QUANTITATIVE CHARACTERISTICS OF CLUSTERING IN MODERN MICROSCOPIC NUCLEAR MODELS

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In collaboration with

A. Volya
MOTIVATIONS

1. A large body of experimental information concerning cluster decay widths of resonance states is accumulated.

2. Redefinition of the cluster spectroscopic characteristics has changed the view on clustering significantly.

3. Supercomputing era came. Advanced approaches to nuclear structure producing wave functions of nuclei which make it possible to describe nuclear spectra, moments, electromagnetic transitions, etc. with rather high quality are created.
A global intension is to create a theory of clustering suited to the requirement of supercomputing era.

A particular program is to build techniques for description of the cluster observables for the wave functions of such a type in the case that they are representable in the form of the oscillator expansion.

Contrary to the modern approaches to clustering concentrating attention on the qualitative manifestation of clustering in strongly clustered states we try to make a quantitative theory and to consider all states as the objects.
Fermionic molecular dynamics (H. Feldmeier, T. Neff).

\[ \Psi = \frac{1}{A!} \hat{A}\{\prod q_i\}; \quad |q_i\rangle = \sum_j \exp\left(-\frac{(\vec{x} - \vec{b}_{ij})^2}{2a_{ij}}\right) \chi_i \varepsilon_i \]

Density contours of 13C nucleus states (internal CS)
NUCLEAR PROCESSES AND MANIFESTATION OF CLUSTERING

I. Spontaneous cluster decay.

II. Cluster transfer reactions.

III. Cluster knock-out.

IV. RESONANCE SCATTERING OF COMPOSITE PARTICLES AND RESONANCE REACTIONS.

In particular studies in the framework of resonance processes by thick target technique in the inverse kinematics. The investigations are:
1. Modern, being in progress, promising.
2. Providing broad and rich spectra.
CLUSTERING IN THE SHELL MODEL (MANG, 1957)

A basic concept of the approach is the definition of measures of clustering in arbitrary A-nucleon model (cluster characteristics) [H.J. Mang Z. Phys. 148, 556 (1957); V.V. Balashov et al. JETP 37, 1385 (1959); a set of works by SINP MSU and VSU groups]:

a) the spectroscopic amplitude

\[ C_{MDC}^{nl} = \langle \Psi_M | \hat{A} \{ \Psi_D \phi_{nl}(\tilde{\rho}) \Psi_C \} \rangle; \]

b) the projection of the nuclear wave function onto the cluster channel – the cluster form factor and its norm – spectroscopic factor

\[ \Phi_l(\rho) = \langle \Psi_M | \hat{A} \{ \Psi_D \frac{1}{\rho^2} \delta(\rho - \rho') Y_{lm}(\Omega_{\rho'}) \Psi_C \} \rangle; \]

\[ S_{MDC} \equiv \int |\Phi(\rho)|^2 \rho^2 d\rho = \sum_n \left( C_{MDC}^{nl} \right)^2; \]
In the case that C is the X-nucleon cluster, the WFs of the mother and the daughter nuclei $\Psi_M(R_M)$ and $\Psi_D(R_D)$ are superpositions of the oscillator WFs, the CM motions of the nuclei described by these WFs are zero oscillations the formula

$$F_{MDC} = \sum F_{MDC}^{nl} = \sum (-1)^n \left( \frac{A}{A - X} \right)^{n/2} X_{nl} F_{MD}^R (XN)$$

takes place. Here first two multipliers present the recoil factor and the multiplier

$$X_{nl} = \langle \Psi_{XN} | \phi_{nl}(\vec{R}_C) \Psi_C \rangle$$

denotes cluster coefficient.
Multi-nucleon fractional parentage coefficient of the $X$-nucleon configuration $\Psi_{XN}$ is defined as:

$$F^R_{MD}(XN) = <\Psi_M(R_M)\hat{A}\{\Psi_D(R_D)\Psi_{XN}\}>$$

where the notation: $\Psi_{M(D)}(R_{M(D)})$ stands for the WF of the traditional shell model containing the redundant center-of-mass (CM) coordinate.

