Case of almost redundant components in 3α Faddeev equations

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The 3α orthogonality condition model using the Pauli-forbidden bound states of the Buck, Friedlich, and Wheatly $\alpha\alpha$ potential can yield a compact 3α ground state with a large binding energy, in which a small admixture of the redundant components can never be eliminated.

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As a typical example of quantum-mechanical three-body systems, the three-alpha-particle (3α) model for ^{12}C has been extensively studied from various viewpoints [1]. It is well known that the microscopic structure of the α cluster plays an important role to create damped inner oscillations in the relative wave functions of the two α clusters, which can be described phenomenologically as the short-range repulsive core in the 2α system. In the 3α system, the amplitudes of these inner oscillations can be enhanced by the existence of the third α cluster, resulting in the formation of the compact shell model like ground state of ^{12}C [2]. On the other hand, the loosely bound nature of the 2α pair is still preserved in the excited 0^+ state at $E_x=7.65$ MeV, for which much interest is recently paid as a possible candidate of the α condensation state [3,4]. This structure change of the 3α system can most easily be simulated in the orthogonality condition model (OCM), first proposed by Saito [5].

In a separate publication [6], we have discussed a new type of the Faddeev formalism for the 3α system, in which pairwise α clusters interact via the Buck, Friedlich, and Wheatly potential (BFW potential) [7]. In this model, the Pauli-forbidden states between the two α clusters are composed of the lowest two S-wave bound states and one D-wave bound state of the BFW potential. We found that the 3α ground-state energy is -19.897 MeV for this potential, which is contradictory to the very small binding energy, $E_{3\alpha}=-0.26$ MeV, from the variational calculations carried out by Tursunov, Baye, Descouvemont, and Daniel in Refs. [8,9]. The same situation also happens when we neglect the Coulomb force between α clusters. Namely, we have obtained $E_{3\alpha}=-27.748$ MeV, while theirs -6.003 MeV [10]. These authors comment that our result for the 3α ground-state solution, using the BFW bound-state Pauli-forbidden states, does not completely eliminate the Pauli-forbidden components. Unlike their work our Faddeev solution contains a small admixture of the redundant components. Suppose $\Psi=\varphi_\alpha+\varphi_\beta+\varphi_\gamma$ be the total wave function of the 3α system, composed of the three Faddeev components φ_α, φ_β, and φ_γ. If one sets $f_u=\langle u|\Psi\rangle$ with u being one of the Pauli-forbidden bound-state solutions, $N_R=\Sigma_u\langle f_u|f_u\rangle$ for all three Pauli-forbidden states is only $(2.6-2.7)\times10^{-4}$. This is a big contrast to the result for the harmonic oscillator (h.o.) Pauli-forbidden states $|u\rangle$, since in this case $N_R\sim10^{-12}$ [6]. The purpose of this brief report is to show that, if one wants to keep the shell-model like compact 3α ground state, one cannot help but allowing a small admixture of the redundant components. In other words, it is impossible to eliminate this small admixture in the present framework without giving up the solution with the dominant shell-model like [3] (04) component with the total h.o. quanta $N=8$. This implies that their solution corresponds to our second (excited-state) solution. The energy of this second solution is about -6 MeV, and it has a small (04) component and $N_R\sim10^{-6}$.

A main problem arises from the second [21]-symmetric component in the 3α Faddeev equation, which now becomes no longer an exact redundant component, but "an almost redundant component" of the Faddeev equation. Here we use the Faddeev terminology and the notations used in our previous publications, Refs. [11,6], but the same analysis is also possible in the various variational approaches. In Ref. [11], we first solve the eigenvalue equation of the rearrangement matrix

$$\langle u|S|uf^\tau\rangle=\tau|f^\tau\rangle, \tag{1}$$

where $S=(123)+(123)^2$ and $|f^\tau\rangle$ is normalized as $\langle f^\tau|f^{\tau'}\rangle=\delta_{\tau,\tau'}$. The solution $|f^\tau\rangle$ with $\tau=-1$ gives a [21]-symmetric redundant solution $\varphi_\tau=G_0|uf^\tau\rangle$ of the Faddeev equation, where G_0 is the free three-body Green function. The Faddeev component φ_τ trivially satisfies

$$\lambda(E)\varphi=G_0\widetilde{T}S\varphi, \quad \text{with} \quad \lambda(E)=1, \tag{2}$$

due to the orthogonality property, $\widetilde{T}G_0|u\rangle=-|u\rangle$, of the redundancy free $\widetilde{T}$-matrix and the commutability $G_0S=SG_0$. For this reason we add an extra term as in Eq. (9) below, and determine the bound-state energy E with $\lambda(E)=1$. After E is

