Solving Three-Cluster OCM Equations in the Faddeev Formalism

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Abstract. Two different types of orthogonality condition models (OCM) are equivalently formulated in the Faddeev formalism. One is the OCM which uses pairwise orthogonality conditions for the relative motion of clusters, and the other is the one which uses the orthogonalizing pseudo-potential method. By constructing a redundancy-free $T$-matrix, one can exactly eliminate the redundant components of the total wave function for the harmonic-oscillator Pauli-forbidden states, without introducing any limiting procedure. As an example, a three-α-particle model interacting via the deep αα potential by Buck, Friedrich and Wheatley is investigated.

1 Introduction

The Faddeev formalism for three composite particles has always suffered from the insufficient treatment of the Pauli principle. For example, in the three-alpha (3α) Faddeev study by one of the authors [1] one-term separable αα potentials are used to reproduce the damped inner oscillations of the relative wave functions, which are the most important effect of the Pauli principle between two α (2α) clusters. Due to the insufficient treatment of the Pauli principle among 3α clusters, some of the obtained states ($0^+_2$ and $1^-$ states) were concluded to be spurious since they contain a large amount of redundant components. On the other hand, a large binding energy of the shell-model like ground state and the excited $0^+$ state with well-developed cluster structure are simultaneously reproduced, which can never be realized by Ali-Bodmer’s phenomenological αα potential with the repulsive core. The large overbinding of the 3α ground state with $E_{3\alpha} = -17$ MeV (without the Coulomb force) is most easily understood by considering that the damped inner oscillations of the 2α relative motion are enhanced in the compact 3α system, and the attractive nature in the short-range part of the core-less potential overwhelms the large kinetic energies. [2] The same situation is also found in the work by Oryu and Kamada [3]. They started directly from the microscopic 2α-cluster kernel of the resonating-group method (RGM), and converted it to the
many-rank separable potentials which are suitable for the Faddeev calculations. Although their admixture of the redundant components is relatively small, the ground-state energy is extremely large with \( E_{3\alpha} \sim -20 \text{ MeV} \). Since the fish-bone optical model proposed by Schmid [5] also gives a large ground-state energy, these authors claim that some sort of \( 3\alpha \) force is definitely necessary in the \( 3\alpha \)-particle model to obtain a reasonable agreement with the experimental observation. [6] We think that this repulsive 3-cluster force can be partly avoided by the complete elimination of the \( 3\alpha \) redundant components, which cannot be excluded at the \( 2\alpha \) potential level. From the microscopic viewpoint based on the \( 3\alpha \) RGM, the model space for the relative motion of the \( 3\alpha \) clusters has a well-defined notion solely determined from the assumed internal wave functions of the \( \alpha \) clusters. The standard interpretation of the 3-cluster force may be the one which stems from the interaction kernel connected to the full antisymmetrization among the three clusters. [7]

Recently, we have developed 3-cluster Faddeev formalism which employs 2-cluster RGM kernel directly. [8, 9] In this formulation, we first write down the RGM equation in the form of the Schrödinger-type equation. The resultant interaction term becomes non-local and energy-dependent. This linear energy dependence in the interaction term originates from splitting the overlap kernel into the direct term and the exchange normalization kernel. The two-cluster RGM equation sometimes involves redundant components. In such a case, the complete off-shell \( T \)-matrix is not well-defined in the standard procedure. [10] Our strategy is to distinguish between the energy \( \varepsilon \) in the interaction term and the starting energy \( \omega \) involved in the 2-cluster Green function. Assuming the energy \( \varepsilon \) involved in the interaction term as a mere parameter, we can define the full \( T \)-matrix, \( T(\omega, \varepsilon) \), through the standard procedure. Although \( T(\omega, \varepsilon) \) is singular when \( \omega = \varepsilon \), there is no harm in solving the Faddeev equation for the bound states since \( \omega \) is negative and \( \varepsilon \) is usually positive. Our finding is that the modified \( T \)-matrix, \( \tilde{T}(\omega, \varepsilon) \), obtained by subtracting this divergent term is the proper "RGM \( T \)-matrix", which should be used in the Faddeev equation. The remaining energy-dependence in \( \tilde{T}(\omega, \varepsilon) \) should be determined self-consistently by calculating the expectation value of the 2-cluster Hamiltonian with the resultant total wave-function of the Faddeev equation. In Ref. [8], we proved that this formalism is completely equivalent to the 3-cluster orthogonality condition model (OCM) with pairwise orthogonality conditions (as proposed by Horiuchi [11, 12]), using the RGM interaction term as the pairwise interaction. The energy dependence in the interaction term should be determined self-consistently even in this 3-cluster equation.

In this paper, we will show that this Faddeev formalism developed for 2-cluster RGM kernel is also applicable to the usual 3-cluster OCM. In this case, the corresponding "OCM \( T \)-matrix" no longer involves the \( \varepsilon \)-dependence, although the interaction term of the Schrödinger-type OCM equation is still energy dependent. We will also show that this 3-cluster Faddeev equation is equivalent to the Faddeev equation formulated for the "redundancy-free" \( T \)-matrix obtained from the original OCM potential by applying Kukulin's method of orthogonalizing pseudo-potentials [13]. Through these procedures, we can prove the equivalence
between Horiuchi-type 3-cluster OCM with the pairwise orthogonality conditions and the method of orthogonalizing pseudo-potentials. A nice point of the present approach is that one no longer needs the process to take the strength parameter, \( \lambda \) in Eq. (2.30), infinity, which may cause a serious numerical instability if the model space to solve the 3-cluster equation is too small in the variational-type calculations. We think that this is a great merit of using the \( T \)-matrix formalism. As a typical example, we investigate the \( 3\alpha \) system in which the pair \( \alpha \)'s interact via the deep local potential proposed by Buck, Friedrich and Wheatley (BFW potential) \[14\]. According to the general idea of the point-like \( \alpha \)-particle models, the redundant components of the \( 2\alpha \) system are assumed to be the bound states of the \( 2\alpha \) Hamiltonian. In this case, the Pauli projection operator \( P \) needs a careful treatment to select a physical model space. We find that the ground-state energy of this system is far below the experimental value. This is a different conclusion from that reached in Refs. \[15\] and \[16\], which was based on the variational calculations in the method of orthogonalizing pseudo-potentials.

In the next section, the Faddeev formalism for the 3-cluster OCM is developed after a brief recapitulation of the previous Faddeev formalism using the 2-cluster RGM kernel \[8, 9\]. An application to the BFW potential with the bound-state Pauli-forbidden states is also given, together with a new feature influenced by the almost forbidden components of the Faddeev equation. The relationship of the \( T \)-matrices derived in this particular case is easily generalized for more general types of the Pauli-forbidden states composed of the harmonic-oscillator (h.o.) wave functions. The third section discusses the numerical examples of the present Faddeev formalism for the \( 3\alpha \) system interacting via the BFW potential. The last section is devoted to a summary. A simple formula for \( T \)-matrices is given in the Appendix.

2 Formulation

2.1 3-cluster Faddeev equation using the 2-cluster RGM kernel

We start from a two-cluster RGM equation for the relative wave function \( \chi \), expressed as

\[
\left[ \omega - H_0 - V_{\text{RGM}}(\omega) \right] \chi = 0 ,
\]

(2.1)

where \( \omega \) is the total energy in the center-of-mass (c.m.) system, measured from the two-cluster threshold, \( \omega = E - E^{\text{int}} \), \( H_0 \) is the relative kinetic-energy operator, and

\[
V_{\text{RGM}}(\omega) = V_D + G + \omega K ,
\]

(2.2)

is the RGM kernel composed of the direct potential \( V_D \), the sum of the exchange kinetic-energy and interaction kernels, \( G = G^K + G^V \), and the exchange normalization kernel \( K \). For simplicity, we assume a single-channel RGM and that there exists only one Pauli-forbidden state \(|u\rangle \) (normalized as \( \langle u|u\rangle = 1 \)), which satisfies the eigen-value equation \( K|u\rangle = \gamma |u\rangle \) with the eigen-value \( \gamma = 1 \). The projection operator on the Pauli-allowed space for the relative motion is denoted
by \( \Lambda = 1 - |u\rangle\langle u| \). Using the basic property of the Pauli-forbidden state \(|u\rangle\), 
\((H_0 + V_D + G)|u\rangle = 0\) and \(\langle u|(H_0 + V_D + G) = 0\), we find that Eq. (2.1) is equivalent to 
\[ \Lambda \left[ \omega - H_0 - V_{RGM}(\omega) \right] \Lambda \chi = 0 \quad (2.3) \]
or 
\[ \Lambda \left[ \omega - H_0 - v(\omega) \right] \Lambda \chi = 0 \quad . \quad (2.4) \]
Here, we have defined 
\[ v(\varepsilon) = \Lambda V_{RGM}(\varepsilon) \Lambda = \Lambda (V_D + G) \Lambda + \varepsilon \Lambda K \Lambda , \quad (2.5) \]
by generalizing \( \omega \) in \( v(\omega) \) to \( \varepsilon \). The OCM approximation consists of 
\[ \Lambda \left[ \omega - H_0 - V_D \right] \Lambda \psi = 0 \quad , \quad (2.6) \]
or more favorably changing the direct potential \( V_D \) to a suitable effective local potential \( V_{\text{eff}} \). [17, 18]

