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Two-Cluster Potential Energy and the Pauli Principle

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Abstract. The aim of this paper is to investigate effects of the Pauli principle on the potential energy of a two-cluster system within a microscopic method. We analysed eigenvalues and eigenfunctions of the two-cluster potential energy matrix constructed with oscillator functions for the following nuclei: ^{6}Li$= \alpha + d$, ^{7}Li$= \alpha +^3$H, ^{7}Be$= \alpha +^3$He, ^{8}Be$= \alpha + \alpha$, ^{5}Li$= \alpha + p$, and ^{5}He$= \alpha + n$. In our calculations we used the Minnesota potential, the modified Hasegawa-Nagata potential and Volkov N2 potential as a nucleon-nucleon potential. In general, the eigenvalues of the folding and exact cluster-cluster potential do not diverge considerably. However, the dependence of the exact cluster-cluster potential on the number of the invoked functions reveals a number of resonance states which are absent in the case of folding potential. Such resonance states are mainly localized in the region of small distances between clusters.

1 Introduction

This report is devoted to study of two-cluster potential energy for the light nuclei with a pronounced two-cluster structure within a microscopic method that takes into account the internal structure of the interacting clusters, correctly treats the Pauli principle and relays on a complete set of the oscillator functions to describe relative motion of clusters. This method is an algebraic version of the resonating group method [1]. The resonating group method (RGM [2]) is a powerful tool for studying properties of two-, three- and many cluster systems. This method works perfectly for describing both bound states and different types of reactions. The main advantages of the method are that (i) it takes into account the internal structure of interacting clusters and (ii) correctly treats the Pauli principle. An important peculiarity of the RGM is that being applied to two- or three-cluster systems it reduces in a self-consistent way the A-body problem to a two- or three-body problem. RGM strongly relies on the translation invariant many-body shell model as this model supplies the wave functions describing the internal structure of clusters. It is natural also to use oscillator wave functions for describing the inter-cluster motion.

The Pauli principle has been investigated many times and from different points of view.Many results have been obtained revealing effects of the anti-

symmetrization on the structure of bound states and dynamics of reactions in two- and three-cluster systems. Meanwhile, we are going to demonstrate that some interesting properties of the Pauli principle were hidden and we are going to reveal some new interesting features. We will demonstrate how the antisymmetrization affects cluster-cluster potential energy.

It is important to notice that the total interaction of two-cluster system originates from nucleon-nucleon interaction and also from the kinetic energy operator. The influence of the Pauli principle on the kinetic energy of relative motion of two clusters has been investigated in Refs. [3–6]. In the present paper will consider only the first part of the cluster-cluster potential.

2 Method

A wave function of A-nucleon systems for the partition $A = A_1 + A_2$ is

$$\Psi_{LM} = \widehat{\mathcal{A}} \left\{ \left[\psi_1 \left(A_1, s_1, b \right) \psi_2 \left(A_2, s_2, b \right) \right]_S f_L \left(q \right) Y_{LM} \left(\widehat{\mathbf{q}} \right) \right\}, \qquad (1)$$

where $\psi_\nu \left(A_\nu, s_\nu, b \right)$ is a fully antisymmetric function, describing internal structure of the νth cluster, $\widehat{\mathcal{A}}$ is the antisymmetrization operator permuting nucleons belonging to different clusters and $\mathbf{q}$ is the Jacobi vector determining distance between interacting clusters. We assume that we deal with the s-clusters only, it means that the intrinsic orbital momentum of each cluster equals to zero. The total spin S is a vector sum of the individual spins s_1 and s_2.