In the most part of papers these WFs are related to the lowest nucleon configuration.
Methods of calculation of the cluster coefficients for various cluster masses and nucleon configurations are developed in many papers. As an example, a general expression for the cluster coefficients of light d, t, h, and α clusters takes the form:

\[
X_{(n0)} = \langle \prod_{i=1}^{X} n_i (n0) : 000 | \phi_{(n0)}(R_C) \Phi_C > = \\
X^{-n/2} \left( \frac{n!}{\prod_{i=1}^{X} n_i !} \right)^{1/2} \left( X! \prod_{j=1}^{k} \alpha_j ! \right)^{1/2} .
\]

[Ichimura et al. Nucl. Phys. A 204, 225 (1973)]. The SU(3)-coupling of the one-nucleon WFs is implied here. The components of the symmetry \((n0); n = \sum n_i\) contribute to the expression only.
REDEFINITION OF THE CLUSTERING MEASURES.
“NEW” CLUSTER CHARACTERISTICS.

In the paper [T. Fliessbach and H.J. Mang, Nucl. Phys. A 263, 75 (1976)] the habituated view on the clustering measures was thrown doubt. The matter is that a certain matching procedure (point or integral) is required to deduce the amplitude and the width of a cluster channel.

The values of one and the same sense can solely be matched (compared).
So the cluster form factor

\[ \Phi_l(\rho) = \langle \Psi_M | \hat{A} \Psi_D \frac{1}{\rho^2} \delta(\rho - \rho') Y_{lm}(\Omega_{\rho'}) \Psi_C \rangle \]

must be matched with the same projection of the cluster channel WF. Not:

\[ \Phi_l(\rho) \not\leftrightarrow f_l(\rho), \]

\( f(\rho) \) – a solution of two-body problem, with the traditional norm, but:

\[ \Phi_l(\rho) \leftrightarrow \Phi'_l(\rho) \]

where:

\[ \Phi'_l(\rho) = \langle \Psi_{D+C} | \hat{A} \Psi_D \frac{1}{\rho^2} \delta(\rho - \rho') Y_{lm}(\Omega_{\rho'}) \Psi_C \rangle \]
And the channel wave function:

$$\Psi_{D+C} = \hat{A}\{\Psi_D \Phi(\vec{\rho}) \Psi_C\} -$$

microscopic solution of A-nucleon problem which may be RGM, OCM, etc. In the case that it is normalized as usual:

$$\langle \Psi_{D+C} | \Psi_{D+C} \rangle = \begin{pmatrix} 1 \\ \delta(E - E'), \delta(k - k'), etc. \end{pmatrix}$$

the WF of the relative motion must be normalized as:

$$\langle \hat{N}^{1/2}_\rho \Phi(\vec{\rho}) | \hat{N}^{1/2}_\rho \Phi(\vec{\rho}) \rangle = \begin{pmatrix} 1 \\ \delta(E - E'), \delta(k - k'), etc. \end{pmatrix}$$

where:

$$\hat{N}_\rho \Phi(\rho) \equiv \int N(\rho', \rho) \Phi(\rho') \rho'^2 d\rho'$$
\[ N(\rho', \rho'') = \left\langle \hat{A} \left\{ \Psi_{A_1} \Psi_{A_2} \frac{1}{\rho^2} \delta(\rho - \rho') Y_{lm}(\Omega_\rho) \right\} \right\rangle \left\langle \hat{A} \left\{ \Psi_{A_1} \Psi_{A_2} \frac{1}{\rho^2} \delta(\rho - \rho'') Y_{lm}(\Omega_\rho) \right\} \right\rangle. \]

As a result:

\[ \Phi'_l(\rho) = \hat{N}_\rho \phi_l(\rho) = \hat{N}^{1/2}_\rho \phi_l(\rho). \]

\[ \Phi_l(\rho) \quad \longleftrightarrow \quad \hat{N}^{1/2}_\rho \phi_l(\rho). \]

\[ \hat{N}_\rho^{-1/2} \Phi_l(\rho) \quad \longleftrightarrow \quad \phi_l(\rho) \]

\[ S'_MDC = \int |\hat{N}_\rho^{-1/2} \Phi(\rho)|^2 \rho^2 d\rho \]

