Study of Cluster Ceactions in Advanced Shell Model Approaches.

Yury M. Tchuvil'sky[a] **and Alexander Volya**[b]

[a] *Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, 119991 Moscow, Russia*

[b] *Department of Physics, Florida State University, Tallahassee, FL 32306, USA*

Abstract

In the Cluster-Nucleon Configuration Interaction Model (CNCIM) presented in this work, the many-body cluster techniques are adopted for use in advanced shell model approaches including the modern *ab initio* schemes. The CNCIM is facilitated by the SU(3) symmetry which allows us to built orthogonal cluster channel wave functions with Pauli exclusion principle being taken into account. Multiple results concerning α spectroscopic factors for ground state to ground state transfers in *sd*-shell nuclei, and for transfers from low-lying and highly excited states in ^{16}O and ^{10}Be are presented. The results are in good agreement with experimental data. Clustering properties of the light nuclei are discussed and some predictions are made. We view our results as an important proof of the principle, showing that modern high performance computing permits studies of clustering within configuration interaction approaches.

Keywords: *α-clustering, shell model, resonance states*

1 Introduction

Clustering is an important feature of nuclei. The phenomenon has been investigated extensively over at least half-a-century and a large body of experimental data on this topic is available. Reaction techniques highlighting the clustering properties are being continuously improved. In particular, thick ^{4}He target inverse kinematics technique [1, 2] has recently provided a large amount of data concerning complicated α-particle resonance spectra [3–5].

Theoretical challenges on the subject of nuclear clustering include *ab initio* approach to nuclear structure, emergence of many-body correlations and many-body forces, nuclear reactions involving cluster knock-out, transfer and decay, as well as many questions in astrophysics. Multiple theoretical techniques have been put forward to study nuclear clustering; some selected ones can be found in Refs. [6–10] as well as in a broad review *Clusters in Nuclei* series [11]. However, many of these techniques, such as, a symmetry based approach found in Ref. [12], focus on the structure of highly clustered nuclear states where cluster degrees of freedom are introduced by construction. Moreover, connection to experimental results is often made using observables that are not directly related to clustering, such as nuclear moments of inertia, quadrupole moments, gamma-transitions, etc. This strategy may be inadequate for drawing conclusions about nuclear clustering based on experimental evidences. The current presentation focuses on the Cluster-Nucleon Configuration Interaction

Proceedings of the International Conference 'Nuclear Theory in the Supercomputing Era — 2014' (NTSE-2014), Khabarovsk, Russia, June 23–27, 2014. Eds. A. M. Shirokov and A. I. Mazur. Pacific National University, Khabarovsk, Russia, 2016, p. 57.

http://www.ntse-2014.khb.ru/Proc/Tchuvilsky.pdf.

Model (CNCIM) and its potential to bridge the gap between experimental results and clustering theory.

Nuclear shell model, which is also generally known as the configuration interaction (CI) method, is broadly used in studies of quantum many-body systems. It is a well established microscopic approach, where, within the same formalism, high quality description and good predictive power are obtained for numerous single-particle and collective nuclear properties [13–16]. In the nuclear shell model, cluster degrees of freedom are not introduced explicitly. This makes the shell model an ideal tool to study weakly clustered states and to address questions related to emergence of clustering and interplay of cluster and single nucleon degrees of freedom. Recent advances in computational techniques and exponential growth of computational power [13,17,18] facilitate work in this direction.

Shell-model microscopic approach to clustering has been extensively developed in the past [19–27]; it represents the path combining both microscopic single-nucleon and collective symmetry based properties of nuclear dynamics. In the CNCIM we advance the shell model approach by targeting the cluster spectroscopic characteristics, by implementing the orthogonality conditions model for description of exit and entrance cluster channels, by utilizing the SU(3) symmetry and some other algebraic properties inherent to the harmonic oscillator basis. This report provides a current summary of our recent results, see also Refs. [5, 28–30].

2 Formalism

Shell model configuration interaction approach and SU(3)-symmetric structures

In the shell model approach, the many-nucleon states

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

are linear combinations of configurations, which are Slater determinants of single-particle states $1 \equiv \{n,l,j,m\}$. These single-particle states are built from the radial harmonic oscillator wave function (WF) $\varphi_{n_1,l_1}(r) \equiv \langle r|1\rangle \equiv \langle r|a_1^\dagger|0\rangle$ with angular momentum and spin variables coupled to total angular momentum j. The operator $a_1^\dagger$ is the nucleon creation operator in the second quantization. The numeric coefficient $\langle 1,2\ldots A|\Psi\rangle$ in Eq. (1) determines the weight of each Slater determinant in the linear superposition.

