Ab initio calculation of one-nucleon halo states

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Abstract. We develop an approach to microscopic and ab initio description of clustered systems, states with halo nucleon and one-nucleon resonances. For these purposes a basis combining ordinary shell-model components and cluster-channel terms is built up. The transformation of clustered wave functions to the uniform Slater-determinant type is performed using the concept of cluster coefficients. The resulting basis of orthonormalized wave functions is used for calculating the eigenvalues and the eigenvectors of Hamiltonians built in the framework of ab initio approaches. Calculations of resonance and halo states of $^5$He, $^9$Be and $^9$B nuclei demonstrate that the approach is workable and labor-saving.

1. Introduction

The development of ab initio approaches is one of the basic lines of the advancement of nuclear science. Various versions of ab initio No-Core Shell Model (NCSM) using realistic microscopic NN- and 3N-forces [1 – 5] occupy a prominent place in nuclear structure calculations. A typical basis of this model contains all possible nucleon configurations on equal terms up to a certain truncation border. At the same time, well-known properties of nuclei demonstrate “inequality” of different nucleon configurations. For this reason, methods discarding non-relevant components and, due to that, allowing one to involve additional critically important states are also popular [6 – 8]).

One of the major properties of light nuclei is clustering displaying itself in a certain degree of separation of a nucleus to two or more fragments (core, clusters, and loosely bound nucleons). Moreover an accurate description of nucleon fragmentation is crucial for calculation of nuclear reactions. The description of systems manifesting significant fragment separation by use of ordinary shell-model methods leads to calculation problems: a too large shell-model basis is required.

The goals of this work may be formulated as follows. The first is to build up a basis of translationally-invariant $A$-nucleon wave functions of an arbitrary channel manifesting two-fragment separation $A = A_1 + A_2$. The second is to assemble the partial bases corresponding to various channels, which are distinguished by the internal states of the fragments $A_1$ and $A_2$, together in a unified orthogonal basis. The third one is to add to this clustered basis a (relatively small) number of eigenvectors obtained in ordinary shell-model calculations (called “polarization terms” in monograph...
[9]) and in such a way to build a final basis suitable to describe the states manifesting fragmentation (cluster) properties and, in particular, the entrance and exit channels of nuclear reactions.

It should be noted that an approach aimed at an accurate description of reactions induced by light nuclei collisions has been developed in Ref. [10]. This approach also explores matrix mathematics of microscopic Hamiltonians corresponding to the No-Core Shell Model plus Resonating Group Method (i.e. accounting for the clustering) basis. It was called NCSM/RGM. The differences of this scheme and ours are the following. First, we use the concept of cluster coefficients (CCs) to extract the zero vibrations of the centre of mass (CM) of the system. The cluster coefficients formalism is well developed in refs. [11 – 15]. It provides the means to work with a broad variety of excited and rather heavy fragments. Second, applying this formalism we obtain a convenient purely algebraic approach.

The polarization terms were introduced into NCSM/RGM in refs. [16 – 20]. The new model received the name No-Core Shell Model with Continuum (NCSMC). Our approach remains algebraic after involving the polarization terms. Thus, in some sense, the interrelation between the NCSMC and our approach is analogous to the interrelation between the conventional RGM [9, 21, 22] and its algebraic version [23]. In certain examples, in particular in the cases where multi-cluster or multi-channel problems are considered, our approach looks promising.

In this work we present a mathematical formalism suitable for the description of a general two-fragment system, whose applicability is limited by computer power only.

As an example, we discuss the simplest type of fragmentation – the formation of one-nucleon halo states and one-nucleon resonances. Peculiar features of these states make them a very interesting object for the studies of various nuclear processes.

2. Construction of the basis

Let us consider a two-fragment system \(A_1 + A_2\). The cluster-channel terms of the basis are built in the form:

\[
\Psi_A = \frac{1}{\mathcal{W}} \hat{A} \{ \Psi_{A_1} \Psi_{A_2} \phi_{nlm} (\tilde{r}) \}_{JM, J},
\]

(1)

where \(A = A_1 + A_2\), \(\hat{A}\) is the antisymmetrizer, \(\Psi_{A_i}\) is a translationally-invariant wave function (WF) of the fragment; \(\phi_{nlm} (\tilde{r})\) is the oscillator WF of the relative motion.

These terms are labeled by the quantum numbers of the internal cluster states and indices \(n, l, m\).