The basic procedure to define the “RGM T-matrix” is to separate \( V_{RGM}(\omega) \) into two distinct parts 
\[ V_{RGM}(\varepsilon) = V(\varepsilon) + v(\varepsilon) \quad (2.7) \]
with 
\[ V(\varepsilon) = (\varepsilon - H_0) - \Lambda (\varepsilon - H_0) \Lambda = \varepsilon |u\rangle\langle u| + \Lambda H_0 \Lambda - H_0 \quad , \quad (2.8) \]
and to assume \( \varepsilon \) in \( v(\varepsilon) \) as a mere parameter which should be determined by the surroundings of the interacting two clusters. Then we can derive a formal solution of the \( T \)-matrix equation 
\[ T(\omega, \varepsilon) = V_{RGM}(\varepsilon) + V_{RGM}(\varepsilon) G_0^{(+)}(\omega) T(\omega, \varepsilon) \quad (2.9) \]
with \( G_0^{(+)}(\omega) = 1/(\omega - H_0 + i0) \) as follows: [8]
\[ T(\omega, \varepsilon) = \tilde{T}(\omega, \varepsilon) + (\omega - H_0)|u\rangle \frac{1}{\omega - \varepsilon} \langle u|(\omega - H_0) \quad , \quad (2.10) \]
\[ \tilde{T}(\omega, \varepsilon) = T_v(\omega, \varepsilon) - \left[ 1 + T_v(\omega, \varepsilon) G_0^{(+)}(\omega) \right] \frac{|u\rangle}{\langle u| G_0^{(+)}(\omega) \langle \omega, \varepsilon) |u\rangle} \]
\[ \times \langle u| \left[ 1 + G_0^{(+)}(\omega) T_v(\omega, \varepsilon) \right] , \quad (2.10) \]
where \( T_v(\omega, \varepsilon) \) is defined by 
\[ T_v(\omega, \varepsilon) = v(\varepsilon) + v(\varepsilon) \frac{G_0^{(+)}(\omega) T_v(\omega, \varepsilon)}{G_0^{(+)}(\omega) T_v(\omega, \varepsilon)} \quad , \quad (2.11) \]
and \( G_v^{(+)}(\omega, \varepsilon) \) is the corresponding full Green function.

The introduction of the parameter \( \varepsilon \) in Eq. (2.9) is not strange if we consider the practical method to solve equations like Eqs. (2.1) and (2.6) with a redundant solution \(|u\rangle\). In these equations we are actually solving \( \Lambda \chi \) or \( \Lambda \psi \). The original Saito’s suggestion [17, 18] for solving the OCM equation Eq. (2.6) is to assume 
\[ \Lambda \psi = \psi \quad \text{or} \quad \langle u|\psi \rangle = 0 \quad \text{and solve} \]
\[ \omega \psi = \Lambda (H_0 + V_D) \Lambda \psi \quad . \quad (2.12) \]
In fact, the solution of Eq. (2.12) is the redundancy-free solution of Eq. (2.6) when \( \omega \neq 0 \). Generally speaking, the trivial solution \(|u\rangle\) needs not be a zero-energy solution. One can also move this exceptional energy to an arbitrary (usually positive) value \( \varepsilon \). This can be achieved by simply adding \( \varepsilon \langle u|\psi\rangle \) term in the right-hand side of Eq. (2.12):

\[
\omega \psi = \Lambda (H_0 + V_D) \Lambda \psi + \varepsilon \langle u|\psi\rangle.
\] (2.13)

One can take the same process in the RGM equation Eq. (2.1). We start from Eq. (2.4) and change \( \omega \) in \( v(\omega) \) to \( \varepsilon \). This is permissible since the energy dependence of the \( v(\varepsilon) \) term is usually very weak due to the structure \( \Lambda K \Lambda \). For example, this term vanishes completely for simple systems like the two di-neutron system. [8] The energy dependence of the RGM interaction in the allowed space is later taken into account by a self-consistency condition. Similarly to Eq. (2.13), we set up with the equation

\[
\omega \chi = \Lambda [H_0 + v(\varepsilon)] \Lambda \chi + \varepsilon \langle u|\chi\rangle.
\] (2.14)

If we use Eq. (2.7), we can easily prove that this equation is nothing but

\[
[\omega - H_0 - V_{RGM}(\varepsilon)] \chi = 0,
\] (2.15)

which no longer has the trivial solution \(|u\rangle\) except for \( \omega = \varepsilon \).

A motivation to use \( \tilde{T}(\omega, \varepsilon) \) in Eq. (2.10) for the Faddeev equation comes from the complete equivalence between the Faddeev equation and the 3-body equation interacting via \( v(\varepsilon) \) in the allowed model space. [8] Namely, for a system composed of three identical spinless particles, we can prove the equivalence between

\[
P \left[ E - H_0 - V_\alpha^{RGM}(\varepsilon_\alpha) - V_\beta^{RGM}(\varepsilon_\beta) - V_\gamma^{RGM}(\varepsilon_\gamma) \right] P \Psi = 0
\] (2.16)

and

\[
\psi_\alpha = G_0^{(+)}(E) \tilde{T}_\alpha^{(3)}(E, \varepsilon_\alpha) (\psi_\beta + \psi_\gamma),
\] (2.17)

where a common self-consistency condition

\[
\varepsilon_\alpha = \langle P \Psi | h_\alpha + V_\alpha^{RGM}(\varepsilon_\alpha) | P \Psi \rangle / \langle P \Psi | P \Psi \rangle,
\] (2.18)

is imposed. In Eq. (2.16), \( H_0 \) is the three-body kinetic energy operator in the c.m. system, \( V^{RGM}_\alpha(\varepsilon_\alpha) \) represents the RGM kernel Eq. (2.2) for the \( \alpha \) pair, and \( P \) is the projection operator onto the \([3]\)-symmetric Pauli-allowed space, as defined in Refs. [8] and [11]. In the Faddeev equation Eq. (2.17), \( \tilde{T}_\alpha^{(3)}(E, \varepsilon_\alpha) \) is essentially the non-singular RGM T-matrix \( \tilde{T}(\omega, \varepsilon) \) defined through Eq. (2.10):

\[
\tilde{T}_\alpha^{(3)}(E, \varepsilon_\alpha) = \tilde{T}_\alpha(E - h_\alpha, \varepsilon_\alpha),
\] (2.19)

where \( h_\alpha \) is the relative kinetic-energy operator between the \( \alpha \)-pair and the third particle. A nice point of the Faddeev equation Eq. (2.17) is that the total wave
function \( \Psi \), constructed from the three Faddeev components, \( \psi_\alpha, \psi_\beta \) and \( \psi_\gamma \) is automatically orthogonal to the Pauli-forbidden state in each pair:

\[
\langle u_\alpha | \Psi \rangle = \langle u_\alpha | P \Psi \rangle = \langle u_\alpha | \psi_\alpha + \psi_\beta + \psi_\gamma \rangle = 0 .
\] (2.20)

This is because of the orthogonality property

\[
\langle u | \left[ 1 + G_0^{(+)}(\omega) \tilde{T}(\omega, \varepsilon) \right] | u \rangle = 0 ,
\] (2.21)

which is derived from the formal solution in Eq. (2.10).

### 2.2 Application to the 3-cluster OCM

The above discussion on the 3-cluster systems interacting via pairwise 2-cluster RGM kernels can be straightforwardly extended to the ordinary 3-cluster OCM interacting via simple energy-independent local potentials. One only needs to modify

\[
v(\varepsilon) \rightarrow v = AV_D A .
\] (2.22)

From Eqs. (2.7) and (2.8), the interaction term for the 2-cluster OCM equation, \( V^{OCM}(\varepsilon) \), turns out to be

\[
V^{RGM}(\varepsilon) \rightarrow V^{OCM}(\varepsilon) = V(\varepsilon) + v = (\varepsilon - H_0) - A(\varepsilon - H_0 - V_D) A = \varepsilon |u\rangle\langle u| + A(H_0 + V_D) A - H_0 .
\] (2.23)

The full \( T \)-matrix of \( V^{OCM}(\varepsilon) \) is defined through

\[
T(\omega, \varepsilon) = V^{OCM}(\varepsilon) + V^{OCM}(\varepsilon)G_0^{(+)}(\omega)T(\omega, \varepsilon) .
\] (2.24)

The formal expression of \( T(\omega, \varepsilon) \) is very similar to Eq. (2.10), but this time the “OCM \( T \)-matrix”, \( \tilde{T}(\omega) \), does not involve the \( \varepsilon \)-dependence. Namely, the \( \varepsilon \)-dependence appears only through the last term in \( T(\omega, \varepsilon) \). Now we can write down two equivalent equations corresponding to Eqs. (2.16) and (2.17):

\[
P \left[ E - H_0 - V_D^{\alpha} - V_D^{\beta} - V_D^{\gamma} \right] P \Psi = 0
\] (2.25)

and

\[
\psi_\alpha = G_0^{(+)}(E) \tilde{T}_\alpha^{(3)}(E) (\psi_\beta + \psi_\gamma) .
\] (2.26)