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TABLE I. Some important overlap amplitudes of the lowest three solutions of Eq. (1) with the shell-model states, when the bound-state $|u\rangle$ of the BFW potential are used for the 2α Pauli-forbidden states. The h.o. width parameter $\nu=0.281\ 25\ \mathrm{fm}^{-2}$ is used for the shell-model wave functions.

τ	−1.00000	−0.999037	−0.099510
$\langle[21]2(20)\|uf^{\tau}\rangle$	0.985929	0.098412	0.000873
$\langle[21]4(40)\|uf^{\tau}\rangle$	0.000764	0.593663	0.024228
$\langle[3]8(04)\|uf^{\tau}\rangle$	0.000657	0.015506	0.001921
$\langle[3]8(04)\|\phi_{\tau}^{[3]}\rangle$		0.865401	0.003506

determined in this way, we again solve the Faddeev equation, Eq. (2), without this second term. Then we get three $\lambda(E)=1$ solutions; one is a real solution and the others are the dual complex solutions having $\mathrm{Re}\{\lambda(E)\}\sim 1$ with a small imaginary part of the order of 10^{-2}. The appearance of the complex eigenvalues having opposite signs in the imaginary part is not excluded since we are working with an eigenvalue problem of the nonsymmetric kernel, $G_0\tilde{T}S$. These three solutions are characterized by the following three SU_3 components; [21]2(20), [21]4(40), and [3]8(04), in the notation $|[f]N(\lambda\mu)\rangle$ or $[f](\lambda\mu)$ with $N=\lambda+2\mu$. However, this classification is for the Faddeev component φ. If we make $\Psi\sim(1+S)\varphi$, all of these three Ψ's become [3]-symmetric total wave functions for the 3α system, as long as they are nonzero. If $|u\rangle$ are the h.o. (0*s*), (1*s*), and (0*d*) states, the first two [21](20) and [21](40) states exactly vanish by the $(1+S)$ operation, which means that these are trivial solutions of Eq. (2) with $\lambda(E)=1$. However, if we use the bound state $|u\rangle$ of the BFW potential, the latter [21](40) state becomes almost redundant. (The same situation also happens for the first [21](20) state, but the residual component after the $(1+S)$ operation is very small and less than 10^{-5}.) In such a case, we can construct the normalized state

$$\phi_{\tau}^{[3]}=\frac{(1+S)|uf^{\tau}\rangle}{\sqrt{3(1+\tau)}}. \tag{3}$$

[Note that $(1+S)^2=3(1+S)$.] This becomes [3](04) dominant state. This can be confirmed by expanding $|uf^{\tau}\rangle$ in the h.o. basis and calculating the overlap of $\phi_{\tau}^{[3]}$ with the shell-model state, $|[3]8(04)\rangle$, in the 3α-cluster representation [11]. Here we use a rather compact α cluster with the h.o. width parameter $\nu=0.281\ 25\ \mathrm{fm}^{-2}$. In Table I, the $\phi_{\tau}^{[3]}$ state generated from the second [21]4(40) dominant solution $|uf^{\tau}\rangle$ with $\tau=-0.999\ 037$ involves the [3]8(04) component with the amplitude 0.865 401. This overlap is obtained from the third overlap in Table I through

$$\begin{aligned}\langle[3]8(04)|\phi_{\tau}^{[3]}\rangle&=\frac{\langle[3]8(04)|(1+S)|uf^{\tau}\rangle}{\sqrt{3(1+\tau)}}\\&=\sqrt{\frac{3}{1+\tau}}\langle[3]8(04)|uf^{\tau}\rangle,\end{aligned} \tag{4}$$

since $S^{\dagger}=S$. The normalization factor $1/\sqrt{3(1+\tau)}$ is the reason for this large overlap. This immediately reminds us of our old experience of the almost forbidden state [12] in two-cluster systems. In that case, the almost forbidden state is the cluster excited state, but in the present case it is the real [3](04) state, which is generated by the 3α symmetrization from the almost redundant solution of Eq. (1), with the dominant [21]-symmetric configuration $|[21]4(40)\rangle$.