NEW SPECTROSCOPIC FACTOR IN A CONFIGURATION MIXING SHELL MODEL

In the case that the WFs $\Psi_D, \Psi_C$ are presented in the form of superposition of the oscillator WFs the calculations of “new” characteristics can be carried out by the following way:

1. The eigenvalues $\varepsilon_k$ and the eigenfunctions $f_{kl}(\rho)$ are found by diagonalization of the norm kernel matrix:

$$\| N_{nn'} \| = < \Psi_D \phi_{nl} (\tilde{\rho}) \Psi_C | \hat{A}^2 | \Psi_D \phi_{nl'} (\tilde{\rho}) \Psi_C > .$$

$$f_{l}^{k} (\rho) = \sum_{n} B_{nl}^{k} \phi_{nl} (\rho) .$$

$$\varepsilon_k = < \Psi_D f_{l}^{k} (\tilde{\rho}) \Psi_C | \hat{A}^2 | \Psi_D f_{l}^{k} (\tilde{\rho}) \Psi_C > . \quad (3)$$
2. The “new” cluster form factor $\Phi'_l(\rho)$ is expanded onto the eigenfunctions of the norm kernel:

$$\Phi'_l(\rho) = \sum_k \varepsilon_k^{-1/2} \langle \Phi'_l(\rho) | f_{kl}(\rho) \rangle f_{kl}(\rho) =$$

$$\sum_k \varepsilon_k^{-1/2} \sum_n C_{MDC}^{nl} B_{nl}^k \phi_{nl}(\rho).$$

the “new” spectroscopic factor takes the form

$$S'_{MDC}^{l'} = \sum_k \varepsilon_k^{-1} \sum_{nn'} C_{MDC}^{nl} C_{MDC}^{n'l'} B_{nl}^k B_{n'l}^k.$$ 

In the particular case that the sole value of $n$ contributes:

$$S'_{MDC} = \frac{S_{MDC}}{\sum_{M'} S_{M' DC}} = \frac{[F_{MD}^R(CN)]^2}{\sum_{M'} [F_{M'D}^R(CN)]^2}$$
Inserting the complete set of the resonance wave functions

\[ 1 = \sum_i |\Psi_{M_i} \propto \Psi_{M_i}| \]

into exp. (3) it is easy to deduce the relationship:

\[ 1 = \varepsilon_k^{-1} \sum_{i,n} C_{M_i DC}^{n l} C_{M_i DC}^{n' l'} B_{n l}^k B_{n' l'}^k \]

Performing summation over \( k \) one can obtain:

\[ \sum_i S_{M_i DC}^{l'} = \text{dim} \| k \| \]

The sum rule of the “new” spectroscopic factors corresponding to a fixed value of \( n \) (cluster strength in \( 2\hbar \omega \) domain turn out to be unity. Thus the statistical properties are described accurately. That is critical for the dense spectra. In average:

\[ S_{M(E) DC}^{l} \sim \rho_l^{-1}(E) \]
SHELL MODEL CALCULATIONS

As usual the WFs of the modern versions of the shell model are:

a) presented in the form of a superposition of $A$-nucleon oscillator WFs,

b) fulfill the factorization condition:

$$\Psi_{M(D)}^{(R_{M(D)})} = \phi_{000}^{(R_{M(D)})} \Psi_{M(D)}.$$

Therefore they are convenient in operating in the just presented formalism.
As that is the case for approaches proposed earlier the lowest oscillator wave function of a cluster is used in the approach:

\[ \Psi_\alpha \equiv X = 4N = 0 [f] = [4](\lambda \mu) = (00) L = 0 S = 0 T = 0 > \]

where \([f]\) is the symbol of the permutation symmetry (Young frame) and \((\lambda \mu)\) – the SU(3) symmetry (Elliott symbol). The problem is concentrated on the calculation of the fractional parentage coefficient:

\[ < \Psi_M (R_M) | \hat{A} \{ \Psi_D (R_D) \Psi_{XN} (\lambda \mu) = (n0) \} > \]
To do that within the shell model approach normalized SU(3) states in are constructed by diagonalization of the SU(3) Casimir operator. In the explicit form these operators can be written as:

\[ \hat{C} = (Q \cdot Q) - 3L^2 \]

where the projection of the Hermitian conjugated quadrupole operator takes the form:

\[ Q^n = \sqrt{4\pi/5} \sum_{j=1}^{A} ((\rho_j^2 / \rho_{j0})Y_{2m}(\theta_j, \phi_j) + (p_j^2 / p_{j0})Y_{2m}(\theta_j, \phi_j)) \]

\( L \) – operator of angular momentum.
From the technical point of view Casimir operator is conveniently expressed in the formalism of the fermion second quantization:

\[ \hat{C} = \hat{B}^\dagger \hat{B} \]

\[ \hat{B}^\dagger = \sum_{\{1,2,3,..,X\}} b_{\{1,2,3,..,X\}}^* a_1^\dagger a_2^\dagger a_3^\dagger \ldots a_X^\dagger \]

\[ \hat{B} = \sum_{\{1,2,3,..,X\}} b_{\{1,2,3,..,X\}} a_X a_{X-1} \ldots a_1 \]

To determine the permutation symmetry in each state obtained by this way the operator:

\[ F_{ij} = \frac{1}{2} (1 + P_{ij}^{sp}) \]

is used. Its mean values are different for different Young frames [f].
This approach as a whole was called Cluster-Nucleon Configuration Interaction Model (CNCIM) and presented first time in the paper [A. Volya, Yu.M. Tchuvil’sky. Phys. Rev. C 91, 044319 (2015)].

The Hamiltonian proposed in the paper [Y. Utsuno, S. Chiba, Phys. Rev. C 83, 021301 (2011)] is used.

For (s-d)-shell nuclei presented bellow the core is 16O and the size of the basis (m-scheme) is about $10^4 \times 10^4$.

For 16O and 10Be the core is 4He. The size of the basis is about $10^{7.5} \times 3 \cdot 10^{7.5}$. 
GENERAL TRENDS OF THE SPECTROSCOPIC FACTORS.

Spectroscopic factors of $\alpha$-clusters in 32S states

![Graph showing spectroscopic factors for different $L$ values.](image-url)
α-cluster strength in 32S spectrum

\[ \frac{(I_{\text{max}} - I(E))}{I_{\text{max}}} \] vs. \( E \) [MeV]
CLUSTER-NUCLEON CONFIGURATION
INTERACTION MODEL AND DESCRIPTION OF
EXPERIMENTAL DATA

$\alpha$-clustering in the ground states of (s-d)-shell
nuclei

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<th>$A_F - A_D$</th>
<th>(S_0^{(exp)})</th>
<th>(S_0^{(exp)})</th>
<th>(S_0^{(exp)})</th>
<th>(S_0^{(old)})</th>
<th>(S_0^{(old)})</th>
<th>(S_0^{(new)})</th>
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α-clustering in 16O
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CONCLUSIONS

1. A theoretical approach and mathematics making possible to calculate cluster spectroscopic amplitudes, form factors and spectroscopic factors of arbitrary nuclear states in advanced versions of the shell model including no-core one is built.
2. It is proved that this the expedient allows one to describe accurately the statistical properties of dense cluster spectra.
3. Using this approach pioneering descriptions of the spectroscopic characteristics of dense spectra of highly excited states of nuclei are obtained.
4. The example demonstrating that the cluster observables may be a tool of the test on the quality of a dynamical model is found.
5. The approach already built looks promising for applications in various areas of the cluster physics.