In our work clustering is approached using multi-nucleon structures related to a certain irreducible representation of the SU(3) group. In the present paper we discuss alpha clustering, therefore we construct four-nucleon states

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

Here $\{\mathfrak{n}_i^{\alpha_i}\}$ denotes a 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 states in Eq. (2) are constructed by diagonalization of linear combinations 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.

A direct correspondence between states $|\Psi\rangle$ and creation and annihilation operators $\Psi^\dagger$ and Ψ of the second quantization facilitates evaluation of the overlap integrals involved in fractional parentage coefficients (FPCs)

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

Table 1: Selected FPCs and channel norms for SU(3) states. All WF and operators are for $L = 0$.

Ψ_P	Φ	$\left\|\langle\Psi_P\|\Phi^\dagger\|\Phi\rangle\right\|^2$	$\langle 0\|\Phi\Phi\Phi^\dagger\Phi^\dagger\|0\rangle$
$(p)^8\,(0,4)$	$(p)^4\,(4,0)$	1.42222*	1.42222
$(sd)^8\,(8,4)$	$(sd)^4\,(8,0)$	0.487903	1.20213
$(fp)^8\,(16,4)$	$(fp)^4\,(12,0)$	0.292411	1.41503
$(sdg)^8\,(24,4)$	$(sdg)^4\,(16,0)$	0.209525	1.5278

*For the p shell this result agrees with the value of $64/45 = 1.42222$ found in Ref. [31].

Here $\hat{\mathcal{A}}$ is the antisymmetrization operator and $|\Psi_P\rangle$ and $|\Psi_D\rangle$ are arbitrary states of type (1).

The FPCs for some selected states of SU(3) symmetry are shown in Table 1. The channel norms shown in the last column, provide a measure of bosonic enhancement. Indeed, if a four-nucleon $L = 0$ operator $\Phi^\dagger \equiv \Phi^\dagger_{(n,0):0}$ is thought of as a boson creation operator then $\Phi\Phi^\dagger = 1 + N_b$, where N_b is the boson number operator. Therefore for ideal bosons the norm of the one-boson channel state $\langle 0|\Phi\Phi\Phi^\dagger\Phi^\dagger|0\rangle$ should be 2. The numbers in the last column are less than 2, showing that the four-nucleon configurations are not true bosons. These objects are comprised of fermions, and residual Pauli blocking effects are noticeable. The blocking effects are naturally reduced for larger shells, which brings the norm closer to 2.

Cluster form factors and spectroscopic factors

The cluster form factor (CFF), also commonly known as the spectroscopic amplitude,

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

is one of the most basic measures of clustering. In Eq. (4), Ψ'_P, Ψ'_D, and Ψ'_α are WFs of the parent (P), the daughter (D) and the α-cluster, respectively, which are internal, translationally invariant, and free of the center of mass (c. m.) coordinate. Here and in what follows 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 nucleus motion; a proper coupling to a relative angular momentum l is established.

In our shell model calculations the parent and daughter states are computed implementing a Glockner–Lawson procedure [32] leading the c. m. motion being in the lowest oscillator state $\varphi_{00}(R)$. The oscillator frequency in harmonic oscillator WF depends in the usual way on the mass number. In order to describe α channels we assume that the α-particle's translationally invariant WF is represented by the lowest four-nucleon oscillator function written through the Jacobi coordinates:

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

Therefore in the WF $|\Phi_{(n,0):l}\rangle$ we are interested in a component that includes the intrinsic 4-nucleon state (5) with the c. m. variable being in the oscillator state $\varphi_{nl}(R_\alpha)$. This component, referred to as cluster coefficient, is known analytically [21, 22, 33],