It is interesting to note that the transition from $N=4$ to 8 takes place, since [3](04) is the only Pauli-allowed state with the lowest h.o. quanta $N=8$. The reason for this transition is naturally understood if we recall how we construct the Pauli-forbidden states in the pairwise OCM for the 3α system. Let us assume for the time being that $|u\rangle$ is the h.o. Pauli-forbidden states. We first enumerate the translationally invariant [3]-symmetric h.o. states by the Moshinsky rule [13]. The elimination of the Pauli-forbidden state by the diagonalization procedure for the projection operator $P=\Sigma_{\alpha}|u_{\alpha}\rangle\langle u_{\alpha}|$ gives that the lowest Pauli-allowed state of the 3α system is only (04) for $N=8$, and (62) and (24) for $N=10$, etc. [14] On the other hand, the construction of the 3α Pauli-forbidden states in Eq. (1) is exactly equivalent to this elimination procedure of the Pauli-forbidden state, as long as the [3]-symmetric basis states are concerned. Since the [3]-symmetric Pauli-forbidden states are already enumerated by Eq. (3) for the solutions of Eq. (1) with $\tau>-1$ in the h.o. limit, $\phi_{\tau}^{[3]}$ with $\tau\sim-1$ should be an extra state which is orthogonal to all of these [3]-symmetric Pauli-forbidden states. Therefore, $\phi_{\tau}^{[3]}$ in Eq. (3) generated from the small deviation from the pure h.o. limit should be the [3]-symmetric *allowed* state with the smallest number of oscillations, namely, $N=8$ (04) state.

To be more specific, let us expand the Faddeev component φ by the following basis states.

[21]-symmetric basis: $\phi_{-1}^{[21]}=|uf^{-1}\rangle$ and the other orthonormalized basis $\phi_{\alpha}^{[21]}$.

[3]-symmetric basis: $\phi_{\tau}^{[3]}$ with $\tau>-1$, given in Eq. (3), and the other orthonormalized basis $\phi_{\beta}^{[3]}$. Here it is important to construct these as

$$\langle\phi_{\tau}^{[3]}|\phi_{\beta}^{[3]}\rangle=0 \quad \forall\ \tau>-1 \text{ and } \beta. \tag{5}$$

We expand φ in Eq. (2) with $\lambda(E)=1$ as

$$\varphi=C_{-1}^{[21]}|uf^{-1}\rangle+\sum_{\alpha}C_{\alpha}^{[21]}\phi_{\alpha}^{[21]}+\sum_{\tau>-1}C_{\tau}^{[3]}\phi_{\tau}^{[3]}+\sum_{\beta}C_{\beta}^{[3]}\phi_{\beta}^{[3]}, \tag{6}$$

and multiply the resultant equation by $\langle u|$ from the left. Then, because of the basic relationship, $\langle u|G_0\tilde{T}=-\langle u|$, the [21]-symmetric part vanishes by $\langle u|(1+S)|[21]\rangle=0$, and we obtain

$$\begin{aligned}0&=\langle u|\Psi\rangle=\langle u|(1+S)|\varphi\rangle\\&=\sum_{\tau>-1}C_{\tau}^{[3]}\sqrt{3(1+\tau)}|f^{\tau}\rangle+\sum_{\beta}3C_{\beta}^{[3]}\langle u|\phi_{\beta}^{[3]}\rangle.\end{aligned} \tag{7}$$

Here we further take the matrix element with some particular $\langle f^{\tau}|$ with $\tau>-1$. Then the basis construction in Eq. (5) gives

that the last term of Eq. (7) disappears and we are left with

$$C_\tau^{[3]}\sqrt{3(1+\tau)}=0 \quad \forall\ \tau>-1. \tag{8}$$

This implies that the exact solution of Eq. (2) with $\lambda(E)=1$ should not contain any of the $\phi_\tau^{[3]}$ components with $\tau>-1$; namely, the 3α Pauli-forbidden components. However, this is correct only within the accuracy of numerical calculations. For the solution with τ far apart from -1, $C_\tau^{[3]}\sim 0$ is certainly true. But, for the second solution of Table I with $\tau=-0.999\,037$, $C_\tau^{[3]}$ could be appreciably large, since $C_\tau^{[3]}\times 0.054=0$. (Note that the imaginary part of the dual complex eigenvalues for the Faddeev equation is of the order of 10^{-2}.) In fact, we have a good reason to believe that our ground-state solution has a dominant $\phi_\tau^{[3]}$ component with $\tau=-0.999\,037$, since both of them have a large [3](04) component. In a practical calculation, we can classify this $|uf^\tau\rangle$ solution to the complete redundant state with $\tau=-1$ and solve a "modified" Faddeev equation