Inter-cluster wave function $f_L \left(q \right)$ is a solution to the integro-differential equation. This equation can be much easily solved, when the function (1) is expanded into a complete set of the the antisymmetric cluster basis functions

$$\left| nL \right\rangle_C = \widehat{\mathcal{A}} \left\{ \left[\psi_1 \left(A_1, s_1, b \right) \psi_2 \left(A_2, s_2, b \right) \right]_S \Phi_{nL} \left(q, b \right) Y_{LM} \left(\widehat{\mathbf{q}} \right) \right\}, \qquad (2)$$

where n is the number of radial quanta, b is the oscillator length b. Functions $\left| nL \right\rangle_C$ are normalized not to unity, but to eigenvalues Λ_{nL} of the norm kernel:

$$\left\langle nL | \widetilde{n} L \right\rangle_C = \Lambda_{nL} \delta_{n,\widetilde{n}}.$$

By using the cluster basis functions (2), one obtains the two-cluster Schrödinger equation in the form

$$\sum_{m=0} \left\{ \left\langle nL \left| \widehat{H} \right| mL \right\rangle_C - E \Lambda_{nL} \delta_{n,m} \right\} C_{mL} = 0, \qquad (3)$$

where $\left\langle nL \left| \widehat{H} \right| mL \right\rangle_C$ is a matrix element of a microscopic two-cluster Hamiltonian, C_{nL} is the expansion coefficient.

If we omit the antisymmetrization operator in the expression for the wave function, we have got the so-called folding approximation.

$$\Psi_{LM}^{(F)} = \left[\psi_1 \left(A_1, s_1, b \right) \psi_2 \left(A_2, s_2, b \right) \right]_S f_L^{(F)} \left(q \right) Y_{LM} \left(\widehat{\mathbf{q}} \right). \qquad (4)$$

This approximate form is valid when the distance between clusters is large and effects of the Pauli principle is negligible small. The exact two-cluster potential is a nonlocal operator, as opposed to the folding cluster-cluster potential. The idea is to compare the exact and folding two-cluster potentials via separable representation of the potentials. As a tool for this study we employ the method suggested in our recent paper [7]. We will construct matrix of potential energy and then analyze its eigenvalues and eigenfunctions of the matrix. The eigenfunctions will be analyzed in the oscillator, coordinate and momentum representations. Involving three different spaces allows us to get more complete picture on the nature and properties of potential energy eigenfunctions.

Having constructed matrix of potential energy $\left\|\left\langle nL\left|\widehat{V}\right|mL\right\rangle\right\|$ of dimension $N\times N$, we can calculate eigenvalues λ_α (α=1, 2, ..., N) and corresponding eigenfunctions $\{U_n^\alpha\}$ of the matrix. Diagonalization of the potential energy matrix generates a new set of inter-cluster functions ϕ_α and two-cluster wave functions Ψ_α

$$\phi_\alpha\left(q,b\right)=\sum_n U_n^\alpha\Phi_{nL}\left(q,b\right) \tag{5}$$

$$\Psi_\alpha=\widehat{\mathcal{A}}\left\{\psi_1\left(A_1\right)\psi_2\left(A_2\right)\phi_\alpha\left(q,b\right)Y_{LM}\left(\widehat{\mathbf{q}}\right)\right\}. \tag{6}$$

The functions $\phi_\alpha\left(q,b\right)$ and eigenvalues λ_α enable us to construct inter-cluster nonlocal potential

$$\widehat{V}_N\left(q,\widetilde{q}\right)=\sum_{\alpha=1}^{N}\phi_\alpha\left(q,b\right)\lambda_\alpha\phi_\alpha\left(\widetilde{q},b\right). \tag{7}$$

In what follows we are going to study properties of the eigenvalues and eigenfunctions of the potential energy operator in the oscillator representation $\{U_n^\alpha\}$, coordinate $\phi_\alpha\left(q,b\right)$ and momentum $\phi_\alpha\left(p,b\right)$ spaces.

For a two-body case, the eigenfunctions $\phi_\alpha\left(q,b\right)$ or $\phi_\alpha\left(p,b\right)$ would immediately define a wave function and t-matrix, as it was demonstrated in Ref. [7]. However, in two-cluster systems the antisymmetrization is known to affect the kinetic energy and norm kernel and thus the kinetic energy and norm kernel participate in creating the effective cluster-cluster interaction as well.