6. We see ways of great improvement of the developed approach such as: involving of realistic cluster wave functions, description of heavy cluster channels, creation of hybrid models, etc.
THANK YOU FOR ATTENTION!
Alpha-particle states of $^{32}$S nucleus (K.-M.Källman et al.).
There is a possibility to rearrange it in a Schrödinger-like form:

\[
\begin{pmatrix}
\mathcal{N}^{}(ho', \rho'') \\
\mathcal{T}^{}(ho', \rho'') \\
\mathcal{V}^{}(ho', \rho'')
\end{pmatrix}
= 
\begin{pmatrix}
1 \\
\hat{T} \\
\hat{V}
\end{pmatrix}
\begin{pmatrix}
\mathcal{A}^{}_{A_1} \mathcal{A}^{}_{A_2} \frac{1}{\rho^2} \delta(\rho - \rho') Y_{lm}(\Omega_\rho) \\
\mathcal{A}^{}_{A_1} \mathcal{A}^{}_{A_2} \frac{1}{\rho^2} \delta(\rho - \rho'') Y_{lm}(\Omega_\rho)
\end{pmatrix}.
\]

There is a possibility to rearrange it in a Schrödinger-like form:

\[
(\hat{N}_\rho^{-1} \hat{T}_\rho + \hat{N}_\rho^{-1} \hat{V}_\rho - E') \phi(\rho) = 0
\]

but the resulting Hamiltonian turn out to be non-Hermitian one.
FIG. 3: The excitation function for $^{14}$C+$\alpha$ elastic scattering at $180^\circ$ in c.m. frame for the entire energy range measured in this experiment. The solid curve is the best R-matrix fit.

Window of observability.
results in two-body equation of another type:

$$(\hat{T}_\rho + \hat{V}_\rho - E' \hat{N}_\rho)\varphi(\tilde{\rho}) = 0,$$

$$E' = E - E_1 - E_2, \quad \tilde{\rho} = \frac{1}{A_1} \sum_{i=1}^{A_1} \tilde{r}_i - \frac{1}{A_2} \sum_{j=A_1+1}^{A_2} \tilde{r}_j.$$  

where

$$\left\langle \hat{N}^{1/2}_{\rho} \varphi(\tilde{\rho}) \left| \hat{N}^{1/2}_{\rho} \varphi(\tilde{\rho}) \right\rangle = \begin{pmatrix} 1 \\ \delta(E - E'), \delta(k - k'), \text{etc.} \end{pmatrix}$$

and

$$\begin{pmatrix} \hat{N}_\rho \\ \hat{T}_\rho \\ \hat{V}_\rho \end{pmatrix} \varphi(\rho) \equiv \int \begin{pmatrix} N(\rho', \rho) \\ T(\rho', \rho) \\ V(\rho', \rho) \end{pmatrix} \varphi(\rho') \rho'^2 d\rho'.$$
The wave function of the resonating group model is chosen in the form:

\[ \Psi_{A_1 + A_2} = \hat{A}\{\Psi_{A_1} \Psi_{A_2} \varphi(\vec{p})\}, \]

where

\[ \hat{A} = \left( \begin{array}{c} A \\ A_1 \end{array} \right)^{-1/2} \left( 1 + \sum_{p} (-1)^p \hat{P} \right) \]

The A-fermion Schrödinger equation

\[ \hat{H} \Psi_{A_1 + A_2} = E \Psi_{A_1 + A_2}, \quad \hat{H} = \hat{T} + \hat{V}, \]

\[ \hat{T} = \sum_{i=1}^{A_1 + A_2} \frac{\hat{p}_i^2}{2m}, \quad \hat{V} = \sum_{i < j=1}^{A_1 + A_2} V(\vec{r}_i - \vec{r}_j) \]
Introducing a new wave function:

\[ \phi(\tilde{\rho}) = \hat{N}^{1/2}_\rho \varphi(\tilde{\rho}) \]

one can obtain the Schrödinger-like equation with Hermitian Hamiltonian.

