Journal of Physics: Conference Series **111** (2008) 012055 doi:10.1088/1742-6596/111/1/012055

Faddeev type of equations for three-cluster systems with full treatment of the Pauli principle

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Abstract. We analyze peculiarities of the Pauli principle in thrre-cluster system. We demonstrated that the antisymmetrization operator, being a source of the three-body interaction, can be decomposed into components involving either permutations between all three clusters, or permutations between two clusters only. Introducing this into the Faddeev equations, one obtains three alternative but equivalent formulations. These sets of equations are presented in operator form, for practical applications we will make use full set of the oscillator functions.

1. Introduction

The Resonating Group Method (RGM) is a well-established approach to three-cluster nuclear systems. It leads to both bound and scattering states using a coupled channels approach. It is a rigorous an self-consistent method for taking into account exactly the Pauli principle, but is computationally expensive and has slow convergence properties.

The Faddeev formalism on the other hand has no problems dealing with the non-orthogonality of channels, and is much more suitable for implementing the boundary conditions for two- and three-cluster asymptotics. It was also demonstrated repeatedly that the Faddeev approach is computationally more efficient. This led to numerous attempts to extend the Faddeev formalism to three-cluster systems (see for instance [1], [2], [2], [3], [4], [5], [3], [6], [7],[8], [9]). Because of complexity, which arise from the Pauli principle, many of these attempts were concentrated on simplified and approximate treatment of the Pauli principle.

The key issue to extend the formalism to three-cluster systems is the correct and full treatment of the Pauli principle. It is well-known that full antisymmetrization leads to non-local, energy-dependent inter-cluster interaction. In addition, in a three-cluster system the antisymmetrization operator is a source of three-body interactions originating from the two-body nucleon-nucleon (NN) interaction, but also from the kinetic energy and overlap kernel.

We want to address these difficulties by starting from the RGM wave function, and introduce it in the Faddeev equations. This wave function will then exhibit three Faddeev amplitudes, each with their appropriate set of boundary conditions. The antisymmetrization operator is then decomposed into components involving either permutations between all three clusters, or permutations between two clusters only. Introducing this into the Faddeev equations, one obtains three alternative but equivalent formulations.

In this paper we restrict ourselves to the clusters from s-shell nuclei, i.e. to clusters consisting of $1 \leq A \leq 4$ nucleons. It is made for the sake of simplicity. However, analysis and results, presented here, are valid for any three-cluster system.

Note, that in our previous papers [10], [11], [12] we introduced the Faddeev amplitudes in the Resonating Group Method and made use the formalism of couple-channels equations. In [10], [11] it allowed us to study resonance states of ^4H, ^4He and ^4Li, created by the three-cluster configuration $d+N+N$. In [12] we make use of the Faddeev components to investigate cluster polarization on discrete and continuous spectrum states in ^7Be. These papers confirm the effectiveness of usage of the Faddeev amplitudes within the RGM.

2. Definitions and Notations

In this section we introduce all necessary pieces of three-cluster hamiltonian and wave function. We start with a hamiltonian. The microscopic hamiltonian for a three-cluster configuration is given by

$$\widehat{H} = \widehat{T} + \widehat{V} = \sum_{\alpha=1}^{3} \widehat{H}_{\alpha}^{(1)} + \widehat{T}_r + \sum_{\alpha} \widehat{V}_{\alpha} \tag{1}$$

i.e. a sum of three single-cluster hamiltonians $\widehat{H}_{\alpha}^{(1)}$ describing the internal structure of each cluster, and a term responsible for the inter-cluster dynamics. The latter consists of the kinetic energy operator for relative motion of clusters $\widehat{T}_r$ and the potential energy of interaction between clusters. This hamiltonian can be also expressed as a sum of two-cluster hamiltonians, and a hamiltonian representing the interaction of the third cluster with both other clusters

$$\widehat{H} = \widehat{H}_{\alpha}^{(2)} + \widehat{H}_{\alpha}^{(1)} + \widehat{T}_{\alpha} + \sum_{\beta \neq \alpha} \widehat{V}_{\beta}. \tag{2}$$