In the present paper we consider only the part of the cluster-cluster potential generated by the nucleon-nucleon potential with the focus on the Pauli effects. The first effect of the Pauli principle on two-cluster systems is connected with appearance of the Pauli forbidden states, which correspond to zero eigenvalues of the norm kernel. The second effect of the Pauli principle is related to the eigenvalues of the Pauli-allowed states which are not equal to unity. It has been shown in [3] that the kinetic energy operator of two-cluster relative motion modified by the Pauli principle generates an effective interaction between clusters. It is interesting to analyze how the eigenvalues of the norm kernel change potential energy of two-cluster system.

3 Results and Discussion

The object of the investigation is the lightest nuclei of p-shell with a dominant alpha-cluster channel shown in Table 1.

Table 1. List of nuclei and two-cluster configurations

Nucleus	^{5}He	^{5}Li	^{6}Li	^{7}Li	^{7}Be	^{8}Be
Configuration	^{4}He+n	^{4}He+p	^{4}He+d	^{4}He+^{3}H	^{4}He+^{3}He	^{4}He+^{4}He

We employ three nucleon-nucleon potentials which have been often used in different realizations of the cluster model. In our calculations we involve the Volkov N2 (VP) [8], modified Hasegawa-Nagata (MHNP) [9,10] and Minnesota (MP) [11] potentials. Coulomb forces are also involved in calculations and treated exactly. For the sake of simplicity we neglect the spin-orbit forces, thus the total spin S and the total orbital momentum L are good quantum numbers. Oscillator length b is selected to optimize energy of the lowest decay threshold for each nucleus and for each NN potential. In what follows, it is assumed the energy of two-cluster systems is determined with respect to the two-cluster threshold.

The optimal values of b are shown in Tab 2.

Table 2. Oscillator length b in fm for different nuclei and different potentials.

Nucleus	VP	MHNP	MP
^{5}He, ^{5}Li	1.38	1.32	1.28
^{6}Li	1.46	1.36	1.31
^{7}Li, ^{7}Be	1.44	1.36	1.35
^{8}Be	1.38	1.32	1.28

Figure 1 shows the eigenvalues of the exact and folding potential energy matrix generated by the MHNP for the 1^- state of ^{7}Be.

We can observe from Figure 1 that the eigenvalues of the potential energy matrix calculated with antisymmetrization are very close to those determined in the folding approximation. The lowest eigenvalues almost coincide indicating that both potentials have the same depth. One can also see that exact potential is less attractive at the range $5 < \alpha < 30$. For $\alpha > 50$ the exact potential is very close to the folding potential. Similar behavior of eigenvalues is observed for all lightest nuclei of the p-shell and for all NN potentials involved in our calculations.

In Figure 2 we show dependence of the eigenvalues λ_α on the number of oscillator functions involved in calculations. These results are obtained for $L^\pi = 1^-$ state of ^{7}Be with the MHNP.

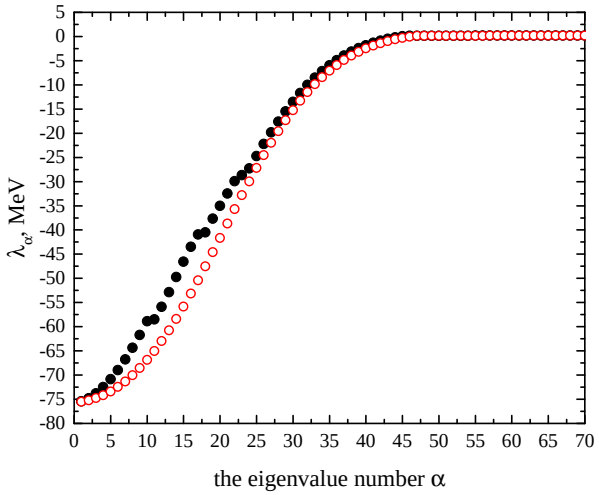

Figure 1. Eigenvalues of the exact (solid circles) and folding (open circles) potential energy matrix for the 1^- state of ^{7}Be. Results are obtained with the MHNP.