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

The following steps (see also Refs. [20–22, 24]) include expansion of the parent state using FPC (3) and recoupling the c. m. variables R_α and R_D into their relative coordinate ρ and the parent c. m. coordinate R_P where the corresponding recoupling coefficient (known as recoil factor) is

$$\mathcal{R}_n = (-1)^n[(m_D + m_\alpha)/m_D]^{n/2}.$$

This leads to the expansion of the CFF (4) in oscillator states,

$$\phi_l(\rho) = \sum_n \mathcal{C}_{nl}\,\varphi_{nl}(\rho), \quad \mathcal{C}_{nl} = X_{nl}\,\mathcal{F}_{nl}\,\mathcal{R}_n. \tag{7}$$

In the past it was common to identify the CFF in Eq. (7) with the observable spectroscopic factors (SFs) $\mathcal{S}_l = \sum_n |\mathcal{C}_{nl}|^2$. However, it was argued in Refs. [34, 35] 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 the Resonating Group Model or, for an easier reduction to the two-body problem, in the form of the Orthogonality Condition Model (OCM) [36]. Therefore the CFF should be redefined as

$$f_l(\rho) \equiv \hat{\mathcal{N}}_l^{-1/2}\phi_l(\rho), \tag{8}$$

where the norm operator

$$\hat{\mathcal{N}}_l\phi_l(\rho) \equiv \int \mathcal{N}_l(\rho',\rho)\phi_l(\rho')\rho'^2 d\rho'$$

contains the overlap norm kernel

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

The validity and importance of this new definition are discussed in details in Refs. [10, 37]. We construct and diagonalize the norm kernel operator as a matrix in oscillator basis

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

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 an 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 SFs 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 $\Phi_{(n,0):l}$) involved. In the one-channel case (such an example is considered in the next section), using 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

$$N_{nl} = \mathcal{R}_n^2 X_{nl}^2 \sum_i (\mathcal{F}_{nl}^i)^2 = \sum_i \mathcal{S}_l^i, \tag{12a}$$

thus

$$S_l^i = \mathcal{S}_l^i / \sum_{i'} \mathcal{S}_l^{i'} = (\mathcal{F}_{nl}^i)^2 / \sum_{i'} (\mathcal{F}_{nl}^{i'})^2. \tag{12b}$$

We refer to the technique outlined here as the Cluster-Nucleon Configuration Interaction Model (CNCIM), and in the following section we demonstrate some of its applications. Additional details can be found in Refs. [5, 29, 30].

3 Applications

Study of the ground state α-clustering in sd-shell nuclei

Transfer and knock-out reactions, such as the ones discussed in Refs. [38–41], provide a wealth of information on α strengths in low-lying states of sd-shell nuclei. Theoretical values of the corresponding SFs obtained in various papers are well-correlated [23,25]. The summary of these results as well as those from our calculations are presented in Table 2. In our calculations of α-particle SFs for ground state to ground state transitions the USDB Hamiltonian [42] was used. The basis is restricted by the sd shell. Within this model only one four-nucleon operator with SU(3) quantum numbers (8,0) contributes, and therefore the relationship (12) holds.

Prior to discussing the results in Table 2, let us clarify some problems associated with evaluation of the absolute values of experimental SFs. First, some problems emerge from poor knowledge of the imaginary part of nucleus-nucleus potential for the types of reactions involved. Second, transfer reactions usually determine only relative values of the SFs, while for knock-out reactions absolute values are commonly provided in the literature (see Table 2, columns 2, 3). Therefore in Table 2 all values evaluated in transfer reactions are normalized to the value of the SF in ^{20}Ne (column 4). Given that the experimental absolute value of SF in ^{20}Ne according to Ref. [43] is very close to 1.0, the remaining relative SFs in column 4 may be interpreted as the absolute ones. Both types of experiments are nevertheless consistent in the general pattern of variation of relative values of SFs with the increase in nuclear mass.

A comparison of theoretical values [23, 25] with the experimental data highlights some problems. First, the theoretical SFs are several times smaller than the measured ones; in certain cases the discrepancy is more than one order of magnitude. To demonstrate this in Table 2 we include the non-renormalized theoretical values of SFs from Ref. [23]. In analogy with the approach taken in experiments with transfer reactions, it is a common practice to renormalize theoretical data using the value of the α-particle SF in ^{20}Ne; and yet this practice needs some rigorous justification. Second, even after the renormalization, the tendency for the values of SFs to decrease rapidly while going from ^{20}Ne to ^{40}Ca, is not confirmed by the data.