The main problem is to present function (1) as a linear combination of the Slater determinants (SDs) containing one-nucleon WFs of the oscillator basis:

\[
\phi_{nlm}^{(s)} (r, \sigma) = R_{nl}(r) \nu_{s}^{(\sigma)} (\theta, \varphi) \Theta_{1/2}^{\mu_{s}} (\sigma).
\]

(2)

For these purposes function (1) is multiplied by the function of the zero vibrations of the CM \(\Phi_{000} (\tilde{R})\). This operation is commutative with the antisymmetrization. Then the Talmi-Moshinsky transformation for particles of different masses [24] is performed:

\[
\Phi_{000} (\tilde{R}) \phi_{nlm}^{(s)} (\tilde{r}) = \sum_{N_1, L_1, M_1, N_2, L_2, M_2} \langle 000 | N_1, L_1, M_1, N_2, L_2, M_2 | \Phi_{N_1 L_1 M_1}^{A_1} (\tilde{R}_1) \Phi_{N_2 L_2 M_2}^{A_2} (\tilde{R}_2) \rangle \Phi_{000}^{\tilde{R}} (\tilde{R}).
\]

(3)

Thus, WF (1) is expressed in the form:

\[
\Phi_{000} (\tilde{R}) \Psi_A = \frac{1}{\mathcal{W}} \sum_{N_1, L_1, M_1, N_2, L_2, M_2} \langle 000 | N_1, L_1, M_1, N_2, L_2, M_2 | \hat{A} \Phi_{N_1 L_1 M_1}^{A_1} (\tilde{R}_1) \Phi_{N_2 L_2 M_2}^{A_2} (\tilde{R}_2) \Psi_{A_1} \Psi_{A_2} \rangle_{JM, J}.
\]

(4)
The critical procedure is to transform the products of the CM and internal WFs corresponding to each fragment into a superposition of SDs

$\Phi_{N_j L_j M_j}^A(\vec{R}_j) \Psi_A = \sum_k X_{N_j L_j M_j}^{A(k)} \Psi_{A,k}^{SD}$.

Overlap $X_{N_j L_j M_j}^{A(k)} = \langle \Psi_{A,k}^{SD} | \Phi_{N_j L_j M_j}^A(\vec{R}_j) \rangle \Psi_A$ is called a cluster coefficient. Mathematics of these objects is presented in detail in [15]. There is a large number of methods elaborated for the calculations of CCs. The most general scheme is based on the method of the second quantization of the oscillator quanta. In this scheme the WF of the CM motion is presented as

$\Phi_{N_j L_j M_j}^A(\vec{R}_j) = N_{N_j L_j}^A \left( \hat{\mu}^+ \right)^{N_j - L_j} Y_{N_j L_j} \left( \hat{\mu}^+ \right) \Phi_{000}^A(\vec{R}_j)$.

where $\hat{\mu}^+$ is the creation operator of the oscillator quantum, and its norm is expressed as

$N_{N_j L_j} = \left( -1 \right)^{N_j - L_j} \frac{4\pi}{\left( N_j - L_j \right)! \left( N_j + L_j + 1 \right)!}$.

Thus the CC turns out to be reduced to a matrix element of the tensor operator presented in (6):

$\langle \Psi_{A,k}^{SD} | \Phi_{N_j L_j M_j}^A(\vec{R}_j) \rangle \Psi_A = N_{N_j L_j} \left( \hat{\mu}^+ \right)^{N_j - L_j} Y_{N_j L_j} \left( \hat{\mu}^+ \right) \Phi_{000}^A(\vec{R}_j)$.

Contrary to pioneering work [25] in which translationally-invariant WFs were written in Jacobi coordinates, the formula

$\Psi_A = \Psi_{A,k}^{shell} / \Phi_{000}^A(\vec{R}_j)$

is considered here as the definition of these functions.

Algebraic methods provide possibilities to obtain compact expressions of the CCs in a lot of particular cases. As an example, a general expression for the cluster coefficients of light d-, t-, h-, and α-clusters ($X = 2, 3, 4$) in their lowest shell-model configurations takes the form:

$\langle \prod_{i=1}^X n_i(n_0) : 000 | \Phi_{000}^A(R_C) \rangle \Psi_C = X^{-n/2} \left( \prod_{i=1}^X n_i ! \right)^{1/2} \left( \prod_{j=1}^X \alpha_j ! \right)^{1/2}$.

Symbol $\alpha$ denotes here the multiplicity of each value of $n_i$ in the configuration $\{n_i\}$. The SU(3)-coupling of the one-nucleon WFs is implied here. For the rearrangement of this configuration to the ordinary SD expression the Clebsh-Gordan coefficients of the SU(3) group having a very simple structure are required.