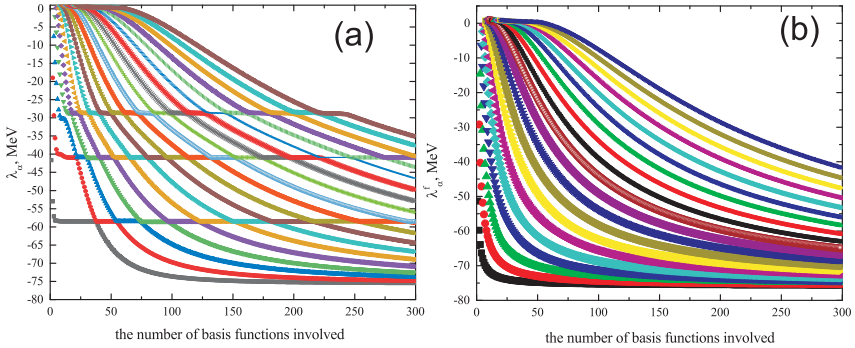

Figure 2. Eigenvalues of the exact (a) and folding (b) potential energy matrix as a function of the number N of oscillator functions involved in calculations. Results are obtained for the 1^- state in ^{7}Be with the MHNP.

As can be seen from Figure 2, the dependence of eigenvalues of the exact potential on the number of functions exhibits resonance behavior. Contrary, none of the eigenstates of the folding potential has a resonance behavior.

In Figure 3 we compare eigenvectors for ^{8}Be and ^{7}Be with and without antisymmetrization for the MHNP.

One can see that they are quite different. The Pauli principle makes zero the first 50 expansion coefficients U^α_n. So, we can conclude that the eigenfunctions of the exact potential corresponding to non-resonance values of α is suppressed at the range $n < 50$ due to the influence of the Pauli principle. The eigenfunc-

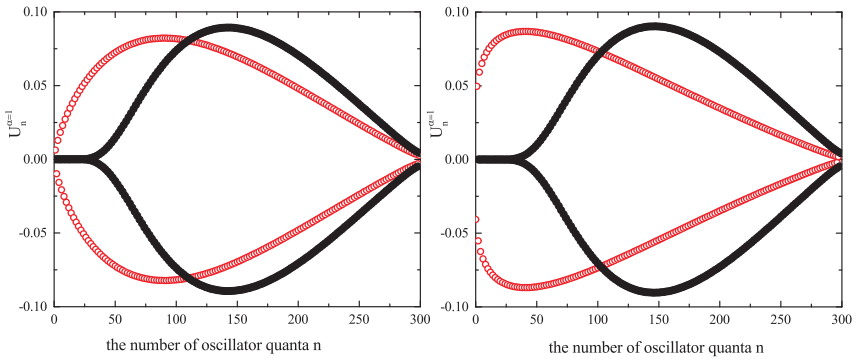

Figure 3. The eigenfunctions of the exact (solid circles) and folding (open circles) potential energy in oscillator representation for the 1^- state in ^{7}Be (left panel) and the 0^+ state in ^{8}Be (right panel). Results are obtained with the MHNP.

tions of the folding potential have a maximum at lower number of quanta than the eigenfunctions of the exact potential. It is also worth noting that different behaviour of the eigenfunctions of the folding potential at small values of n for ^{7}Be and ^{8}Be is caused by different values of orbital momenta.

Figure 4 presents the eigenfunctions of the potential energy operator for the 0^+ state in ^{8}Be in the momentum space for $\alpha = 1$, 2 and 3.

A huge repulsive core in the MHNP and the Pauli principle make eigenfunctions $\phi_\alpha(p)$ to vanish in a large range of $0 < p < 10$ fm^{-1}.