By omitting interaction $\sum_{\beta\neq\alpha} \widehat{V}_{\beta}$,we obtain so-called channel hamiltonian

$$\widehat{H}_{\alpha}^{(c)} = \widehat{H}_{\alpha}^{(2)} + \widehat{H}_{\alpha}^{(1)} + \widehat{T}_{\alpha}, \tag{3}$$

which determine asymptotic properties of three cluster system, when one cluster is far from two-cluster subsystem. Here we used the following notation:

$$\widehat{T}_r = \frac{\hbar^2}{2m}\Delta_{\mathbf{x}_\alpha} + \frac{\hbar^2}{2m}\Delta_{\mathbf{y}_\alpha}, \quad \widehat{T}_{\alpha} = \frac{\hbar^2}{2m}\Delta_{\mathbf{y}_\alpha}, \tag{4}$$

$$\widehat{H}_{\alpha}^{(1)} = \sum_{i\in A_\alpha} \widehat{T}(i) + \sum_{i<j\in A_\alpha} \widehat{V}(ij) \tag{5}$$

$$\widehat{H}_{\alpha}^{(2)} = \sum_{i\in A_\beta + A_\gamma} \widehat{T}(i) + \sum_{i<j\in A_\beta + A_\gamma} \widehat{V}(ij) \tag{6}$$

$$\widehat{V}_{\alpha} = \sum_{i\in A_\beta} \sum_{j\in A_\gamma} \widehat{V}(ij) \tag{7}$$

where $\mathbf{x}_\alpha$ is the Jacobi vector, proportional to the distance between β and γ clusters, while $\mathbf{y}_\alpha$ is a Jacobi vector connecting the α cluster to the center of mass of the β and γ clusters:

$$\mathbf{x}_\alpha = \sqrt{\frac{A_\beta A_\gamma}{A_\beta + A_\gamma}} \left(\frac{1}{A_\beta} \sum_{j\in A_\beta} \mathbf{r}_j - \frac{1}{A_\gamma} \sum_{k\in A_\gamma} \mathbf{r}_k \right) \tag{8}$$

$$\mathbf{y}_\alpha = \sqrt{\frac{A_\alpha (A_\beta + A_\gamma)}{A_\alpha + A_\beta + A_\gamma}} \left(\frac{1}{A_\beta + A_\gamma} \left[\sum_{j\in A_\beta} \mathbf{r}_j + \sum_{k\in A_\gamma} \mathbf{r}_k \right] - \frac{1}{A_\alpha} \sum_{i\in A_\alpha} \mathbf{r}_i \right) \tag{9}$$

The indexes α, β and γ form a cyclic permutation of 1, 2 and 3.

We will also use notation $\widehat{H}_0$ for the sum of internal single-cluster hamiltonians

$$\widehat{H}_0 = \sum_\alpha \widehat{H}_\alpha^{(1)} \tag{10}$$

The wave function for s-shell clusters can be written as

$$\Psi^J = \widehat{\mathcal{A}} \left\{ \Phi_1 \left(A_1 \right) \Phi_2 \left(A_2 \right) \Phi_3 \left(A_3 \right) \left[f_1 \left(\mathbf{x}_1, \mathbf{y}_1 \right) + f_2 \left(\mathbf{x}_2, \mathbf{y}_2 \right) + f_3 \left(\mathbf{x}_3, \mathbf{y}_3 \right) \right] \right\} \tag{11}$$

where $\Phi_\alpha \left(A_\alpha \right)$ is a shell-model wave function for the internal motion of cluster α ($\alpha = 1, 2, 3$) and $f_\alpha \left(\mathbf{x}_\alpha, \mathbf{y}_\alpha \right)$ is a Faddeev amplitude. The expectation values of internal cluster hamiltonian

$$\mathcal{E}_\alpha = \left\langle \Phi_\alpha \left(A_\alpha \right) \left| \widehat{H}_\alpha^{(1)} \right| \Phi_\alpha \left(A_\alpha \right) \right\rangle$$

gives energy of bound state of cluster consisting of A_α nucleons. For the sake of simplicity we assume that each cluster has only one bound state, which is totally correct for s-shell nuclei.

As $\Phi_\alpha \left(A_\alpha \right)$ is an antisymmetric function of A_α nucleon system, then the antisymmetrization operator in eq. (11) permutes nucleons from different clusters. It was indicated in [11], [10] that such an operator can be presented as

$$\widehat{\mathcal{A}} = 1 + \widehat{\mathcal{A}}_{12} + \widehat{\mathcal{A}}_{23} + \widehat{\mathcal{A}}_{31} + \widehat{\mathcal{A}}_{123}, \tag{12}$$

where $\widehat{\mathcal{A}}_{\alpha\beta}$ exchanges nucleons from clusters α and β, and $\widehat{\mathcal{A}}_{123}$ permutes particles from all three clusters. Note that the operator $\widehat{\mathcal{A}}_{\alpha\beta}$ consists of two-particle, three-particle, ..., $\min\left(A_\alpha, A_\beta\right)$-particle permutation operators.