Our results, shown in the last (7th) column in Table 2, appear to resolve the above mentioned long standing theoretical problems in a natural way. Indeed, the

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 $(p, p\alpha)$ [43, 44] and (^{6}Li,d) [45] reactions, traditional S_0 obtained in Ref. [23] and in the current work, and "new" SFs S_0^{new}.

$A_P - A_D$	S^{exp} [43]	S^{exp} [44]	S^{exp} [45]	$\mathcal{S}_0$ [23]	$\mathcal{S}_0$	S_0
^{20}Ne-^{16}O	1.0	0.54	1	0.18	0.173	0.755
^{22}Ne-^{18}O			0.37	0.099	0.085	0.481
^{24}Mg-^{20}Ne	0.76	0.42	0.66	0.11	0.091	0.411
^{26}Mg-^{22}Ne			0.20	0.077	0.068	0.439
^{28}Si-^{24}Mg	0.37	0.20	0.33	0.076	0.080	0.526
^{30}Si-^{26}Mg			0.55	0.067	0.061	0.555
^{32}S-^{28}Si	1.05	0.55	0.45	0.090	0.082	0.911
^{34}S-^{30}Si				0.065	0.062	0.974
^{36}Ar-^{32}S				0.070	0.061	0.986
^{38}Ar-^{34}S			1.30	0.034	0.030	0.997
^{40}Ca-^{36}Ar	1.56	0.86	1.18	0.043	0.037	1

agreement between absolute SFs found in experiment (columns 2–4) and those from CNCIM (column 7) is good without any renormalization. This includes the trend of SFs to drop down towards the middle of the *sd* shell and to increase at the edges.

The values of the traditional spectroscopic factors obtained by us (column 6) and the ones presented in Ref. [23] (column 5) are close, thus showing that renormalization of the channel WFs proposed by Fliessbach is the main reason for this improvement.

Study of α-clustering in ^{16}O

A more advanced investigation using CNCIM is summarized in Table 3. Here we examine α-clustering of the ground and multiple excited states in ^{16}O relative to channels involving ^{12}C nucleus in the ground state. Both parent and daughter systems are treated in the unrestricted *p-sd* configuration space with effective interaction Hamiltonian from Ref. [17]. In Ref. [17] Utsuno and collaborators suggest that this effective Hamiltonian describes well the multi-particle correlations in ^{16}O, thus making it an ideal choice for exploring clustering. The *p-sd* valence space allows for the following SU(3)-classified four-nucleon configurations:

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

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

A broad part of the low-lying ^{16}O spectrum is examined in our study. For over 60 states the experimentally known characteristics that include spin, parity and α-decay reduced widths θ_α^2 turned out to be reasonably described by our model. Focusing on clustering properties in Table 3 we restrict our presentation to the states with SFs $S_\alpha > 0.1$. The table is organized based on the theoretically calculated spectrum of ^{16}O. We made an effort to identify each theoretically predicted state with an experimentally known counterpart. In this process an agreement within a factor of 3 to 4 in SF was the primary criterion, a theory-experiment agreement in excitation energy within about 1 MeV was considered as secondary.

Table 3: The α-particle SFs for states in ^{16}O.

J_i^π	E(sm)	S_l	E(exp)	θ_α^2
0_1^+	0.000	0.794	0.000	0.86[a]
3_1^-	5.912	0.663	6.13	0.41[a]
0_2^+	6.916	0.535	6.049	0.40[a]
1_1^-	7.632	0.150	7.117	0.14
2_1^+	8.194	0.500	6.917	0.47[a]
2_2^+	9.988	0.349	9.844[b]	0.0015
4_1^+	10.320	0.313	10.356	0.44
0_3^+	10.657	0.216	11.26	0.77
2_3^+	11.307	0.158	11.52[b]	0.033
4_2^+	11.334	0.203	11.097[b]	0.0014

continued

J_i^π	E (sm)	S_l	E(exp)	θ_α^2
2_4^+	12.530	0.123	—[c]	
6_1^+	13.286	0.465	14.815	0.17
4_3^+	13.308	0.160	14.62	0.19
3_3^-	13.733	0.144	14.1	0.21
2_6^+	14.646	0.102	14.926[b]	0.0098
1_4^-	15.298	0.174	16.2	0.085
4_5^+	15.474	0.152	16.844	0.13
5_1^-	15.945	0.289	14.66	0.55
6_2^+	16.304	0.415	16.275	0.43

[a] Recalculated value of the SF from [46] (see the text).