This time, we do not need the self-consistency condition Eq. (2.18), and Eq. (2.19) becomes

\[
\tilde{T}_\alpha^{(3)}(E) = \tilde{T}_\alpha(E - h_\alpha) .
\] (2.27)

Since the orthogonality condition in Eq. (2.21) is still valid for \( \tilde{T}(\omega) \), we can prove that the solution of Eq. (2.26) satisfies the orthogonality of the total wave function, Eq. (2.20).
If the Pauli-forbidden state \(|u\rangle\) is a real bound state of \(V_D\), our expression for \(V_{OCM}(\varepsilon)\) in Eq. (2.23) is further simplified. We assume that \(|u\rangle = |u_B\rangle\) is the bound-state wave function, satisfying

\[
(\varepsilon_B - H_0 - V_D)|u_B\rangle = 0 ,
\]

with \(\varepsilon_B (\leq 0)\) being the bound-state energy. Here, \(H_0\) is the 2-cluster kinetic-energy operator, and only one bound state is assumed to exist. Then, one can easily show that \(V_{OCM}(\varepsilon)\) is reduced to

\[
V_{OCM}(\varepsilon) = V_D + (\varepsilon - \varepsilon_B)|u_B\rangle\langle u_B| ,
\]

which is nothing but the Kukulin’s pseudo-potential

\[
V^{ps} = V_D + \lambda|u_B\rangle\langle u_B|
\]

with \(\lambda = \varepsilon - \varepsilon_B\). By using the general formula given in Appendix, we can find that the \(T\)-matrix defined through Eq. (2.24) is given by

\[
T(\omega, \varepsilon) = T_D(\omega) + \frac{1}{|u_B\rangle\langle u_B|} \left(1 - \frac{1}{\omega - \varepsilon} \right) G_D^{(+))(\omega)}|u_B\rangle\langle u_B| ,
\]

where

\[
T_D(\omega) = V_D + V_D G_0^{(+))(\omega)} T_D(\omega)
\]

and

\[
G_D^{(+))(\omega)} = [\omega - H_0 - V_D + i0]^{-1} = G_0(\omega) + G_0(\omega) T_D(\omega) G_0(\omega) .
\]

On the other hand, \((\omega - H_0 - V_D)|u_B\rangle = (\omega - \varepsilon_B)|u_B\rangle\) yields

\[
G_D^{(+))(\omega)}|u_B\rangle = \frac{1}{\omega - \varepsilon_B}|u_B\rangle ,
\]

if \(\omega \neq \varepsilon_B\). By using Eq. (2.34), the second term of Eq. (2.31) in the right-hand side is greatly simplified through the relationship like

\[
[1 + T_D(\omega)G_0(\omega)]|u_B\rangle = (\omega - H_0)G_D^{(+))(\omega)}|u_B\rangle = (\omega - H_0)|u_B\rangle \frac{1}{\omega - \varepsilon_B} .
\]

We find

\[
T(\omega, \varepsilon) = T_D(\omega) - (\omega - H_0)|u_B\rangle \frac{1}{\omega - \varepsilon_B} \langle u_B|(\omega - H_0) + (\omega - H_0)|u_B\rangle \frac{1}{\omega - \varepsilon} \langle u_B|(\omega - H_0) .
\]

If we define \(\tilde{T}(\omega)\) through

\[
T(\omega, \varepsilon) = \tilde{T}(\omega) + (\omega - H_0)|u_B\rangle \frac{1}{\omega - \varepsilon} \langle u_B|(\omega - H_0) ,
\]

then

\[
\tilde{T}(\omega) = T_D(\omega) - \frac{1}{\omega - \varepsilon_B} \langle u_B|(\omega - H_0) \frac{1}{\omega - \varepsilon} \langle u_B|(\omega - H_0) .
\]
we obtain
\[ \tilde{T}(\omega) = T_D(\omega) - (\omega - H_0)|u_B\rangle \frac{1}{\omega - \varepsilon_B} \langle u_B|(\omega - H_0) , \] (2.38)
or
\[ \tilde{T}(\omega) = \lim_{\varepsilon \to \infty} T(\omega, \varepsilon) . \] (2.39)

Adding the separable term to \( V_D \) in Eq. (2.29) removes the bound-state pole of the \( T \)-matrix \( T_D(\omega) \) and moves it to the positive energy \( \varepsilon \) in Eq. (2.37). In \( \tilde{T}(\omega) \) in Eq. (2.38), this positive energy pole is even removed. In order to see this, we use the spectral decomposition of \( G_D^{(+)}(\omega) \):
\[ G_D^{(+)}(\omega) = \left[ \omega - H_0 - V_D + i0 \right]^{-1} \]
\[ = |u_B\rangle \frac{1}{\omega - \varepsilon_B + i0} \langle u_B| + \int \frac{dk}{2\pi} \frac{1}{\omega - \frac{k^2}{2\mu} + i0} \langle \phi^{(+)}| . \] (2.40)

Using this in \( T_D(\omega) = V_D + V_D G_D^{(+)}(\omega) V_D \) and in Eq. (2.38), we find
\[ \tilde{T}(\omega) = \lambda V_D \alpha - |u_B\rangle \langle u_B| (\omega - H_0)|u_B\rangle \langle u_B| \]
\[ + \int \frac{dk}{2\pi} V_D |\phi^{(+)}\rangle \frac{1}{\omega - \frac{k^2}{2\mu} + i0} \langle \phi^{(+)}| V_D , \] (2.41)
which has no singularities if \( \omega < 0 \).

Let us consider a three-body system composed of three identical spinless particles with the mass \( M \). One of such examples is the \( 3\alpha \) system interacting via the BFW potential, discussed in the next section. The pairwise interaction is assumed to be the Kukulin’s pseudo-potential \( V^{ps} \) with \( \lambda = \varepsilon - \varepsilon_B \) in Eq. (2.30). The three-body Schrödinger equation reads
\[ \left( E - H_0 - V^{ps}_\alpha - V^{ps}_\beta - V^{ps}_\gamma \right) \Psi = 0 . \] (2.42)

This equation is transformed to the Faddeev equation by the standard procedure:
\[ \psi_\alpha = G_0 T_\alpha (\psi_\beta + \psi_\gamma) , \] (2.43)
where \( G_0 = G_0^{(+)}(E) \) with \( E < 0 \), \( T_\alpha = T_\alpha(E - h_\alpha) \), and \( \psi_\alpha \) etc. are the three Faddeev components yielding the total wave function \( \Psi = \psi_\alpha + \psi_\beta + \psi_\gamma \). Using Eq. (2.37), we find
\[ \psi_\alpha = G_0 \left( \tilde{T}_\alpha + (E - H_0)|u^B_\alpha\rangle \frac{1}{E - \frac{3}{4} \frac{\hbar^2}{M} q^2 - \varepsilon} \langle u^B_\alpha|(E - H_0) \right) (\psi_\beta + \psi_\gamma) \]
\[ = G_0 \tilde{T}_\alpha (\psi_\beta + \psi_\gamma) + |u^B_\alpha\rangle \frac{1}{E - \frac{3}{4} \frac{\hbar^2}{M} q^2 - \varepsilon} \langle u^B_\alpha|(E - H_0)|\psi_\beta + \psi_\gamma| . \] (2.44)

Here, \( q \) is the momentum Jacobi coordinate between a pair and the third particle. If we multiply Eq. (2.44) by \( \langle u^B_\alpha| \) from the left-hand side, we obtain
\[ \langle u^B_\alpha| \psi_\alpha = -\langle u^B_\alpha| \psi_\beta + \psi_\gamma \rangle + \frac{1}{E - \frac{3}{4} \frac{\hbar^2}{M} q^2 - \varepsilon} \langle u^B_\alpha|(E - H_0)|\psi_\beta + \psi_\gamma| , \] (2.45)
or
\[
\langle u^B_\alpha | \Psi \rangle = \frac{1}{E - \frac{1}{2 \alpha^2} q_\alpha^2 - \varepsilon} \langle u^B_\alpha | E - H_0 | \psi_\beta + \psi_\gamma \rangle .
\] (2.46)

If we take the limit \( \lambda \to \infty \) or \( \varepsilon \to \infty \), we obtain
\[
\psi_\alpha = G_0 \tilde{T}_\alpha (\psi_\beta + \psi_\gamma) ,
\] (2.47)

and
\[
\langle u^B_\alpha | \Psi \rangle = 0 .
\] (2.48)

Since \( \tilde{T} \) does not depend on \( \varepsilon \) or \( \lambda \), we can achieve the solution of Eq. (2.42) with \( \lambda \to \infty \), by solving Eq. (2.47) without any limiting procedure. On the other hand, we have proven that Eq. (2.47) is equivalent to the Horiuchi’s OCM Eq. (2.25), using \( V_D \). We can thus prove the equivalence between Eq. (2.42) with \( \lambda \to \infty \) and Eq. (2.25); namely, the equivalence between the Kukulin’s OCM and the Horiuchi’s OCM, when the Pauli-forbidden state \( |u\rangle \) is the exact eigen-state for the local potential \( V_D \). In fact, this equivalence is also valid even when the \( |u\rangle \) is not the eigen-state of \( V_D \) but the h.o. Pauli-forbidden state of the normalization kernel \( K \), which is proved in the next subsection.