If we omit the antisymmetrization operator or take the simplest form of the operator $\widehat{\mathcal{A}} = 1$, then we go over to the well-known folding approximation. In this approximation wave function is

$$\Psi = \left\{ \Phi_1 \left(A_1 \right) \Phi_2 \left(A_2 \right) \Phi_3 \left(A_3 \right) \left[f_1 \left(\mathbf{x}_1, \mathbf{y}_1 \right) + f_2 \left(\mathbf{x}_2, \mathbf{y}_2 \right) + f_3 \left(\mathbf{x}_3, \mathbf{y}_3 \right) \right] \right\} \tag{13}$$

It can be easily shown that in case of folding approximation a three-cluster system is reduced to the three-body system with a local two-body folding interaction and the Faddeev equations can be easily formulated for this case.

It is important to note that the structure of the antisymmetrization operator, presented in eq. (12), means that the total wave function, being totally antisymmetric, contains parts which have different permutational symmetry. For instance, first two terms of the antisymmetrization operator $(1 + \widehat{\mathcal{A}}_{12})$ being applied to the three-cluster wave function (13) make this function antisymmetric with respect to permutations of nucleons from the first and second clusters.

3. Faddeev equations for three-cluster systems

When considering many-cluster or many-channel nuclear or atomic systems, one usually works with symmetric (with respect to particle permutations) hamiltonian and antisymmetric wave functions. Antisymmetrization operator is making use to construct fully antisymmetric wave functions. In fact, the operator is a projection operator, which transform or project non antisymmetric many-particle functions to part of the Hilbert space, spanned by antisymmetric functions. There is other possibility to consider system of identical particles. We may work with arbitrary non antisymmetric many-particle function, provided that hamiltonian is antisymmetric one. It can be done by multiplying microscopical hamiltonian by the antisymmetrization operator. The Schrödinger equation for three-cluster system can be presented in the form

$$\left(\widehat{H}_0 + \widehat{T} + \widehat{V} - E \right) \Psi = 0 \tag{14}$$

for antisymmetric function

$$\Psi = \widehat{\mathcal{A}}\left\{\Phi_1\Phi_2\Phi_3 f\left(\mathbf{x},\mathbf{y}\right)\right\}$$

and

$$\left(\widehat{\mathcal{A}}\widehat{H}\widehat{\mathcal{A}} - E\widehat{\mathcal{A}}\right)\underline{\Psi} = 0 \tag{15}$$

or

$$\left(\widehat{H}\widehat{\mathcal{A}} - E\widehat{\mathcal{A}}\right)\underline{\Psi} = 0 \tag{16}$$

for non antisymmetric function

$$\underline{\Psi} = \Phi_1\Phi_2\Phi_3 f\left(\mathbf{x},\mathbf{y}\right)$$

We underline non antisymmetric functions ($\underline{\Psi}$) in order to distinguish them from fully antisymmetric functions (Ψ). Modified hamiltonian $\widehat{\mathcal{A}}\widehat{H}\widehat{\mathcal{A}}$, or $\widehat{H}\widehat{\mathcal{A}}$ will be acting as a projection operator. We will show that such form of the Schrödinger equation (eq. (15) or (16)) is more suitable for analysis of three-cluster system and for formulation of exact and approximate form of the Faddeev-type of equations. Note that equations (15) and (16) are identical because of the idempotent properties of the antisymmetrization operator $\widehat{\mathcal{A}}^2 = \widehat{\mathcal{A}}$ and because $\left[\widehat{H},\widehat{\mathcal{A}}\right] = 0$.

Remain that the operator of potential energy is a sum of three terms $\widehat{V} = \sum_\alpha \widehat{V}_\alpha$and operator $\widehat{\mathcal{A}}$ is

$$\widehat{\mathcal{A}} = 1 + \sum_\alpha \widehat{\mathcal{A}}_\alpha + \widehat{\mathcal{A}}_{123}$$

where $\widehat{\mathcal{A}}_\alpha$ stands for the operator $\widehat{\mathcal{A}}_{\beta\gamma}$ from eq. (12). Consider operator $\widehat{V}\widehat{\mathcal{A}}$. It can be presented as

$$\widehat{V}\widehat{\mathcal{A}} = \sum_\alpha \widehat{V}_\alpha + \widehat{V}\sum_\alpha \widehat{\mathcal{A}}_\alpha + \widehat{V}\widehat{\mathcal{A}}_{123}$$