The next step is to build a basis of orthonormalized WFs which includes both the polarization terms and the terms of several cluster channels. The related norm kernel is obtained by the diagonalization of matrix

$\left[ \begin{array}{c} \langle \Psi_{pol}^{(j)} | \Phi_{pol}^{(j)} \rangle \\ \langle \Psi_{pol}^{(j)} | \hat{A} \prod_{i=1}^{l=2} \Phi_{N_j L_j M_j}^A(\vec{R}_j) \Psi_A \rangle \\ \langle \Psi_{pol}^{(j)} | \hat{A} \prod_{i=1}^{l=2} \sum_{i,l=2} \Phi_{N_j L_j M_j}^A(\vec{R}_j) \Psi_A \rangle \end{array} \right] \left[ \begin{array}{c} \prod_{i=1}^{l=2} \Phi_{N_j L_j M_j}^A(\vec{R}_j) \Psi_A \end{array} \right] = \left[ \begin{array}{c} \prod_{i=1}^{l=2} \Phi_{N_j L_j M_j}^A(\vec{R}_j) \Psi_A \end{array} \right] \left[ \begin{array}{c} \prod_{i=1}^{l=2} \Phi_{N_j L_j M_j}^A(\vec{R}_j) \Psi_{pol}^{(j)} \end{array} \right] \left[ \begin{array}{c} \prod_{i=1}^{l=2} \Phi_{N_j L_j M_j}^A(\vec{R}_j) \Psi_{pol}^{(j)} \end{array} \right]$,

in which the square brackets denote the submatrices and the cluster-channel terms symbolically presented in (11) as the products are, in fact, expressed in the form of superpositions of SDs with the help of formula (5). The eigenvectors of the matrix normalized by its eigenvalues give the desirable
basis. Each term of the basis takes the form of a SDs linear combination. Thus the form of such a term is identical to the form of the terms of the ordinary shell-model basis.

Therefore the next step – the computation of the matrix elements of both the kinetic and the potential energy in the discussed basis – is identical in design to the ordinary shell-model computation. Thus, an arbitrary microscopic (ab initio or effective, including two-, three-, etc. nucleon forces) Hamiltonian may be explored. The calculations of the matrix elements of the operators, the estimates of error bars etc. are also analogous to those in the shell-model. The only difference is the list of the basis vectors. This list is significantly shorter compared to the shell-model one. The limitations on the use of the approach are imposed by the dimensionality of the basis vectors. At the same time these restrictions seem to be not so strong compared to the limitations of the canonical NCSMC in the case, where long inter-cluster distances are considered.

This approach as a whole is very flexible due to the possibilities to vary: $A$-, $A_1$-, $A_2$- nucleon shell-model spaces determined by the corresponding truncation border parameters ($N_{\text{max}}^0$), determining the maximal value of the total number of the oscillator quanta in each system, as well as the maximal value of $n$. For example, even the insertion of “unphysical” channels containing the WFs of clusters in their lowest shell-model configurations into the basis turns out to be a step forward in the spectral computations. The basis built before procedure (10) may be orthogonal, non-orthogonal and, if necessary, overloaded. This gives a way to take into account various halo, cluster and other properties of a system. The multi-dimensional ($N_{\text{max}}^0, n, \hbar \omega$)-dependence of the computation results provides a possibility for their extrapolation to the infinite basis space along each discrete variable separately and thus for more reliable estimates of their error bars compared to the shell-model calculation results.

### 3. One-nucleon halo and resonance systems, results and discussion

To demonstrate the capabilities of our approach, in this section we present the results of total and nucleon binding (resonance) energies calculations. The ground states of five- and nine-nucleon systems are considered. Ab initio Hamiltonian Daejeon16 [26] was chosen for these calculations. Widely-used code Antoine is explored for NCSM computations of the internal WFs of the clusters and the polarization terms. For all WFs of nuclei under study the value of the oscillator parameter $\hbar \omega = 15$ MeV was chosen. The computational procedure of each example involves about $10^6$ SDs.

#### 3.1 Five-nucleon system. Lowest resonance state of $^5$He nucleus

The two channels of $^4$He+n fragmentation corresponding to $0^+_1$ and $0^+_2$ states of the core nucleus respectively are considered in these calculations. The truncation border parameter for the polarization terms of nucleus $^4$He is chosen to be $N_{\text{max}}^{^4\text{He}} = 7(9)$. For the clustered terms, the truncation border of the core nucleus $^4$He WF is $N_{\text{max}}^{^4\text{He}} = 2$.