For solving the 3\( \alpha \) Faddeev equation, it is important to note that there exist some trivial solutions related to the orthogonality condition Eq. (2.21) for the \( \tilde{T} \) \( T \)-matrix. As is discussed in Ref. [9] in detail, the eigen-value solutions of the rearrangement matrix \( S \) among the three different types of the Jacobi coordinates with the eigen-value \( \tau = -1 \) are the redundant solutions of the Faddeev equation Eqs. (2.17) or (2.26). For the h.o. Pauli-forbidden state \( |u\rangle \), this eigen-value equation reads
\[
\langle u|S|uf^{\tau} \rangle = \tau |f^{\tau} \rangle \quad \text{with} \quad \tau = -1 .
\] (2.49)

We find that the Faddeev component
\[
\psi_0^{\tau} = G_0 |uf^{\tau} \rangle \quad \text{with} \quad \tau = -1
\] (2.50)
is a trivial solution with the total wave function \( \Psi_0^{\tau} = (1 + S) \psi_0^{\tau} = 0 \) for \( \tau = -1 \). The non-zero \( \psi_0^{\tau} \) is the [21]-symmetric function with respect to the permutation of the 3\( \alpha \) particles. We have two such trivial solutions for the 3\( \alpha \) system with the total angular momentum \( L = 0 \). For this reason, the Faddeev equation (2.17) or (2.26) should be modified to\(^1\)
\[
\lambda \psi = \left[ G_0 \tilde{T} S - \sum_{\tau = -1} G_0 |uf^{\tau} \rangle \frac{1}{\langle uf^{\tau}|G_0|uf^{\tau} \rangle} \langle uf^{\tau}| \right] \psi ,
\] (2.51)
in order to find a unique solution with \( \lambda = 1 \). The solution of Eq. (2.51) with \( \lambda = 1 \) automatically satisfies
\[
\psi = G_0 \tilde{T} S \psi , \quad \langle u|(1 + S)|\psi \rangle = 0 , \quad \langle uf^{\tau}|\psi \rangle = 0 \quad \text{for} \quad \tau = -1 .
\] (2.52)

\(^1\)The inverse of the matrix elements in the last terms of Eq. (2.51) and Eq. (2.56) should be understood as the matrix inverse.
When the bound-state solution $|u_B\rangle$ is used for $|u\rangle$, these $\tau = -1$ eigen-values of Eq. (2.49) are no longer exactly $\tau = -1$, but move to the $\tau > -1$ values. The $[3]$-symmetric basis states constructed from

$$\Psi_0 = \frac{1}{\sqrt{3(1+\tau)}}(1+S)|u_B f^{\tau}\rangle \quad \text{with} \quad \tau \sim -1$$

(2.53)

involve some of the important shell-model like components such as $|[3](04)\rangle$ etc. [19] If these configurations are excluded, one cannot describe a compact shell-model like structure of $^{12}$C. The original $3\alpha$ OCM equation should, therefore, be formulated by using

$$\tilde{P} = |\Psi_0\rangle\langle\Psi_0| + P ,$$

(2.54)

instead of $P$ in Eq. (2.25). Since $|\Psi_0\rangle$ involves a small admixture of the redundant components as

$$\langle u_B|\Psi_0\rangle = \sqrt{1+\tau}3 |f^{\tau}\rangle \quad \text{with} \quad \tau \sim -1 ,$$

(2.55)

the ground-state solution of the $3\alpha$ system with the dominant $|\Psi_0\rangle$ components naturally involves a small admixture of the redundant components. We can also formulate an equivalent Faddeev equation to this modified $3\alpha$ OCM equation with $\tilde{P}$, which has a slightly different form from Eq. (2.51):

$$\lambda \psi = \left[ G_0 \tilde{T} S + \sum_{\tau \sim -1} |u f^{\tau}\rangle \langle u f^{\tau}|(E - H_0 - V_D)|u f^{\tau}\rangle \langle u f^{\tau}|(E - H_0)S \right] \psi .$$

(2.56)

The derivation of this equation and a detailed discussion of the almost redundant components of the Faddeev equation will be given elsewhere. [19]

2.3 Equivalence between pairwise orthogonality conditions and the method of orthogonalizing pseudo-potentials in the 3-cluster systems

In this subsection, we will prove the equivalence between the Horiuchi’s OCM and the Kukulin’s OCM, even when the Pauli-forbidden state $|u\rangle$ is not the eigen-state of the pairwise potential $V_D$, but the original h.o. Pauli-forbidden state of $K$. The essential point is that the OCM $T$-matrix $\tilde{T}(\omega)$ defined through $T(\omega, \varepsilon)$ in Eq. (2.24) is nothing but the $\tilde{T}$-matrix generated from the pseudo-potential $V^{ps}$ in Eq. (2.30) with $|u_B\rangle \rightarrow |u\rangle$ and $\lambda \rightarrow \infty$.

Let us assume that $|u\rangle$ is not the eigen-state of $V_D$, but the h.o. eigen-state of $K$ with the eigen-value $\gamma = 1$. The $T$-matrix generated from $V^{ps}$ with $\lambda \rightarrow \infty$ is, from Eq. (2.31),

$$\tilde{T}(\omega) = T_D(\omega) - (\omega - H_0)G_D(\omega)|u\rangle \frac{1}{\langle u|G_D(\omega)|u\rangle} \langle u|G_D(\omega)(\omega - H_0) ,$$

(2.57)

where $T_D(\omega)$ and $G_D(\omega)$ are the $T$-matrix and the full Green function of $V_D$, respectively. On the other hand, we separate $V^{OCM}(\varepsilon)$ in Eq. (2.23) as

$$V^{OCM}(\varepsilon) = (\varepsilon - H_0) - \Lambda(\varepsilon - H_0 - V_D)\Lambda = V_1 + \lambda_1|u\rangle\langle u|$$

(2.58)
Then, we find that

\[ V_1 = V_D - (H_0 + V_D)|u\rangle \langle u| - |u\rangle \langle u|(H_0 + V_D) , \]

\[ \lambda_1 = \varepsilon + \langle u|H_0 + V_D|u \rangle . \]  

Then, the general formula in Appendix gives the \( T \)-matrix as

\[ T(\omega, \varepsilon) = t_1 + (1 + t_1 G_0)|u\rangle \langle u| = \frac{1}{\lambda_1 - \langle u|G_0 + G_0 t_1 G_0|u \rangle} \langle u|(1 + G_0 t_1) \]

\[ = t_1 + (\omega - H_0) G_1|u\rangle \langle u| G_1(\omega - H_0) , \]  

where \( t_1 \) and \( G_1 \) are the \( T \)-matrix and the full Green function of \( V_1 \). Here we take \( \varepsilon \to \infty \) (\( \lambda_1 \to \infty \)) and obtain

\[ \tilde{T}(\omega) = \lim_{\varepsilon \to \infty} T(\omega, \varepsilon) = t_1 - (\omega - H_0) G_1|u\rangle \langle u| G_1(\omega - H_0) . \]  

We note that \( \omega - H_0 - V_1 \) is expressed as

\[ \omega - H_0 - V_1 = \omega - H_0 - V_D + (H_0 + V_D)|u\rangle \langle u| + |u\rangle \langle u|(H_0 + V_D) \]

\[ = \omega - A(h_0 + V_D) \Lambda + |u\rangle \langle u| (H_0 + V_D) + |u\rangle \langle u| \]

\[ = A(\omega - H_0 - V_D) \Lambda + |u\rangle \langle u|(H_0 + V_D) + |u\rangle \langle u| \].  