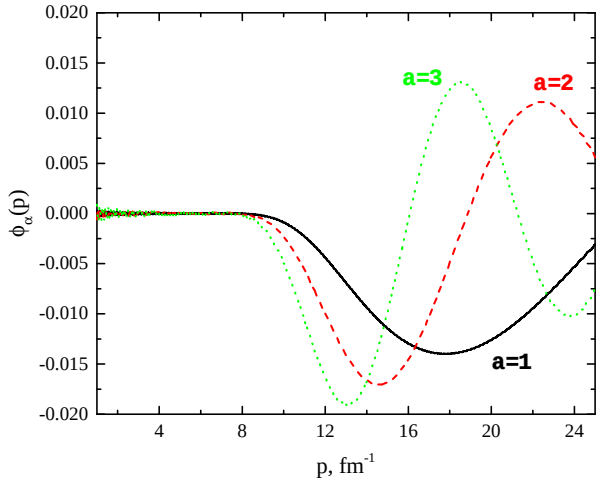

Figure 4. The eigenfunctions of the potential energy operator for the 0^+ state in ^{8}Be in the momentum representation. Results are obtained with the MHNP.

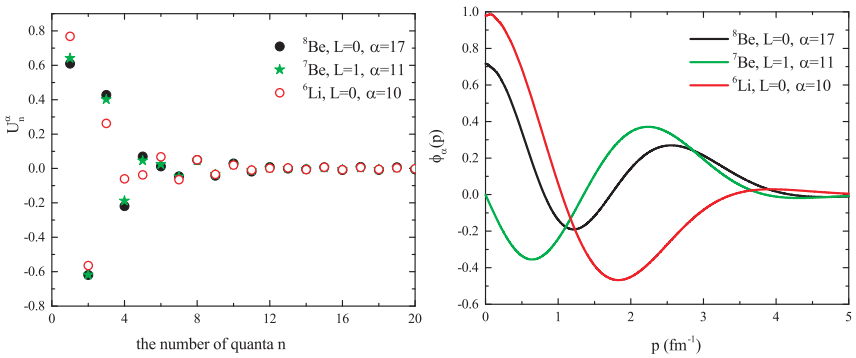

Figure 5. Wave functions of the resonance states in ^{8,7}Be and ^{6}Li in oscillator representation (left panel) and momentum representation (right panel). Results are obtained with the MHNP

Now let us consider wave functions of trapped and resonance states in the two-cluster systems. Wave functions of the resonance states in ^{8,7}Be and ^{6}Li in oscillator and momentum representation are shown in Figure 5.

We can conclude that the eigenfunctions of resonance states describe a compact configuration, because they are localized at low values of oscillator quanta and momentum.

Eigenvalues of the potential energy matrix generated by the Volkov N2 potential are shown in Figure 6 for the 1^- state of ^{5}He.

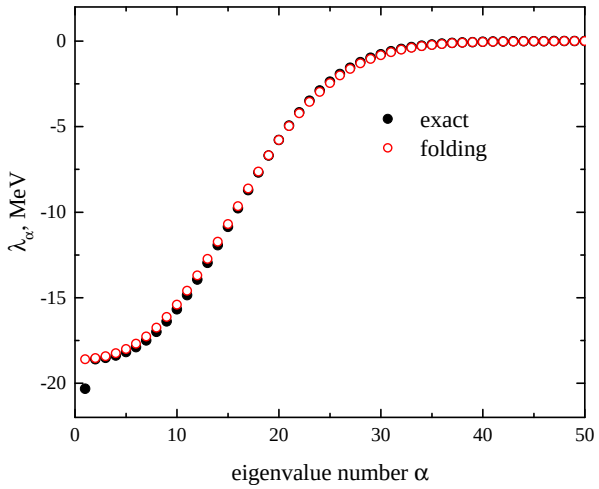

Figure 6. Eigenvalues of the exact (solid circles) and folding (open circles) potential energy matrix for the 1^- state of ^{5}He. Results are obtained with the VP.