First two terms on the right hand side of this equation have a simple meaning. This term is a sum of three folding potentials, i. e. potential energies of two-cluster interaction when the antisymmetrization is switched off. The second term can be presented as

$$\widehat{V}\sum_\alpha \widehat{\mathcal{A}}_\alpha = \sum_\alpha \widehat{V}_\alpha\widehat{\mathcal{A}}_\alpha + \sum_\alpha \left(\widehat{V} - \widehat{V}_\alpha\right)\widehat{\mathcal{A}}_\alpha$$

The first term $\widehat{V}_\alpha\widehat{\mathcal{A}}_\alpha$ is potential energy of two cluster subsystem when antisymmetrization is within this two-cluster subsystem only. The second term $\left(\widehat{V} - \widehat{V}_\alpha\right)\widehat{\mathcal{A}}_\alpha$ is a folding potential energy of interacting of third cluster with two-cluster subsystem. We call this term folding potential because antisymmetrization between nucleons of third cluster and nucleons of two-cluster subsystem is absent. It is well known, that in order to determine folding interaction, one needs to know density distribution of neutron and proton matter in interacting clusters. Last term of this equation represent interaction between two clusters when permutations of nucleons from all three clusters are in action (enable). This term is a part of three-body type of interaction between clusters. The other parts of three-body type of interaction are connected with the kinetic energy operator, overlap and internal hamiltonians $\widehat{H}_\alpha^{(1)}$. It means, as pointed out above, that three-body interaction originated from those terms of the total hamiltonian and overlap, where three-cluster exchange term $\widehat{\mathcal{A}}_{123}$ is presented.

To proceed with formulating and solving three-cluster equations of Faddeev type, one needs to solve two-cluster equations in order to define energies of bound states (which determine the threshold energies) and wave functions of bound states, if they exist. Two-cluster hamiltonian to be used with nonantisymmetric wave function is

$$\widehat{\mathcal{A}}_\alpha^{(2)}\widehat{H}_\alpha^{(2)}\widehat{\mathcal{A}}_\alpha^{(2)} = \widehat{H}_\alpha^{(2)}\widehat{\mathcal{A}}_\alpha^{(2)}$$

Antisymmetrization operator $\widehat{\mathcal{A}}_\alpha^{(2)} = \left(1 + \widehat{\mathcal{A}}_\alpha\right)$ will eliminate the Pauli forbidden states and make two-cluster function antisymmetric with respect to permutation of any pair of nucleons of $A_\beta + A_\gamma$ - nucleons system. This operator can be also sandwiched between non antisymmetric functions of three-cluster system. Two-cluster channel hamiltonian is simplified form of three-cluster hamiltonian in which interaction of third cluster with two-cluster subsystem and total antisymmetrization is neglected.

Before formulating the Faddeev equations for three-cluster systems let us consider the Faddeev equations for three structureless particles. In the differential form these equations can be written as

$$\left(\widehat{T} + \widehat{V}_\alpha - E\right)\Psi_\alpha = -\widehat{V}_\alpha\left[\Psi_\beta + \Psi_\gamma\right] \tag{17}$$

The left hand side of this set of equations contains the asymptotic form of the equation for amplitude Ψ_α. This is because that at certain conditions the right hand side can be neglected (see details for instance in [13], [14]). The asymptotic part of the amplitude Ψ_α contains two components, first of them describes scattering of particle with an index α on bound state of two-body subsystem consisting of particles β and γ. The second component of the amplitude Ψ_α describes three-body breakup process.

One may expect the similar asymptotic regimes in the case of three-cluster systems. First regime is connected with scattering of a cluster with index α on bound state(s) of two-cluster subsystem, the second regime corresponds to three-cluster decay of the compound three-cluster system. In the former case two-cluster antisymmetrization operator $\widehat{\mathcal{A}}_\alpha^{(2)}$ has to be taken into account. In the latter case all three cluster are well separated and thus one can neglect the antisymmetrization operator.

By concluding these statements, we can suggest three different sets of the Faddeev type of equations for three-cluster systems. In first case the left had side of the Faddeev equations will not contain antisymmetrization operator. In the second case the left had side of the Faddeev equations will contain two-cluster antisymmetrization operator. The asymptotic part of such equations will describe both two and three-body regimes of three-cluster systems. The left had side of the third set of Faddeev equations will contain the total antisymmetrization operator $\widehat{\mathcal{A}}$. This is done in order to reduce the coupling between different channels of three-cluster system. We have to stress that all three sets of the Faddeev equation are equivalent. The difference between them arises from those part of the total antisymmetrization operator which generates three-body inter-cluster forces. It was shown in [15] (see also [14]) that there several equivalent way of including three-body forces in the Faddeev equations.

Omitting details of deducing the Faddeev equations for three-cluster system we present final results.