[b] Identified states are, probably, of different nature.

[c] No experimental analog has been found.

The most part of the experimental information was taken from the spectroscopic tables [47, 48]. Measured excitation energies and α spectroscopic strengths θ_α^2 are listed in Table 3 in the last two columns. The α-decay reduced widths were calculated using standard equations of resonance reaction theory. For evaluation of the SFs of sub-threshold states, the experimental data from (^{6}Li,d) reaction [46] were 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 known α-decay width.

The results displayed in Table 3 are encouraging. The model includes no additional parameters, nor fits, and yet for most levels observed in experiments theoretical partners may be found. Over 2/3 of states predicted to have strong clustering properties have been identified experimentally. Many states with lower α SF (not listed in Table 3) are also reproduced by the theory. Other properties of the ^{16}O states that include electric quadrupole transitions and possible identification of rotational bands are also well-described, see further details in Ref. [29].

The lack of configurations from the pf shell appears to be a reason for discrepancy related to α-decaying states 1^- E(exp)=9.585 MeV and 3^- E(exp)=11.6 MeV. Disagreements similar in nature were seen in ^{18}O, Ref. [5]. Some cases, such as those marked in Table 3 by ^{b}, point toward deficiencies of the Hamiltonian.

Study of α-clustering in ^{10}Be

^{10}Be is another popular system for studies of clustering because it is one of the lightest nuclei where the interplay between cluster and nucleon degrees of freedom is manifested. Apart from that, ^{10}Be provides a path for a better understanding of the exotic isobar-analogous system of ^{10}C [49]. The α-cluster properties of ^{10}Be are not easy to measure because ^{6}He beams lack intensity and there is no other convenient projectile for such studies. The lack of information has motivated active discussions and numerous loosely validated qualitative conclusions, that could benefit from additional theoretical work.

The study of ^{10}Be is similar to that of ^{16}O described in the previous section. We use the same unrestricted *p-sd* configuration space with the effective interaction Hamiltonian from Ref. [17], and consider the same set of four-nucleon operators in Eq. (13). A large number of the states with natural parity was obtained, and for each state the SF for the α+^{6}He channel was computed from Eq. (11). The results are summarized in Table 4 which includes all theoretically predicted states up to 10 MeV of excitation. In the region between 10 and 15 MeV only the states with $S_l > 0.01$ are listed, and this list includes all high-spin states ($J \geq 4$). For higher excitation energy low-spin levels are tabulated in the case where $\Gamma_\alpha > 300$ keV and high-spin levels where $\Gamma_\alpha > 100$ keV.

The three lowest states, 0_1^+, 2_1^+, and 4_2^+, in ^{10}Be are strongly clustered, which are the only states with $S_l > 0.3$. The clustering is explained by the large $|(1p)^6[42], (\lambda,\mu) = (2,2), L, S = 0,\ T = 1\rangle$ component, the weight of this component is 0.65, 0.53 and 0.35 for 0_1^+, 2_1^+, and 4_2^+, respectively. These states do not form a rotational band because the 0_1^+ ground state in the algebraic model has a value of projection $K = 0$, and this value of intrinsic angular momentum projection is not presented in the 4^+ state related to $(\lambda,\mu) = (2,2)$ SU(3) representation. Clustering effects are weak in high-spin states. For all 6^+ states $S_l < 0.04$; all 7^- and 8^+ states are found to have near zero SFs, to be specific, $S_l < 10^{-6}$.

The experimental information presented in Table 4 comes from Refs. [50–54]. As it is the case for the ^{16}O example presented in Table 3, agreement in spectroscopic factors is the primary criterion in establishing theory-experiment correspondence for ^{10}Be as presented in Table 4; the theory-experiment agreement in excitation energy is considered secondary. The traditional R-matrix relations, see for example Ref. [51],

Table 4: Results of the CNCIM calculations for ^{10}Be compared with the available experimental information. Energies are given in MeV; decay widths are in keV, or as indicated.