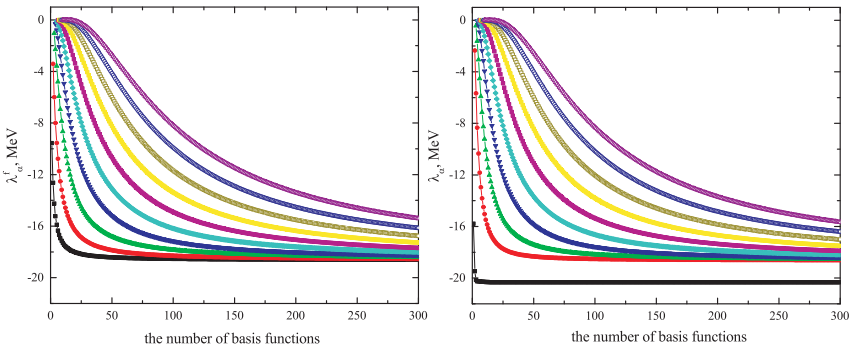

Figure 7. Eigenvalues of the exact (right pane) and folding (left panel) potential energy matrix as a function of the number of oscillator functions involved in calculations. Results are obtained for the 1^- state in ^{5}He with the VP.

The eigenvalues of the exact VP differ from those of the folding potential at a single point $\alpha = 1$. The eigenvalue $\lambda_{\alpha=1}$ corresponds to a "trapped" state. This conclusion follows from Figure 7, where the dependence of the eigenvalues of the potential energy matrix as a function of the number of oscillator functions involved in calculations is shown for the 1^- state in ^{5}He.

Figure 7 shows fast convergence of the first eigenvalue of the exact potential energy matrix.

Wave functions of the trapped state in ^{5}He, ^{6}Li and ^{7}Be in oscillator representation are shown in Figure 8.

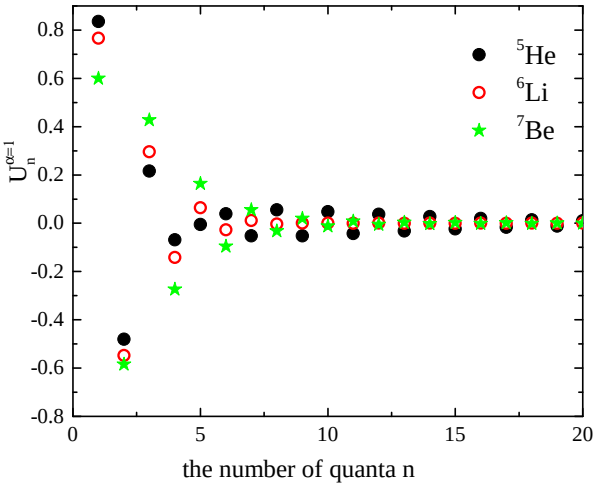

Figure 8. Wave functions of the trapped state in ^{5}He, ^{6}Li and ^{7}Be in oscillator representation. Results are obtained with the VP.

The wave functions of the trapped state have an exponential asymptotic behavior. Thus, there is a full resemblance of these functions with a true bound state wave function which is usually observed in coordinate space. The asymptotic part of the wave functions of resonance states has an oscillatory behavior (Figure 5). The node of the trapped state wave functions appears due to the orthogonality of this state to the Pauli forbidden states in two-cluster systems.

It is interesting to note that a trapped state in the VP appears only for the cluster configurations characterized by the eigenvalues of the norm kernel $\Lambda_n > 1$. Namely, the VP generates a "trapped" state in the states of normal parity in ^{5}He, ^{5,6,7}Li and ^{7}Be. MP also produces a "trapped" state in ^{6}Li.

4 Conclusion

We investigated effects of antisymmetrization on the potential energy of cluster-cluster interaction within a microscopic method – an algebraic version of the resonating group method. For this aim we have studied eigenfunctions and eigenvalues of the potential energy matrix, calculated within a basis of the cluster oscillator functions. It was shown that the eigenvalues of the potential energy calculated with the full antisymmetrization do not differ much from the eigenvalues obtained in the folding approximation. However, the eigenfunctions in those cases are quite different.

Dependence of eigenvalues of the exact potential on the number of functions exhibits resonance behavior, contrary to the eigenvalues of the folding potential. The Pauli exclusion principle can produce trapped and resonance states in two-cluster potential energy. Both trapped and resonance states have a compact wave function of two-cluster systems. This compactness is observed in the oscillator, momentum and coordinate spaces. The trapped states have an exponential asymptotic tail, while the resonance states have an oscillating asymptotic tail.

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