The first sets of the Faddeev equations can be written as

$$\begin{aligned}&\left[\left(\widehat{H}_0 + \widehat{T} - E\right)\left(1 + \widehat{\mathcal{A}}_\alpha + \tfrac{1}{3}\widehat{\mathcal{A}}_{123}\right) + \widehat{V}_\alpha + \widehat{V}\widehat{\mathcal{A}}_\alpha + \tfrac{1}{3}\widehat{V}\widehat{\mathcal{A}}_{123}\right]\underline{\Psi}_\alpha \\ &= -\left[\widehat{V}_\alpha + \widehat{V}\widehat{\mathcal{A}}_\alpha + \tfrac{1}{3}\widehat{V}\widehat{\mathcal{A}}_{123} + \left(\widehat{H}_0 + \widehat{T} - E\right)\left(\widehat{\mathcal{A}}_\alpha + \tfrac{1}{3}\widehat{\mathcal{A}}_{123}\right)\right]\textstyle\sum_{\beta\neq\alpha}\underline{\Psi}_\beta\end{aligned} \tag{18}$$

The second set of the Faddeev equations reads as

$$\begin{aligned}&\left[\left(\widehat{H}_0 + \widehat{T} + \widehat{V} - E\right)\widehat{\mathcal{A}}_\alpha^{(2)} + \widehat{V}_\alpha + \widehat{V}\widehat{\mathcal{A}}_\alpha + \tfrac{1}{3}\widehat{V}\widehat{\mathcal{A}}_{123}\right]\underline{\Psi}_\alpha \\ &= -\left[\left(\widehat{H}_0 + \widehat{T} + \widehat{V} - E\right)\left(1 + \widehat{\mathcal{A}}_\alpha + \tfrac{1}{3}\widehat{\mathcal{A}}_{123}\right)\right]\textstyle\sum_{\beta\neq\alpha}\underline{\Psi}_\beta\end{aligned} \tag{19}$$

The third set of the Faddeev equations we present as

$$\begin{aligned}&\left[\left(\widehat{H}_0 + \widehat{T} - E\right)\widehat{\mathcal{A}} + \widehat{V}_\alpha + \widehat{V}\widehat{\mathcal{A}}_\alpha + \tfrac{1}{3}\widehat{V}\widehat{\mathcal{A}}_{123}\right]\underline{\Psi}_\alpha \\ &= -\left[\widehat{V}_\alpha + \widehat{V}\widehat{\mathcal{A}}_\alpha + \tfrac{1}{3}\widehat{V}\widehat{\mathcal{A}}_{123}\right]\textstyle\sum_{\beta\neq\alpha}\underline{\Psi}_\beta\end{aligned} \tag{20}$$

This is the Faddeev type of equations for three-cluster system. One can easily verify that the equations (18), (19) and (20) transform into ordinary set of the Faddeev equation when one switch off the antisymmetrization operator, i.e. by assuming that $\widehat{\mathcal{A}}_\alpha = \widehat{\mathcal{A}}_{123} = 0$ and $\widehat{\mathcal{A}} = 1$.

All sets of the Faddeev type of equations are obtained in the operator form. To solve these equations we will sandwich all operators, appearing in these equations, between the cluster oscillator functions. The effectivenees of the Faddeev equations, deduced for three cluster system, will be be demonstrated elsewhere.

4. Conclusion

We deduced three different but equivalent sets of the Faddeev type of equations for a three-cluster system. Within these equations the Pauli principle is treated correctly. We demonstrated the antisymmetrzation operator, which provides total antisymmetric of a wave function of three-cluster system, can be decomposed in four terms. First three terms consist of permutation operators interchanging nucleons from selected pair of clusters. Each of these terms make total function antisymmetric with respect of permutations of nucleons belonging to the selected pair of clusters. Last term of the antisymmetrization involves permutations of nucleons of all clusters and thus generates three-body interaction between clusters. This term leads to different sets of the Faddeev equations.

We deduced the Faddeev equation in the operator form. This form can be transformed to integro-differential form of the standard Resonating Group Method or algebraic (or J-Matrix) form by using full set of the oscillator functions.

Acknowledgments

Support from the Fonds voor Wetenschappelijk Onderzoek Vlaanderen (FWO), G0488-03N, and the AfdelingTechnologie en Innovatie van het Ministerie van het Vlaams Gewest is gratefully acknowledged. V.S. Vasilevsky is grateful to the Department of Mathematics and Computer Science of the University of Antwerp (UA) for hospitality.

This work was supported in part by the Program of Fundamental Research of the Physics and Astronomy Department of the National Academy of Sciences of Ukraine.

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