The results of the calculations are presented in Tab. 1.

| $N_{\text{max}}^{^5\text{He}}$ | NCSM | $n_{\text{max}} = 7$ | $n_{\text{max}} = 9$ | $n_{\text{max}} = 11$ | Exp. |
|---|---|---|---|---|---|
| $N_{\text{max}}^{^5\text{He}} = 7$ | $E_{^5\text{He}}$ | 26.37 | 26.40 | 26.51 | 26.57 |
| | $E_n$ | $-1.85$ | $-1.82$ | $-1.71$ | $-1.65$ |
| $N_{\text{max}}^{^5\text{He}} = 9$ | $E_{^5\text{He}}$ | 26.83 | – | 26.87 | 26.92 | 27.41 |
| | $E_n$ | $-1.50$ | – | $-1.46$ | $-1.41$ | $-0.89$ |
The contents of the table demonstrate that the contribution of the additional cluster terms to the total binding energy of $^5$He turns out to be relatively small compared to this energy. Nevertheless, the shift of the resonance energy value by 0.20 MeV or 0.09 MeV respectively caused by the inclusion of the additional cluster terms is not negligible. Having been achieved by using rather modest computational means, this result looks reasonable and therefore the prospects to merge the presented method of one-nucleon resonance states study with the approach developed in [27] are expected to be good.

3.2 Nine-nucleon system

A six-channel model is used for the description of the $^8$Be+n and $^8$Be+p fragmentations of $^9$Be and $^9$B nuclei. These channels contain $0^+_1$, $0^+_2$, $1^+_1$, $1^+_2$, $2^+_1$, $2^+_2$ states of $^8$Be respectively. The truncation border parameter $N(9)_{\text{max}}=9$ is chosen for the performed NCSM calculations, the value of the truncation border parameter of $^8$Be in all cluster channels is chosen to be 4, i.e. the lowest configurations of the core nucleus in the channel WFs are considered.

The results of the calculations are presented in Tab. 2.

|                        | NCSM $(N(9)_{\text{max}}=9)$ | $n_{\text{max}}=5$ | $n_{\text{max}}=7$ | $n_{\text{max}}=9$ | Exp. |
|------------------------|-----------------------------|---------------------|---------------------|---------------------|------|
| $E_{^9\text{Be}}$      | 53.51                       | 37.66               | 37.74               | 37.76               | 58.16|
| $E_n$                  | 1.34                        | 1.46                | 1.54                | 1.56                | 1.66 |
| $E_{^9\text{B}}$       | 51.58                       | 35.74               | 35.84               | 35.91               | 56.31|
| $E_p$                  | –0.59                       | –0.47               | –0.37               | –0.29               | –0.19|
| $\Delta E$            | 1.93                        | 1.93                | 1.90                | 1.85                | 1.85 |

These results allow one to make the following conclusions. First, the calculations using a basis of cluster-channel WFs containing relatively lower configurations of core nucleus result in a significant underestimation of the total binding energies. Thus, taking into account the polarization terms is necessary for an accurate reproduction of these values. At the same time the “differential” quantities: the nucleon binding and resonance energies, the Coulomb energy differences etc. turn out to be well-reproduced in the case, where one and the same truncation border parameter of the core nucleus WFs is used for the construction of the cluster-channel basis and for the computation of the binding energy of the core nucleus. Moreover, it is the differential characteristics of the reaction channels that determine the cross-sections of the respective nuclear reactions. Thus, the method developed here provides a convenient and labor-saving means of ab initio studies of resonance and direct nuclear reactions.

4. Summary

We demonstrate that the formalism of cluster coefficients is a convenient tool to construct a basis that takes into consideration the cluster properties of nuclear systems. This basis looks promising for further ab initio calculations of their characteristics because the adoption of this basis allows one to get rid of most of the components, inherent for the shell model, which do not contribute to the wave functions of the clustered states.
The developed approach is versatile. The basis of this approach includes the shell-model WFs together with various cluster-channel ones, i.e. different versions of the basis conform to the properties of systems under study.

Thus, the approach is suitable for the ab initio computation of clustered systems, halo systems and narrow resonances. The calculations of resonance and halo states of $^5\text{He}$, $^9\text{Be}$ and $^9\text{B}$ nuclei demonstrate the prospects of this approach for nuclear reaction studies.

Our approach may be considered, in parallel with the approaches presented in [10, 16 – 20], as a step towards realizing an ab initio version of a general theory developed by K. Wildermuth and Y.C. Tang that received the name “A Unified Theory of the Nucleus” [9].

Acknowledgments
The work was supported by Russian Science Foundation (RSF), grant No. 16-12-10048.

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