Then, we find that \( G_1 = (\omega - H_0 - V_1)^{-1} \) is expressed as

\[ G_1 = G_A + |u\rangle \langle u| \frac{1}{\omega + \langle u|H_0 + V_D|u \rangle} , \]  

where \( G_A \) is defined by

\[ G_A = G_D - G_D|u\rangle \langle u| G_D , \]  

with \( G_D = (\omega - H_0 - V_D)^{-1} \), and satisfies

\[ A(\omega - H_0 - V_D) \Lambda G_A = G_A \Lambda(\omega - H_0 - V_D) \Lambda = \Lambda . \]  

Since we have

\[ G_1|u\rangle = |u\rangle \frac{1}{\omega + \langle u|H_0 + V_D|u \rangle} \quad \text{etc. } , \]  

Eq. (2.61) becomes

\[ \tilde{T}(\omega) = t_1 - (\omega - H_0)|u\rangle \langle u| \frac{1}{\omega + \langle u|H_0 + V_D|u \rangle} \langle u|(\omega - H_0) . \]  

On the other hand, \( G_1 = G_0 + G_0 t_1 G_0 \) yields

\[ t_1 = (\omega - H_0) G_1(\omega - H_0) - (\omega - H_0) = (\omega - H_0) G_A(\omega - H_0) - (\omega - H_0) \]

\[ + (\omega - H_0)|u\rangle \langle u| \frac{1}{\omega + \langle u|H_0 + V_D|u \rangle} \langle u|(\omega - H_0) , \]  

\[ \text{etc.} \]
where the last term in the right-hand side cancels with the last term of Eq. (2.67). Thus, we find

\[
\tilde{T}(\omega) = (\omega - H_0)G_A(\omega - H_0) - (\omega - H_0) \\
= (\omega - H_0)G_D(\omega - H_0) - (\omega - H_0) - (\omega - H_0)G_D|u\rangle \langle u|G_D(\omega - H_0) \\
= T_D - (\omega - H_0)G_D|u\rangle \frac{1}{\langle u|G_D|u\rangle} \langle u|G_D(\omega - H_0) ,
\]

(2.69)

which is nothing but Eq. (2.57). We can also prove that the bound state pole of \(V_D\) is eliminated from Eq. (2.69), by using the spectral decomposition of \(G_D\) in Eq. (2.40). This proves the equivalence between the Kukulin’s OCM and our Faddeev OCM, hence the equivalence between the Kukulin’s OCM and the Horiuchi’s OCM for the h.o. Pauli-forbidden state \(|u\rangle\).

3 3α OCM for the BFW αα potential

As an example, we consider the 3α system interacting via the deep αα potential

\[
V_{BFW}(r) = -122.6225 \ e^{-0.22 \ r^2} + 4e^2 \ \text{erf}(0.75 \ r)/r \quad \text{(MeV)}
\]

(3.1)

with \(r\), being the relative coordinate between 2α’s in fm. In Eq. (3.1), \(\text{erf}(x) = (2/\sqrt{\pi}) \int_0^x e^{-t^2} dt\) is the error function. The Pauli principle between 2α particles are taken into account in terms of the bound states of \(V_{BFW}(r)\). Since the Coulomb force is not exactly treated in the Faddeev formalism, we replace the folded Coulomb term of Eq. (3.1) with the cut-off Coulomb force

| momen. rep. | 0s       | 1s       | 0d       |
|-------------|----------|----------|----------|
| with Coulomb| -72.6257 | -25.6186 | -22.0005 |
| without Coulomb | -76.7051 | -28.7325 | -25.0908 |
| Coulomb cont. | 4.0794   | 3.1139   | 3.0903   |
| RKG         | 0s       | 1s       | 0d       |
| with Coulomb| -72.6255 | -25.6186 | -22.0005 |
| without Coulomb | -76.7050 | -28.7325 | -25.0908 |
| Coulomb cont. | 4.0795   | 3.1139   | 3.0903   |
\( v^C(r) = \frac{4e^2}{r} \theta(R_C - r) \) with \( R_C = 10 \) fm, introduced at the nucleon level. Here \( \theta(x) \) is the Heaviside step function. For this type of the Coulomb force between protons, the \( \alpha \) Coulomb potential in Eq. (3.1) is replaced with

\[
V^C_{\alpha\alpha}(r) = 4e^2 \left\{ \text{erf}(0.75 \, r) - \frac{1}{2} \left[ \text{erf}(0.75 \, (r + R_C)) + \text{erf}(0.75 \, (r - R_C)) \right] \right\} / r. \tag{3.2}
\]

In the following, we use \( \hbar^2 / M_\alpha = 10.4465 \) MeV \( \cdot \) fm\(^2\) and \( e^2 = 1.44 \) MeV \( \cdot \) fm for the comparison with Ref. [15], unless otherwise specified. Table 1 shows the bound-state energies obtained by diagonalizing the negative-energy \( T \)-matrix in the momentum representation. We have two bound states, \((0s)\) and \((1s)\), in the relative \( S \)-state and one bound state, \((0d)\), in the \( D \)-state, when the Coulomb force is included. The relative momentum \( p \) is discretized using the Gauss-Legendre \( n_1 \)-point quadrature formula for each of the four intervals of 0 - 1 fm\(^{-1}\), 1 - 3 fm\(^{-1}\), 3 - 6 fm\(^{-1}\), and 6 - 12 fm\(^{-1}\). The large value of \( p \) beyond \( p_0 = 12 \) fm\(^{-1}\) is also taken into account by using the Gauss-Legendre \( n_3 \)-point quadrature formula through the mapping \( p = p_0 + \tan \{ \pi (1 + x)/4 \} \). We choose \( n_1 = 15 \) and \( n_3 = 5 \), so that 65 points are used for solving the bound-state wave functions and the necessary \( T \)-matrix for solving the Faddeev equation.

The second Jacobi coordinate \( q \) is also discretized with the Gauss-Legendre \( n_2 \)-point quadrature formula with \( n_2 = 10 \) in the similar way to \( p \), but in this case choosing only three major dividing points with \( q = 1 \) fm\(^{-1}\), 3 fm\(^{-1}\), and 6 fm\(^{-1}\) is good enough. The Gauss-Legendre \( n_3 \)-point quadrature formula with \( q = q_0 + \tan \{ \pi (1 + x)/4 \} \) is also applied to \( q \geq q_0 = 6 \) fm\(^{-1}\). In Table 1, the result of the coordinate-space calculation using the Runge-Kutta-Gill method is also shown for comparison. In this case, we use the full Coulomb force in Eq. (3.1). We find that the choice \( R_C = 10 \) fm in the momentum-representation calculation is accurate enough with the error less than 1 keV. This is also true even in the \( 3\alpha \) Faddeev calculations. The \( \alpha \alpha \) phase shifts by the BFW potential in Eq. (3.1) is very well reproduced, as is shown in the original paper [14].

Table 2 shows the solutions of the \( 3\alpha \) Faddeev equation (2.56) for the \( L = 0 \) ground and excited states, obtained by using the BFW potential and the cut-off Coulomb force with \( R_C = 10 \) fm. The demarcation “b.s.” implies that the bound-state wave functions of the BFW potential are used for the Pauli-forbidden states. Partial waves up to \( \ell_{\text{max}} \) are included in \( 2\alpha \) and \( (2\alpha) - \alpha \) relative motion. The convergence of the ground state energy is very rapid when we increase \( \ell_{\text{max}} \) from 4 to 10. The inaccuracy in \( \ell_{\text{max}} = 8 \) is within 1 keV. Table 2 also shows the results of the variational calculations for Eq. (2.25) with \( V_D \rightarrow V_{\text{BFW}} \) and \( P \) being replaced by \( \tilde{P} \) in Eq. (2.54). Here we use the translationally invariant h.o. basis for the variational functions, [8, 9] with the maximum value of the total h.o. quanta \( N_{\text{max}} = 72 \). Agreement with the Faddeev calculation is satisfactory for the ground state. For the excited \( 0^+ \) state, it deteriorates since \( N_{\text{max}} = 72 \) is still insufficient. We find a very large binding energy of 19.897 MeV for the \( 3\alpha \) bound state, which is different from the result in Refs. [15] and [16]. This difference originates from the fact that we have used \( \tilde{P} \) instead of \( P \). We have also calculated

\*These \( n_3 \) points for \( p \) are not included for solving the Faddeev equation (2.51) or (2.56), since these cause a numerical inaccuracy for the interpolation.
where the SU model as \[9\] the overlap amplitude of the ground-state wave function, \(c\). Partial waves up to \(\ell_{\text{max}}\) are included in \(2\alpha\) and \((2\alpha)\)-\(\alpha\) relative motion. The heading \(n_1-n_2-n_3\) is the number of the momentum discretization points (see the text for details); “dim.” stands for the full dimensionality of the diagonalizing matrix for the Faddeev equation (i.e., \(4n_1(3n_2 + n_3)(\ell_{\text{max}}/2 + 1)\)); \(\varepsilon_{2\alpha}\) is the expectation value of the \(2\alpha\) Hamiltonian with respect to the \(3\alpha\) bound-state solution; \(E_{3\alpha}\) is the \(3\alpha\) bound-state energy; \(c_{(04)}\) is the overlap amplitude between the \(3\alpha\) bound-state wave function and the SU3 (04) configuration with the \(\text{h.o.}\) width parameter \(\nu = 0.28125 \text{ fm}^{-2}\); and \(|f|f\rangle\) in the last column is the squared norm of the redundant components. The results of the variational calculations, using the translationally invariant \(\text{h.o.}\) basis with the maximum \(\text{h.o.}\) quanta \(N_{\text{max}} = 72\), is also shown in the last rows for comparison.

