and its relation to α-clustering is not trivial in many-body systems. However, in this example, it appears that increased pairing also favors clustering. Moreover, for strong pairing almost all the α-clustering strength is concentrated in the ground state.

Study of α-clustering in ^{16}O
A more complicated investigation in the framework of the CNCIM is summarized in Tab. 3. Here we examine α-clustering of the ground and multiple excited states in ^{16}O relative to channels

$A_P - A_D$	S_0	$\mathcal{S}_0$	S_0 [35]	S_0 [36]	S_0 [37][a]
^{20}Ne-^{16}O	0.755	0.173	1.0	0.54	1
^{22}Ne-^{18}O	0.481	0.085			0.37
^{24}Mg-^{20}Ne	0.411	0.091	0.76	0.42	0.66
^{26}Mg-^{22}Ne	0.439	0.068			0.20
^{28}Si-^{24}Mg	0.526	0.080	0.37	0.20	0.33
^{30}Si-^{26}Mg	0.555	0.061			0.55
^{32}S-^{28}Si	0.911	0.082	1.05	0.55	0.45
^{34}S-^{30}Si	0.974	0.062			
^{36}Ar-^{32}S	0.986	0.061			
^{38}Ar-^{34}S	0.997	0.030			1.30
^{40}Ca-^{36}Ar	1	0.037	1.56	0.86	1.18

Table 2. Ground state to ground state α-particle SFs, "new" S_0 and "old" $\mathcal{S}_0$ and the experimental SFs extracted from the cross sections of (p,pα) [35, 36] and (^{6}Li,d) [37] reactions. [a] The values of the SFs are normalized by the SF of ^{20}Ne. Taking into account that the experimental absolute value of SF in ^{20}Ne according to [35] is very close to 1.0 (see column 4), they may be considered as absolute ones.

Figure 1. SF (new) for the lowest 0^+ states in ^{28}Si for the $l = 0$ channel of the α-particle with ^{24}Mg in the ground state. The SFs are stacked because their total sum equals to unity in this model space. The USDB [34] shell model Hamiltonian is used with all $T = 1$; $J = 0$ pairing matrix elements being scaled. The scaling parameter is shown on the x-axis.

involving ^{12}C nucleus in the ground state. Both parent and daughter systems are treated in the unrestricted p-sd configuration space with the effective interaction Hamiltonian from [19]. The study in Ref. [19] suggests that this effective Hamiltonian describes well the multi-particle correlations in ^{16}O which makes it a good choice for exploring clustering. The p-sd valence space permits the following SU(3)-classified four-nucleon configurations:

$$\Phi_{(n,0):l}(R) = |R; (0p)^q (2s - 1d)^{4-q} [4](n,0) : l, S = 0, T = 0\rangle, \qquad (13)$$

where $q = 0, 1...4$; $n = 8 - q$; $l = n, n - 2, ..., 1$ or 0; and $\pi = (-1)^l$.

In our study the spectrum of ^{16}O has been calculated in a broad energy region. Experimentally known characteristics – spin, parity and α decay reduced widths θ_α^2 – of more than sixty states are reasonably described. For the sake of brevity in Tab. 3 we exemplify our results only for the states with SFs $S_\alpha > 0.1$.

J_i^π	E(sm)	S_l	E(exp)	θ_α^2					
0_1^+	0.000	0.794	0.000	0.86^a			continued		
3_1^-	5.912	0.663	6.13	0.41^a	J_i^π	E (sm)	S_l	E(exp)	θ_α^2
0_2^+	6.916	0.535	6.049	0.40^a	2_4^+	12.530	0.123	$—^c$	
1_1^-	7.632	0.150	7.117	0.14	6_1^+	13.286	0.465	14.815	0.17
2_1^+	8.194	0.500	6.917	0.47^a	4_3^+	13.308	0.160	14.62	0.19
2_2^+	9.988	0.349	9.844^b	0.0015	3_3^-	13.733	0.144	14.1	0.21
4_1^+	10.320	0.313	10.356	0.44	2_6^+	14.646	0.102	14.926^b	0.0098
0_3^+	10.657	0.216	11.26	0.77	1_4^-	15.298	0.174	9.585	0.67
2_3^+	11.307	0.158	11.52^b	0.033	4_5^+	15.474	0.152	16.844	0.13
4_2^+	11.334	0.203	11.097^b	0.0014	5_1^-	15.945	0.289	14.66	0.55
					6_2^+	16.304	0.415	16.275	0.43

Table 3. The α-particle SF for states in ^{16}O. See text for additional details.
^{a} Recalculated value of the SF from [38] (see the text).
^{b} Identified states are, probably, of different nature.
^{c} No experimental analog has been found.

Tab. 3 is based on the theoretically calculated spectrum of ^{16}O. We attempted to identify each theoretically predicted state with an experimentally known state. Experimentally observed excitation energy E(exp) and α spectroscopic strength θ_α^2 are listed in the last two columns. The most part of the experimental information is taken from the spectroscopic tables [39, 40]; α decay reduced widths were calculated using ordinary formulas typical for resonance reaction theory. For evaluation of the SFs of sub-threshold states the experimental data from (^{6}Li,d) reaction [38] are used, where SFs relative to 4_1^+ 10.356 MeV are presented. Taking into account some inconsistencies in determination of absolute values of the sub-threshold SFs, we rescale this data using an over-threshold reference state with a known α decay width. It should be noted that in this compilation of data the accuracy of the θ_α^2 values is very limited. Thus, in establishing theory-experiment correspondence in Tab. 3 an agreement within a factor of 3 to 4 in SF is the primary criterion, a theory-experiment agreement in excitation energy within about 1 MeV is considered secondary. Overall, we find the accord between theory and experiment displayed in Tab. 3 encouraging. Indeed, about $^2/_3$ of theoretical results obtained without introducing any parameters or fitting procedures turn out to be supported by the experimental data. Many states with lower α SFs (not listed in Tab. 3) are also reproduced by this theory. For most levels observed in experiments theoretical partners may be found. Other properties of the ^{16}O states that include electric quadrupole transitions and possible identification of rotational bands are also well-described. The details can be found in Ref. [29]. Discrepancies between theory and observations in Tab. 3 shed new light on the nature of states and provide guidance for further development of microscopic approaches to nuclear clustering. The expansion of the basis is the most obvious direction towards an improvement of the method. The lack of configurations from the pf-shell appears to be an origin of the serious discrepancy in the energy and the width of the 1_4^- E(exp)=9.585 MeV.

4. Summary

In this contribution we summarize our recent progress with the Cluster-Nucleon Configuration Interaction Model. The approach expands the modern configuration interaction versions of the nuclear shell model towards clustering. Large configuration-space studies, interplay between cluster and nucleon degrees of freedom, cluster strength distribution at high excitation energies, and numerous opportunities for extension and development are the particularly appealing sides of this technique. Here we provide a brief description of CNCIM and discuss the SU(3) properties

of α-cluster channels. We demonstrate the effects that follow from the Orthogonality Condition Model which appear to resolve a long-standing problem of underestimation of α spectroscopic factors in sd-shell nuclei. We briefly touch on an issue of interplay between nuclear pairing and clustering. The ^{16}O nucleus is selected as an example of a large scale study. Comparison of theoretical results and experimental data represents an affirmative assessment to the approach.

Acknowledgments

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