J^π_s	S_l	E^{th}_x	Γ^{th}_α	E^{exp}_x	Γ^{exp}_α	$\theta^2_\alpha(r_1)$	$\theta^2_\alpha(r_2)$
0^+_1	0.686	0.000		0			
2^+_1	0.563	3.330		3.368			
0^+_2	0.095	4.244		6.197			
2^+_2	0.049	5.741		5.958			
2^+_3	0.052	6.123					
1^-_1	0.027	6.290		5.96			
3^-_1	0.098	6.926		7.371		$0.42^{a,b}$	
2^+_4	0.116	7.650	0.3 eV	7.542	0.5 eV	$1.1^{a,b}$	0.19
0^+_3	0.023	8.068	17				
4^+_1	0.049	8.933	4.7				
1^-_2	0.045	9.755	180	10.57			
3^-_2	0.046	9.897	61				
2^+_5	0.027	10.819	50	9.56	141^d		0.074
2^+_6	0.023	11.295	43				
0^+_5	0.153	11.403	800				
4^+_2	0.370	11.426	180	10.15	185^b	1.5^b	0.38
5^-_1	0.148	11.440	150	11.93	200		0.20
1^-_5	0.013	12.650	76				
6^+_1	0.013	13.134	24	13.54^b	99	1.0^b	0.051
5^-_2	0.128	13.545	250				
2^+_{10}	0.040	13.789	240				
4^+_3	0.011	13.992	20	11.76	121		0.066
4^+_4	0.022	14.233	40				
0^+_6	0.018	14.252	120				
3^-_7	0.014	14.468	77				
5^-_3	0.059	14.992	180				
4^+_5	0.161	15.071	800	$15.3(6^-)^c$	800^d		0.16
2^+_{13}	0.046	15.534	330				
4^+_6	0.033	15.809	180				
4^+_7	0.03	16.426	150				
4^+_9	0.200	17.510	1300				
4^+_{11}	0.041	18.566	290				
5^-_8	0.017	19.448	110				
5^-_9	0.018	19.840	120				
5^-_{11}	0.017	21.395	130				
6^+_4	0.037	19.101	170				

[a] Widths deduced from the isobaric analog channel ^{10}B $\rightarrow ^6$Li$(0^+)+\alpha$ [50, 51].

[b] Results from Ref. [51].

[c] Results from Ref. [52].

[d] Total width Γ^{tot}.

are used to obtain theoretical predictions for the decay width Γ_α^{th}, and inversely, to obtain the reduced widths θ_α^2 from the experimentally observed α decay width Γ_α^{exp}. The R-matrix relations depend on the excitation energy and on the channel radius r. If the energy of the level is known experimentally, the observed value is used to compute Γ_α^{th}. Some significant dependence of the decay width on the channel radius is demonstrated by the last two columns in Table 4. For example, the reduced widths θ_α^2 presented in Ref. [51] (7th column) appear to be in disagreement, but those results were obtained using the channel radius r_1=4.77 fm, typical for stable nuclei. In the last column of Table 4 we demonstrate that another choice of the channel radius, $r_2 = 6.0$ fm, brings all values of θ_α^2 to a good agreement with calculated SFs. Moreover, the choice of a larger channel radius is more natural for a halo ^{6}He nucleus.

The calculated energy spectrum is consistent with the recent experimental findings. There are some discrepancies: somewhat noticeable deviations in excitation energy are observed for the 0_2^+ level and the doublet $4_{3,4}^+$. In addition to that, a number of theoretically predicted levels has not been observed in experiments; those, however, can often be explained by small decay widths, such as in the case of the 2_3^+ state.

Being encouraged by the success of the CNCIM, we are compelled to take part in discussions related to interpretation of recent experimental data. Our results summarized in Table 4 confirm that the branching ratio $\Gamma_\alpha/\Gamma_{tot}$ for the state at $E_x^{exp} = 7.543$ MeV is close to $1.3{\cdot}10^{-4}$ [51]. The conclusion of Refs. [51, 53] that the level 10.15 MeV is 4^+ and not 3^- [52] is also confirmed. Results in Table 4 suggest that the state at $E_x = 13.54$ MeV [51] is actually a 6^+ and 5^- doublet of resonances. The state at $E_x = 15.3$ MeV is characterized in Ref. [52] as J^π=6^- based on an expectation to see a $K = 1$ "band" member in this energy region; according to our results it is probably a 4^+ state. A number of theoretical results in Table 4 can potentially guide future experimental investigations.