|\(\ket{u}\)| \(\ell_{\text{max}}\) | \(n_1-n_2-n_3\) | \(\text{dim.}\) | \(\varepsilon_{2\alpha}\) (MeV) | \(E_{3\alpha}\) (MeV) | \(c_{(04)}\) | \(|f|f\rangle\) |
|---|---|---|---|---|---|---|---|
| | 4 | 15-10-5 | 6,300 | 14.610 | -19.595 | 0.9652 | 2.7 \times 10^{-4} |
| b.s. | 6 | 15-10-5 | 8,400 | 14.485 | -19.894 | 0.9613 | 2.7 \times 10^{-4} |
| 0_{1}^{+} | 8 | 15-10-5 | 10,500 | 14.483 | -19.897 | 0.9612 | 2.7 \times 10^{-4} |
| 0_{1}^{+} | 10 | 15-10-5 | 12,600 | 14.483 | -19.897 | 0.9612 | 2.7 \times 10^{-4} |
| | | | | | | | |
| b.s. | 4 | 15-10-5 | 6,300 | 7.886 | -0.370 | 0.1302 | 1.9 \times 10^{-6} |
| 0_{2}^{+} | 6 | 15-10-5 | 8,400 | 8.431 | -0.485 | 0.1410 | 1.7 \times 10^{-6} |
| 0_{2}^{+} | 8 | 15-10-5 | 10,500 | 8.500 | -0.475 | 0.1419 | 1.7 \times 10^{-6} |
| 0_{2}^{+} | 10 | 15-10-5 | 12,600 | 8.522 | -0.471 | 0.1422 | 1.7 \times 10^{-6} |
| | | | | | | | |
| b.s. | 9 | 9.950 | -0.241 | 2.0 \times 10^{-6} |

the overlap amplitude of the ground-state wave function, \(c_{(04)} = \langle \Psi_{L=0}^{(04)} | \Psi \rangle\), where the SU3 (04) shell-model wave function is expressed in the 3\(\alpha\) cluster model as [9]

\[
\Psi_{L=0}^{(04)} = [U_{(40)}(p)U_{(40)}(q)]_{(04)0} = \frac{8}{15} R_{20}(p, b_1) R_{20}(q, b_2) Y_{0(00)}(\hat{p}, \hat{q})
\]

\[
- \frac{4}{3\sqrt{5}} R_{12}(p, b_1) R_{12}(q, b_2) Y_{2(22)}(\hat{p}, \hat{q}) + \frac{3}{5} R_{04}(p, b_1) R_{04}(q, b_2) Y_{4(44)}(\hat{p}, \hat{q}) .
\]

(3.3)

Here, \(U_{(40)}(p)\) and \(U_{(40)}(q)\) are the single-particle SU3 states with the SU3 coupling \((40) \times (40) \rightarrow (04)\), \(R_{mf}(x, \nu)\) is the radial part of the h.o. wave function, and \(Y_{3\alpha L}(\hat{p}, \hat{q})\) is the coupled angular-momentum function. The width parameters of the h.o. radial wave functions in the momentum representation are given by \(b_1 = 1/4\gamma\) and \(b_2 = 3/16\gamma\) with \(\gamma = \mu \nu = 2\nu\). For the present calculation,
we have used the h.o. width parameter $\nu = 0.28125 \text{ fm}^{-2}$ in the configuration space.\textsuperscript{3} Since the binding energy is very large, the $c_{(04)}$ value is very close to 1, and is about 0.96. The squared norm of the redundant components defined by $\langle f|f \rangle$ with $|f\rangle = \langle u_B|\Psi \rangle = \langle u_B|(1 + S)|\psi \rangle$ are also shown in the last column in Table 2.

Table 3 shows results of the $3\alpha$ Faddeev calculations when the Coulomb force is switched off. We find that the Coulomb contribution in the present $3\alpha$ ground

\textsuperscript{3}This $\nu$ value corresponds to a rather compact $\alpha$ cluster with the rms radius $r_\alpha = (3/4\sqrt{\nu}) = 1.414 \text{ fm}.$

Table 3. The same as Table 2, but when the Coulomb force is switched off. In the upper half, denoted by “h.o.”, the results for the h.o. Pauli-forbidden states $|u\rangle$ with the width parameter $\nu = 0.28125 \text{ fm}^{-2}$ are shown.

| $|u\rangle$ | $\ell_{\text{max}}$ | $n_1-n_2-n_3$ | dim. | $\varepsilon_{2\alpha}$ (MeV) | $E_{3\alpha}$ (MeV) | $c_{(04)}$ | $\langle f|f \rangle$ |
|----------|----------------|--------------|------|----------------|----------------|-------------|----------------|
| h.o.     | 4              | 15-10-5      | 6,300 | 12.405     | $-25.296$     | 0.9740      | $1.3 \times 10^{-12}$ |
| $0_1^+$  | 6              | 15-10-5      | 8,400 | 12.262     | $-25.563$     | 0.9707      | $1.3 \times 10^{-12}$ |
| 10       | 8              | 15-10-5      | 10,500 | 12.259    | $-25.565$     | 0.9706      | $1.3 \times 10^{-12}$ |
| h.o. variation |             |              |       |            |                |             |                       |
| h.o.     | 4              | 15-10-5      | 6,300 | 6.836      | $-6.181$      | 0.1343      | $5.7 \times 10^{-12}$ |
| $0_2^+$  | 6              | 15-10-5      | 8,400 | 7.117      | $-6.404$      | 0.1423      | $5.8 \times 10^{-12}$ |
| 10       | 8              | 15-10-5      | 10,500 | 7.125     | $-6.417$      | 0.1426      | $5.8 \times 10^{-12}$ |
| h.o. variation |             |              |       |            |                |             |                       |
| b.s.     | 4              | 15-10-5      | 6,300 | 12.722     | $-27.431$     | 0.9738      | $2.6 \times 10^{-4}$ |
| $0_1^+$  | 6              | 15-10-5      | 8,400 | 12.582     | $-27.745$     | 0.9700      | $2.6 \times 10^{-4}$ |
| 10       | 8              | 15-10-5      | 10,500 | 12.580    | $-27.748$     | 0.9700      | $2.6 \times 10^{-4}$ |
| h.o. variation |             |              |       |            |                |             |                       |
| b.s.     | 4              | 15-10-5      | 6,300 | 9.062      | $-5.731$      | 0.1121      | $3.1 \times 10^{-6}$ |
| $0_2^+$  | 6              | 15-10-5      | 8,400 | 9.327      | $-6.060$      | 0.1213      | $2.5 \times 10^{-6}$ |
| 10       | 8              | 15-10-5      | 10,500 | 9.329     | $-6.077$      | 0.1217      | $2.5 \times 10^{-6}$ |
| h.o. variation |             |              |       |            |                |             |                       |


Table 4. Result of the 3α OCM with pairwise orthogonality conditions (Horiuchi-type 3α OCM) for the 3α ground state, using the translationally invariant h.o. basis. The BFW potential for α is used with \( \hbar^2/M_N = 41.7860 \text{ MeV} \cdot \text{fm}^2 \) and \( \nu = 0.28125 \text{ fm}^{-2} \). The Coulomb force is switched off. The heading \( N_{\text{max}} \) is the maximum value of the total h.o quanta included in the calculation; \( E_{2\alpha} \) is the lowest 2α diagonalization energy; \( \varepsilon_{2\alpha} \) is the expectation value of the 2α Hamiltonian with respect to the 3α ground-state solution; \( E_{3\alpha} \) is the 3α ground-state energy; and \( c_{(04)} \) is the overlap amplitude between the 3α ground-state wave function and the \( SU_3 \) (04) configuration. The Faddeev result in Table 3 with the h.o. \( |u\rangle \) is also shown in the bottom row for comparison.

| \( N_{\text{max}} \) | \( E_{2\alpha} \) (MeV) | \( \varepsilon_{2\alpha} \) (MeV) | \( E_{3\alpha} \) (MeV) | \( c_{(04)} \) |
|-----------------|----------------|----------------|----------------|---------|
| 4               | 9.81970        | -              | -              | -       |
| 6               | 6.23729        | -              | -              | -       |
| 8               | 2.34421        | 14.0067        | -22.6177       | 1       |
| 10              | 0.85837        | 14.3470        | -22.6745       | 0.9993  |
| 12              | -0.11812       | 12.9759        | -25.2357       | 0.9811  |
| 14              | -0.67019       | 12.7748        | -25.2768       | 0.9797  |
| 16              | -1.03181       | 12.4909        | -25.5086       | 0.9740  |
| 18              | -1.26800       | 12.3918        | -25.5244       | 0.9729  |
| 20              | -1.43122       | 12.3215        | -25.5528       | 0.9716  |
| 30              | -1.77280       | 12.2608        | -25.5649       | 0.9707  |
| 40              | -1.86319       | 12.2584        | -25.5652       | 0.9706  |
| 50              | -1.89424       | 12.2583        | -25.5652       | 0.9706  |
| 60              | -1.90664       | 12.2583        | -25.5652       | 0.9706  |
| Faddeev         | 12.2594        | -25.5653       | 0.9706         |         |

state with the BFW potential is 7.85 MeV, which implies that our 3α ground state is rather compact compared with the microscopic 3α cluster model. In the latter case, the standard value is 5 ~ 6 MeV. When the Coulomb force is neglected, we find that the second 0^+ state appears around \( E_{3\alpha} \sim -6 \text{ MeV} \). In Table 3, we also show in the upper half, denoted by “h.o.”, the results when the h.o. Pauli-forbidden states are used for \( |u\rangle \), instead of the bound-state wave functions \( |u_B\rangle \) of the BFW potential. The h.o. width parameter \( \nu = 0.28125 \text{ fm}^{-2} \) is again used for this calculation. We find that the 3α ground state is less bound, but the energy difference is only 2 MeV. In this case, the elimination of the Pauli-forbidden states of the 3α system is rather easy, if we use the translationally invariant h.o. basis in the variational calculation. In Ref. [8], we have examined the equivalence between such a variational calculation and the present Faddeev calculation using the 2α RGM kernel. Table 4 shows the results of the 3α OCM with pairwise orthogonality conditions (namely, Eq. (2.25) with \( V_D \rightarrow V_{\text{BFW}} \) and \( P \) constructed from the h.o. \( |u\rangle \)), using the translationally invariant h.o.
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Table 5. The same as Table 4, but for the $3\alpha$ OCM, using the Kukulin’s method of orthogonalizing pseudo-potentials (namely, Eq. (2.42)) for the h.o. Pauli-forbidden states $|u\rangle$. The $\lambda$ parameter, $\lambda = 10^5$ MeV, is used to eliminate the h.o. Pauli-forbidden components. The parenthesized numbers indicate the values for the modification of the last two digits when $\lambda = 10^5$ MeV is used.