\[
\left( \hat{N}^{-1/2}_\rho \hat{T}_\rho \hat{N}^{-1/2}_\rho + \hat{N}^{-1/2}_\rho \hat{V}_\rho \hat{N}^{-1/2}_\rho - E' \right) \phi(\rho) = 0, 
\]

where the habituated orthonormalization conditions take place:

\[ \langle \phi(\tilde{\rho}) | \phi(\tilde{\rho}) \rangle = 1 \] - for states of discrete spectra,

\[ \langle \phi_E(\tilde{\rho}) | \phi_{E'}(\tilde{\rho}) \rangle = \delta(E - E'), \text{ etc.} \] - for continuum states.
OUTGROWS OF RGM

   \[ \Psi = \sum_{A_1, i, A_2, j} A \{ \Psi_{A_1}^i \Psi_{A_2}^j \phi_{ij}(\vec{r}) \} + \sum_k \Psi_{\text{shell}}^k \]

2. Algebraic version of RGM (G.F. Filippopv et al).


4. Many-body RGM (M. Kamimura).

5. Approximate methods
   a) Brink’s method (1957).
   b) Cluster model (B.F. Beyman, A. Bohr, 1958)
   c) Orthogonality conditions model (S. Saito, 1969).
I. Translationally- invariant shell model (TISM)

Cluster fractional parentage coefficient (FPC) is defined as:

\[ F_{MDC}^{nl} = \langle \Psi_M | \hat{A} \{ \Psi_D \phi_{nl}(\tilde{\rho}) \Psi_C \} \rangle \]  

(1)

where: \( \phi_{nl}(\rho) \) – wave function (WF) of the relative motion, \( \Psi_M, \Psi_D, \Psi_C \) – internal translationally-invariant wave functions (WFs) of the mother, daughter nuclei and the cluster respectively. Thus FPC TISM coincides with the SA.
\[ \alpha \text{-clustering in } 10\text{Be} \]

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\(^{(a)}\) The existence of this state is suggested by the existence of 8.070 MeV state in \(^{10}\text{B}\) which could be the isobaric analog, see conceptual discussion in Ref. [20];
\(^{(b)}\) Widths deduced from the isobaric analog channel 
\(^{10}\text{B} \rightarrow ^{6}\text{Li}(0^+) + \alpha\) [21,22];
\(^{(c)}\) results from Ref. [22];
\(^{(d)}\) results from Ref. [23].
\(^{(e)}\) Total width \(\Gamma^{tot}\).
\(^{(f)}\) In Ref. [22] the state was assigned spin-parity 6^+. 

Alpha cluster spectroscopic factors in $^{24}\text{Mg}$

Theoretical calculations in SD shell

Experimental results


Counts/75 keV

Excitation Energy [MeV]

Rotational Structures

Energy $E_{rot}$ [MeV]

J [$\hbar$]
QUANTITATIVE CHARACTERISTICS OF CLUSTERING IN MODERN MICROSCOPIC NUCLEAR MODELS

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Modern studies of the clustering phenomena are dividable into two groups. Typical investigations of the first type are the antisymmetrized molecular dynamics [1] and the fermionic molecular dynamics [2]. In these approaches clustering properties of some low-laying nuclear states are qualitatively confirmed to emerge directly from $NN$-interactions. The cluster structures turn out to be visible as humps in the density distribution in the body-fixed coordinate frame.

Another type of the approaches to clustering explores the quantitative concepts such as the cluster spectroscopic amplitudes, form factors spectroscopic factors, etc. These values provide possibilities to investigate various processes of cluster decay, resonance cluster scattering, cluster break-up and transfer of composite particles. The discussed characteristics are calculated in various versions of the shell model. Binary cluster channels are described in the framework of simple two-body or advanced orthogonality conditions model. In near future one might expect that high-quality resonating group model would be involved.

The present talk demonstrates methods of calculation of the cluster characteristics in modern shell-model approaches such as configuration interaction technique [3] and no-core shell model [4]. The compatibility of the resulted wave functions and two-body channel wave functions is discussed. The cluster decay properties of multitude of low-laying and highly excited states of nuclei are investigated in one and the same procedure with the excitation energies, electromagnetic moments and other characteristics of these states [5,6].