4 Summary

In this work we develop formalism and methods for conducting studies of nuclear clustering using the advanced large-scale shell model technique. The effects of Pauli exclusion principle which, as found in previous works, result in the specific renormalization of wave functions of the cluster channels and require redefinition of traditional cluster characteristics are accurately taken into account. The developed formalism is applicable for all microscopic configuration interaction approaches, including *ab initio* no-core schemes. Cluster transitions between the states of all kinds (ground, excited, resonance; strongly and weakly clustered) can be treated in our approach. The end products of the approach are the cluster spectroscopic characteristics that can be directly compared with experimental observables.

We use a variety of examples to demonstrate the capability of our approach. Reviewing the α spectroscopic factors of ground state to ground state transitions in even-even nuclei of the *sd* shell we resolve a long-standing problem related to underestimation of absolute values of spectroscopic factors and obtain a good agreement with the experimental data.

We perform two large-scale studies of ^{16}O and ^{10}Be nuclei within the *p*-*sd* valence space. The ^{16}O system is chosen because α-decay widths and transfer strengths going to the ground state of ^{12}C nucleus have been measured for many states. The performed calculations provide a good description of both the spectrum and the alpha-decay widths. These results along with the ones related to the traditional single-particle excitations, electromagnetic transitions and cluster rotational bands, obtained both in our calculations and in preceding papers, validate the approach.

With the ^{10}Be study we join the recent debate about the nature of clustering in this exotic nucleus. The widths of known α-decaying resonances of the nucleus turn

out to be well-described in CNCIM. This allows us to discuss structure of these states and to make predictions.

We would like to conclude that the success of the CNCIM reported in this work indicate that in the era of supercomputers the study of clustering physics becomes feasible within the phenomenological or *ab initio* configuration interaction technique.

We thank V. Goldberg, T. Dytrych and G. Rogachev for motivating discussions. This material is based upon work supported by the U.S. Department of Energy Office of Science, Office of Nuclear Physics under Award Number DE-SC-0009883.

References

[1] K. Artemov *et al.*, Sov. J. Nucl. Phys. **52**, 406 (1990).

[2] V. Goldberg and A. Pakhomov, Phys. At. Nucl. **56**, 1167 (1993).

[3] T. Lonnroth *et al.*, Eur. Phys. J. A **46**, 5 (2010).

[4] M. Norrby *et al.*, Eur. Phys. J. A **47**, 73 (2011).

[5] M. Avila *et al.*, Phys. Rev. C **90**, 024327 (2014).

[6] K. Varga, R. G. Lovas and R. J. Liotta, Nucl. Phys. A **550** (1992).

[7] K. Varga and R. J. Liotta, Phys. Rev. C **50**, R1292 (1994).

[8] R. Id Betan and W. Nazarewicz, Phys. Rev. C **86**, 034338 (2012).

[9] A. Insolia, P. Curutchet, R. J. Liotta and D. S. Delion, Phys. Rev. C **44**, 545 (1991).

[10] S. G. Kadmensky, S. D. Kurgalin and Yu. M. Tchuvil'sky, Phys. Part. Nucl. **38**, 699 (2007).

[11] *Clusters in nuclei*, ed. C. Beck, Lecture Notes in Physics **818, 848, 875**. Springer, Berlin, New York, 2010, 2012, 2013.

[12] I. A. Gnilozub, S. D. Kurgalin and Yu. M. Tchuvl'sky, J. Phys. Conf. Ser. **436**, 012034 (2013).

[13] E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves and A. P. Zuker, Rev. Mod. Phys. **77**, 427 (2005).

[14] I. Talmi, *Fifty years of the nuclear shell model — the quest for the effective interaction*, Advances in Nuclear Physics **27**, 1. Kluwer, 2003.

[15] B. A. Brown, Progr. Part. Nucl. Phys. **47**, 517 (2001).

[16] A. Volya, Phys. Rev. C **79**, 044308 (2009).

[17] Y. Utsuno and S. Chiba, Phys. Rev. C **83**, 021301(R) (2011).

[18] *Proc. Int. Conf. Nucl. Theor. Supercomputing Era (NTSE-2013), Ames, IA, USA, May 13–17, 2013*, eds. A. M. Shirokov and A. I. Mazur. Pacific National University, Khabarovsk, 2014, http://ntse-2013.khb.ru/proceedings/.

[19] H. J. Mang, Z. Phys. **148**, 582 (1957).

[20] Yu. F. Smirnov and D. Chlebowska, Nucl. Phys. **26**, 306 (1961).