| $N_{\text{max}}$ | $E_{2\alpha}$ (MeV) | $\varepsilon_{2\alpha}$ (MeV) | $E_{3\alpha}$ (MeV) |
|------------------|----------------------|-----------------------------|----------------------|
| 4                | 9.81970 (56)         | $6.25 \times 10^6$ ($6.25 \times 10^4$) | $1.87 \times 10^7$ ($1.87 \times 10^5$) |
| 6                | 6.23729 (08)         | $3.02 \times 10^7$ ($3.02 \times 10^4$) | $9.07 \times 10^6$ ($9.06 \times 10^4$) |
| 8                | 2.34421 (01)         | 14.0067 (69)                | $-22.6177$ (88)      |
| 10               | 0.85836 (16)         | 14.3470 (77)                | $-22.6745$ (56)      |
| 12               | $-0.11812$ (32)      | 12.9759 (68)                | $-25.2357$ (70)      |
| 14               | $-0.67019$ (37)      | 12.7748 (58)                | $-25.2768$ (80)      |
| 16               | $-1.03181$ (98)      | 12.4909 (19)                | $-25.5086$ (98)      |
| 18               | $-1.26800$ (17)      | 12.3918 (29)                | $-25.5244$ (56)      |
| 20               | $-1.43122$ (38)      | 12.3215 (26)                | $-25.5528$ (40)      |
| 30               | $-1.77280$ (95)      | 12.2608 (19)                | $-25.5649$ (61)      |
| 40               | $-1.86319$ (33)      | 12.2584 (95)                | $-25.5652$ (64)      |
| 50               | $-1.89424$ (38)      | 12.2583 (94)                | $-25.5653$ (65)      |
| 60               | $-1.90664$ (78)      | 12.2583 (94)                | $-25.5653$ (65)      |

basis. The BFW potential for $\alpha\alpha$ is used with $\hbar^2/M_N = 41.7860$ MeV·fm$^2$ and the h.o. Pauli-forbidden states with $\nu = 0.28125$ fm$^{-2}$. The Coulomb force is switched off for simplicity. Since the present $3\alpha$ ground state is very compact, the convergence with respect to the increase of $N_{\text{max}}$ is very fast, and $N_{\text{max}} = 40$ is almost sufficient to obtain the converged result.

We have also examined the $3\alpha$ OCM, using the Kukulin’s method of orthogonalizing pseudo-potentials (namely, Eq. (2.42)) for the h.o. Pauli-forbidden states $|u\rangle$. The results are shown in Table 5 with respect to the cases when the $\lambda$ parameter in Eq. (2.30) is $\lambda = 10^5$ MeV and $\lambda = 10^7$ MeV. For $\lambda = 10^7$ MeV, we find a complete agreement with the results in Table 4 for $N_{\text{max}} \geq 8$. When $\lambda = 10^5$ MeV is used, the energies deviate from the values in $\lambda = 10^7$ MeV in the last two digits, as long as the model space is large enough. This is, of course, a rather expected result, since the h.o. basis can conveniently eliminate the Pauli-forbidden states with some particular h.o. quanta within the finite number of the basis states.

A conclusion derived from the above discussion is that the deeply bound feature of the $3\alpha$ system in the BFW potential does not change appreciably even if one uses the real bound states for the BFW potential as the Pauli-forbidden states $|u\rangle$, as long as the dominant shell-model components are preserved in the Pauli-allowed space by using $\tilde{P}$. This is because the deeply bound states have
very large overlaps with the h.o. Pauli-forbidden states. The strongly attractive feature of the BFW potential in the $3\alpha$ system is related to the short range nature of this potential, in comparison with the usual folding potentials in the OCM formalism. As an example of the usual $3\alpha$ OCM, we show in Table 6 the result of the $\alpha\alpha$ folding potential using the Schmid-Wildermuth force \[20\] with $\nu = 0.257$ fm$^{-2}$. In this case, we use $\hbar^2/M_N = 41.4711$ MeV$\cdot$fm$^2$ for the microscopic $3\alpha$ cluster model. We find that the $3\alpha$ energy is $-10.63$ MeV and it is not overbound, since the Coulomb energy is about 5 - 6 MeV.

The short range nature of the BFW potential can be seen, by directly com-

Table 6. The same as Table 4, but for the $2\alpha$ folding potential obtained from the Schmid-Wildermuth force with $\nu = 0.257$ fm$^{-2}$. As for the spin-isospin dependence, an almost pure Serber force with $X_d = 2.4$ is used. For the reduced mass, the standard value $\hbar^2/M_N = 41.4711$ MeV$\cdot$fm$^2$ for the microscopic $3\alpha$ cluster model is used.

| $N_{\text{max}}$ | $E_{2\alpha}$ (MeV) | $\varepsilon_{2\alpha}$ (MeV) | $E_{3\alpha}$ (MeV) | $\varepsilon_{(04)}$ |
|------------------|----------------------|-----------------|-----------------|-----------------|
| 4                | 14.3525              | $-\varepsilon_{2\alpha}$ | $-\varepsilon_{3\alpha}$ | $-\varepsilon_{(04)}$ |
| 6                | 9.1136               | $-\varepsilon_{2\alpha}$ | $-\varepsilon_{3\alpha}$ | $-\varepsilon_{(04)}$ |
| 8                | 4.9458               | 17.6002          | $-5.8189$      | 1 |
| 10               | 3.0476               | 15.2471          | $-6.5774$      | 0.9873 |
| 12               | 1.8698               | 13.1271          | $-9.1708$      | 0.9528 |
| 14               | 1.1573               | 11.8925          | $-9.6655$      | 0.9293 |
| 16               | 0.6854               | 11.0975          | $-10.1209$     | 0.9085 |
| 18               | 0.3637               | 10.5721          | $-10.3130$     | 0.8946 |
| 20               | 0.1348               | 10.2268          | $-10.4427$     | 0.8845 |
| 30               | $-0.3903$            | 9.6254           | $-10.6095$     | 0.8661 |
| 40               | $-0.5598$            | 9.5415           | $-10.6253$     | 0.8634 |
| 50               | $-0.6313$            | 9.5286           | $-10.6271$     | 0.8630 |
| 60               | $-0.6665$            | 9.5264           | $-10.6274$     | 0.8629 |
| 72               | $-0.6882$            | 9.5259           | $-10.6274$     | 0.8629 |

Table 7. Decomposition of the $3\alpha$ energy $E_{3\alpha}$ into the kinetic-energy and potential-energy contributions. Here the h.o. $|\psi\rangle$ is used.

| $V_{\alpha\alpha}$ | $\varepsilon_{2\alpha}$ (MeV) | $E_{3\alpha}$ (MeV) | $\langle H_0 \rangle$ (MeV) | $\langle V \rangle$ (MeV) |
|---------------------|-------------------------------|-------------------|-------------------------|-------------------------|
| BFW                 | 12.258                        | $-25.565$         | 124.680                 | $-150.245$              |
| SW                  | 9.526                         | $-10.624$         | 78.405                  | $-89.030$               |
Table 8. The correlation between the 3α ground-state energy $E_{3\alpha}$ and the depth of the direct potential $V_0$. For BFW the bound-state $|u_B\rangle$ is used.

| $V_{\alpha\alpha}$ | $V_0$ (MeV) | b (fm) | $E_{3\alpha}$ (MeV) |
|-------------------|-------------|--------|---------------------|
| SW ($\nu = 0.257$ fm$^{-2}$) | -97.7 | 2.26 | -10.62 |
| SW ($\nu = 0.275$ fm$^{-2}$) | -105.4 | 2.21 | -14.66 |
| BFW (b.s. $|u_B\rangle$) | -122.6 | 2.13 | -27.75 |

paring the nuclear part of the $\alpha\alpha$ potentials:

$$V^{BFW} = -122.6225 \ e^{-0.22 \ r^2},$$
$$V_D(SW) = -97.7 \ e^{-0.196 \ r^2}.$$ (3.4)