$$\lambda(E)\varphi=G_0\left[\widetilde{T}S-\sum_{\tau\sim-1}|uf^\tau\rangle\frac{1}{\langle uf^\tau|G_0|uf^\tau\rangle}\langle uf^\tau|\right]\varphi. \tag{9}$$

[Otherwise, we obtain unstable complex solutions and the energy with $\lambda(E)=1$ is not precisely determined.] The 3α ground-state energy obtained by this prescription is $E_{3\alpha}=-27.625$ MeV, which is very close to the exact value -27.748 MeV obtained by solving an improved equation, Eq. (14) or Eq. (22). In this case, the relationship in Eq. (8) is modified to

$$\langle uf^\tau|\Psi\rangle=\langle uf^\tau|1+S|\varphi\rangle=C_\tau^{[3]}\sqrt{3(1+\tau)}=-\langle uf^\tau|\varphi\rangle. \tag{10}$$

For the normalized φ with $3\langle\varphi|1+S|\varphi\rangle=1$, the last matrix element of Eq. (10) for the ground state is found to be 0.1604×10^{-1}. This leads to the value $C_\tau^{[3]}=-0.2984$, which yields the amplitude of the $\phi_\tau^{[3]}$ component contained in the total wave function Ψ as

$$\langle\phi_\tau^{[3]}|\Psi\rangle=\sqrt{\frac{3}{1+\tau}}\langle uf^\tau|\Psi\rangle=3C_\tau^{[3]}=-0.8952. \tag{11}$$

If we assume $\Psi\sim 3C_\tau^{[3]}\phi_\tau^{[3]}$, we can approximate the redundant amplitudes as

$$|f_u\rangle=\langle u|\Psi\rangle\sim 3C_\tau^{[3]}\langle u|\phi_\tau^{[3]}\rangle=C_\tau^{[3]}\sqrt{3(1+\tau)}|f^\tau\rangle, \tag{12}$$

and the redundant component admixed in the ground state is given by

$$\langle f_u|f_u\rangle\sim C_\tau^{[3]2}3(1+\tau)=\langle uf^\tau|\varphi\rangle^2=0.26\times10^{-3}, \tag{13}$$

which agrees very well with the number $(2.6\text{–}2.7)\times10^{-4}$, obtained by solving Eq. (22).

From the definition of $\phi_\beta^{[3]}$ in Eq. (5), it is apparent that none of the $\phi_\beta^{[3]}$ has the large [3](04) component. Therefore, if one rejects the second $\phi_\tau^{[3]}$ in the [3]-symmetric model space, one misses the dominant [3](04) component, and consequently one obtains a broad solution with a smaller binding energy. This is the situation which happens in Refs. [8] and [9].

In order to formulate a precise 3α OCM equation with the almost redundant Faddeev components, we write $\phi_\tau^{[3]}$ with $\tau\sim-1$ as Ψ_0, and define a new projection operator $\widetilde{P}=|\Psi_0\rangle\langle\Psi_0|+P$ with $P=\Sigma_{\lambda=0}|\Phi_\lambda\rangle\langle\Phi_\lambda|$. Here Φ_λ with $\lambda=0$ are the [3]-symmetric Pauli-allowed 3α states and $P|\Psi_0\rangle=0$ is satisfied. The 3α OCM equation solved in the present formalism is

$$\widetilde{P}\left[E-H_0-\sum_\alpha V_\alpha^{\mathrm{BFW}}\right]\widetilde{P}\Psi=0. \tag{14}$$

(On the other hand, the original equation with $\widetilde{P}\to P$ is solved in Refs. [8,9] in the method of orthogonalizing pseudopotentials.) This equation is equivalent with the following two equations:

$$\langle\Psi_0|E-H_0-\sum_\alpha V_\alpha^{\mathrm{BFW}}|\widetilde{P}\Psi\rangle=0, \tag{15a}$$

$$P\left[E-H_0-\sum_\alpha V_\alpha^{\mathrm{BFW}}\right]|\widetilde{P}\Psi\rangle=0. \tag{15b}$$