[21] M. Ichimura, A. Arima, E. C. Halbert and T. Terasawa, Nucl. Phys. A **204**, 225 (1973).

[22] Yu. F. Smirnov and Yu. M. Tchuvil'sky, Phys. Rev. C **15**, 84 (1977).

[23] W. Chung, J. van Hienen, B. H. Wildenthal and C. L. Bennett, Phys. Lett. B **79**, 381 (1978).

[24] O. F. Nemetz, V. G. Neudatchin, A. T. Rudchik, Yu. F. Smirnov and Yu. M. Tchuvil'sky, *Nucleon clusters in atomic nuclei and multi-nucleon transfer reactions*. Naukova Dumka, Kiev, 1988 (*in Russian*).

[25] M. Grigorescu, B. A. Brown and O. Dumitrescu, Phys. Rev. C **47**, 2666 (1993).

[26] Yu. M. Tchuvil'sky, W. W. Kurowsky, A. A. Sakharuk and V. G. Neudatchin, Phys. Rev. C **51**, 784 (1995).

[27] P. Navratil, Phys. Rev. C **70**, 054324 (2004).

[28] A. Volya and Yu. M. Tchuvil'sky, IOP Conf. Proc. (2014), *in press*.

[29] A. Volya and Yu. M. Tchuvil'sky, in *IASEN 2013 Proceedings*. World Scientific, (2014), *in press*.

[30] Yu. M. Tchuvil'sky and A. Volya, in *ARIS-2014 Proceeding*. 2014, *in press*.

[31] I. Rotter, Ann. der Phys. **16**, 242 (1965).

[32] R. D. Lawson, *Theory of the nuclear shell model*. Clarendon Press, Oxford, 1980.

[33] Yu. F. Smirnov and Yu. M. Tchuvil'sky, Czech. J. Phys. **33**, 1215 (1983).

[34] T. Fliessbach and H. Mang, Nucl. Phys. A **263**, 75 (1976).

[35] T. Fliessbach and P. Manakos, J. Phys. G **3**, 643 (1977).

[36] S. Saito, Progr. Theor. Phys. **41**, 705 (1969).

[37] R. G. Lovas, R. J. Liotta, A. Insolia, K. Varga and D. S. Delion, Phys. Rep. **294**, 265 (1998).

[38] W. Oelert, W. Chung, A. Djaloeis, C. Mayer-Böricke and P. Turek, Phys. Rev. C **22**, 408 (1980).

[39] W. Oelert *et al.*, Phys. Rev. C **20**, 459 (1979).

[40] H. W. Fulbright, Ann. Rev. Nucl. Part. Sci. **29**, 161 (1979).

[41] N. Anantaraman, H. W. Fulbright and P. M. Stwertka, Phys. Rev. C **22**, 501 (1980).

[42] B. A. Brown and W. A. Richter, Phys. Rev. C **74**, 034315 (2006).

[43] T. Carey *et al.*, Phys. Rev. C **23**, 576(R) (1981).

[44] T. Carey *et al.*, Phys. Rev. C **29**, 1273 (1984).

[45] N. Anantaraman *et al.*, Phys. Rev. Lett. **35**, 1131 (1975).

[46] F. D. Becchetti, D. Overway, J. J. Knecke and W. W. Jacobs, Nucl. Phys. A **344**, 336 (1980).

[47] D. R. Tilley, H. R. Weller and C. M. Cheves, Nucl. Phys. A **564**, 1 (1993).

[48] Evaluated nuclear structure data file, http://www.nndc.bnl.gov/ensdf/.

[49] V. Z. Goldberg and G. V. Rogachev, Phys. Rev. C **86**, 044314 (2012).

[50] A. N. Kuchera *et al.*, Phys. Rev. C **84**, 054615 (2011).

[51] A. N. Kuchera, *Clustering phenomena in the* $A = 10$ $T = 1$ *isobaric multiplet*, Florida State University, Electronic Theses, Treatises and Dissertations, 2013, Paper 8585, http://diginole.lib.fsu.edu/etd/8585/.

[52] D. R. Tilley *et al.*, Nucl. Phys. A **745**, 155 (2004).

[53] M. Freer *et al.*, Phys. Rev. Lett. **96**, 042501 (2006).

[54] D. Suzuki *et al.*, Phys. Rev. C **87**, 054301 (2013).