In order to calculate the folding potential $V_D(SW)$, we have used the formula

$$V_\alpha^{\alpha\alpha}(r) = 2X_dv_0 \left(\frac{\nu}{\nu + 3\kappa/4}\right)^3 \exp\left\{-\frac{\kappa\nu}{\nu + 3\kappa/4} \ r^2\right\},$$ (3.5)

for the effective two-nucleon interaction $v(r) = v_0 \ w \ e^{-\kappa r^2}$ with $w = W + BP_\sigma - HP_\tau - MP_\sigma P_\tau$. We use an almost pure Serber force with the Majorana parameter $m = 0.505$, which corresponds to $X_d = 8W + 4B - 4H - 2M = 2.4$ in Eq. (3.5). The $1/e$ ranges of these potentials are $b = 2.13$ fm for the BFW potential and $b = 2.26$ fm for the folding potential. Since we have calculated $\varepsilon_{2\alpha}$, we can evaluate the contributions of the kinetic-energy and the potential-energy terms separately through the simple expression: $\langle H_0\rangle = 2(3\varepsilon_{2\alpha} - E)$ and $\langle V\rangle = 3(E - 2\varepsilon_{2\alpha})$. (See, for example, Ref. [21].) Table 7 clearly shows that the large $3\alpha$ energy of the BFW potential is the result of the large cancellation of the kinetic-energy and potential-energy contributions. In the original $3\alpha$ OCM calculation using the Schmid-Wildermuth force, Horiuchi [12] has used the value $\nu = 0.275$ fm$^{-2}$ and the pure Serber force, $X_d = 2.445$. In this case, the direct potential becomes

$$V_D(SW) = -105.4 \ e^{-0.204 \ r^2},$$ (3.6)

with $b = 2.21$ fm and the converged $3\alpha$ bound-state energy is $-14.66$ MeV.\(^4\)

We find that the $3\alpha$ energy is strongly correlated with the depth of the direct potential $V_0$, as shown in Table 8. If we extrapolate the BFW value from the above two results of the SW force, we find $-23.68$ MeV for the BFW potential, which is close to the calculated value $-27.75$ MeV. It is natural that a deep potential gives stronger binding in the $3\alpha$ system, since the effect of the potential term is by factor 1.5 larger than in the $2\alpha$ system, as was pointed out by Horiuchi [12].

\(^4\)In Ref. [12] it is reported as $-14.68$ MeV.
4 Summary

In this study, we have developed the Faddeev formalism for the three cluster systems, which “exactly” takes into account the Pauli-forbidden states. Actually, the exact Pauli-forbidden states of three-cluster systems are defined through the eigen-value problem of the three-cluster normalization kernel with the eigen-value zero. However, the pairwise orthogonality conditions to the total wave functions developed in this paper are known to give a good approximation for the exact Pauli-allowed space obtained by the diagonalization procedure of the normalization kernel. For example, in the $3\alpha$ system composed of the simple $(0s)^4$ harmonic-oscillator (h.o.) shell-model wave functions, this correspondence is completely verified by enumerating the $SU_3$ allowed states in the translationally invariant h.o. basis. [22]

The main result of this paper is that it is this type of three-cluster orthogonality condition model (OCM) with pairwise orthogonality conditions that leads to the complete equivalence to the three-cluster Faddeev equation interacting only by pairwise interactions. The pairwise interaction can be two-cluster RGM kernels with the linear energy dependence, two-cluster folding potentials of the effective two-body force, or the deep phenomenological local potentials like the Buck, Friedrich and Wheatley potential (BFW potential) [14]. In order to formulate the three-cluster Faddeev equation with explicit elimination of the pairwise Pauli-forbidden components, we only need to use the modified $T$-matrix, $\tilde{T}(\omega,\varepsilon)$, which eliminates the off-shell singularity related to the existence of the Pauli-forbidden states. This $T$-matrix is, in general, energy dependent ($\varepsilon$-dependent) for the three-cluster Faddeev equation using two-cluster RGM kernels, and the energy dependence is self-consistently determined by calculating the expectation value of the two-cluster Hamiltonian with respect to the resultant Faddeev solution. [8] On the other hand, in the three-cluster OCM, considered in the present paper, $\tilde{T}(\omega)$ is energy independent. The Pauli-forbidden state in this OCM could be the h.o. wave functions of the microscopic two-cluster system, or the real bound states of the phenomenological local potentials between two clusters. However, the $3\alpha$ Pauli-allowed space should be carefully defined, in order not to exclude the dominant $SU_3$ components for the realistic description of the $^{12}\text{C}$ ground state. We find that the Kukulin’s method of orthogonalizing pseudo-potentials [13] is completely equivalent to the three-cluster OCM with pairwise orthogonality conditions. The latter was first proposed by Horiuchi [11]. We have proven this equivalence through the equivalence between either model and the present three-cluster Faddeev formalism using $\tilde{T}(\omega)$. A nice feature of the present Faddeev formalism is that the $T$-matrix description of the two-cluster interaction allows us to take the limit $\lambda \to \infty$ analytically in the method of orthogonalizing pseudo-potentials, and that the solution of the Faddeev equation automatically guarantees the pairwise orthogonality conditions of the total wave function, owing to the orthogonality property of the $\tilde{T}(\omega)$ $T$-matrix.

As an example, we have applied the present three-cluster Faddeev formalism to the $3\alpha$ system interacting via the BFW $\alpha\alpha$ potential [14]. The Pauli-forbidden states are assumed to be the real bound states of the potential. We have found that this potential yields the $3\alpha$ ground-state energy $-19.897$ MeV, which is a
different result from Refs. [15] and [16], in which the orthogonality to the 2α bound-state solutions |u_B⟩ is very strictly demanded. This feature of the large overbinding does not change even when we use the h.o. Pauli-forbidden states with a reasonable width parameter of the α-clusters. This feature is traced back to the deep and short-range nature of the BFW αα potential, as compared with the folding potentials usually used in the microscopic 3α cluster model. The validity of the 3α boson model described by the BFW αα potential is examined by calculating other physical observables, like the rms radius of 12C, using the obtained 3α ground-state wave function.

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A simple formula for T-matrix

In this Appendix, we will show a general formula of the T-matrix for the sum of two potentials. From a simple calculation, the T-matrix for V = V_1 + V_2 is expressed as

\[ T = T_1 + T_2 \]

where \( T_1 \) and \( T_2 \) are the T-matrices of \( V_1 \) and \( V_2 \), respectively:

\[ T_1 = t_1 + t_1 G_0 T_2 , \quad T_2 = t_2 + t_2 G_0 T_1 , \]

\[ t_1 = V_1 + V_1 G_0 t_1 , \quad t_2 = V_2 + V_2 G_0 t_2 . \]

If we further assume \( V_2 = \lambda |u⟩⟨u| \), we find

\[ t_2 = |u⟩⟨u| \frac{1}{\lambda^{-1} - ⟨u|G_0|u⟩} ⟨u| \] .

Thus, the solution of \( T = V + V G_0 T \) for \( V = V_1 + \lambda |u⟩⟨u| \) is given by

\[ T = t_1 + (1 + t_1 G_0)|u⟩⟨u| \frac{1}{\lambda^{-1} - ⟨u|G_0 + G_0 t_1 G_0|u⟩} ⟨u|(1 + G_0 t_1) . \]

If we further move to \( \lambda \to \infty \), we find

\[ T = t_1 - (1 + t_1 G_0)|u⟩⟨u| \frac{1}{⟨u|G_0 + G_0 t_1 G_0|u⟩} ⟨u|(1 + G_0 t_1) , \]

with \( t_1 = V_1 + V_1 G_0 t_1 \). This expression leads to our basic relationship

\[ ⟨u| 1 + G_0 T⟩ = 0 \quad \text{and} \quad [1 + T G_0]|u⟩ = 0 . \]

As an example, let us use this formula in the method of orthogonalizing pseudo-potentials for \( V_{\text{RGM}}(ε) \). We set

\[ V_1 \to V_{\text{RGM}}(ε) \quad \text{and} \quad t_1 \to T(ω, ε) . \]

If we use the relationship between \( T(ω, ε) \) and \( \tilde{T}(ω, ε) \), given in Eqs. (2.8), (2.9), and (2.10) of Ref. [8], we easily obtain

\[ T = T(ω, ε) - [1 + T(ω, ε)G_0(ω)]|u⟩⟨u| \frac{1}{⟨u|G_0(ω) + G_0(ω)T(ω, ε)G_0(ω)|u⟩} \times ⟨u| 1 + G_0(ω)T(ω, ε)] = T(ω, ε) - (ω - H_0)|u⟩⟨u| \frac{1}{ω - ε} ⟨u|(ω - H_0) = \tilde{T}(ω, ε) , \]

\[ \text{Namely, our RGM T-matrix } \tilde{T}(ω, ε) \text{ is obtained from } V_{\text{RGM}}(ε) \text{ by the method of orthogonalizing pseudo-potentials.} \]
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