From Eq. (15a), we find

$$\langle\Psi_0|H|P\Psi\rangle=(E-E_0)\langle\Psi_0|\Psi\rangle, \tag{16}$$

where $H=H_0+\Sigma_\alpha V_\alpha^{\mathrm{BFW}}$ and $E_0=\langle\Psi_0|H|\Psi_0\rangle$. By multiplying Eq. (15b) by $\langle\Psi|$ from the left and using Eq. (16), we immediately obtain

$$E\langle P\Psi|P\Psi\rangle-\langle P\Psi|H|P\Psi\rangle=\frac{|\langle\Psi_0|H|P\Psi\rangle|^2}{E-E_0}. \tag{17}$$

If $|\Psi_0\rangle$ is an approximate eigenstate of the full Hamiltonian H, the coupling term in Eq. (16) is almost zero. In this case, we find two solutions for E from a simple illustration of the graph for Eq. (17) with respect to E; namely, one is the Ψ_0-dominant ground state with $E\sim E_0$ and the other the excited state with $E\sim\langle P\Psi|H|P\Psi\rangle/\langle P\Psi|P\Psi\rangle$ and a small admixture of the Ψ_0 component.

It is also possible to derive a Faddeev equation which is completely equivalent to Eq. (14). We assume $|u\rangle$ the bound-state solution of V^{BFW} with the energy eigenvalue ε_B. For $\mathcal{V}_\alpha(E)=E-H_0-\Lambda_\alpha(E-H_0-V_\alpha^{\mathrm{BFW}})\Lambda_\alpha$ with $\Lambda_\alpha=1-|u_\alpha\rangle\langle u_\alpha|$, one can prove

$$\mathcal{V}_\alpha(E)-V_\alpha^{\mathrm{BFW}}=|u_\alpha\rangle\langle u_\alpha|(E-h_{\bar{\alpha}}-\varepsilon_B)|u_\alpha\rangle\langle u_\alpha|, \tag{18}$$

where $h_{\bar{\alpha}}$ is the kinetic-energy operator of the third α particle. Owing to this relationship, we can replace V_α^{BFW} in Eq. (15b) by $\mathcal{V}_\alpha(E)$. Following the same procedure as developed in Ref. [14] for $\widetilde{P}\Psi=\varphi_\alpha+\varphi_\beta+\varphi_\gamma$, we can derive

$$\varphi=G_0\widetilde{T}S\varphi+\sum_{\tau\sim-1}|u\widetilde{f}^\tau\rangle\langle\Psi_0|\widetilde{P}\Psi\rangle, \tag{19}$$

where $\widetilde{f}^\tau=\langle u|\Psi_0\rangle=\sqrt{(1+\tau)/3}f^\tau$. In the intermediate step, we also find

$$\left[E - H_0 - \sum_\alpha \mathcal{V}_\alpha(E)\right]\widetilde{P}\Psi = -\sum_\alpha |u_\alpha\rangle\langle u_\alpha|E - H_0|\varphi_\beta + \varphi_\gamma\rangle. \tag{20}$$

We multiply this equation by $\langle\Psi_0|$ from the left, and subtract the resultant equation from Eq. (15a). Then the symmetry of the matrix elements yields $\langle\Psi_0|[\mathcal{V}_\alpha(E) - V_\alpha^{\rm BFW}]|\widetilde{P}\Psi\rangle = \langle u_\alpha\widetilde{f}^\tau_\alpha|E - H_0|\varphi_\beta + \varphi_\gamma\rangle$ for each α and $\tau\sim -1$, or [from Eq. (18) and restoring $V^{\rm BFW}$]

$$\langle\Psi_0|\widetilde{P}\Psi\rangle = \frac{\langle u\widetilde{f}^\tau|(E - H_0)S|\varphi\rangle}{\langle u\widetilde{f}^\tau|E - H_0 - V^{\rm BFW}|u\widetilde{f}^\tau\rangle}. \tag{21}$$

Using this relationship in Eq. (19), we eventually obtain a new type of Faddeev equation

$$\varphi = G_0\widetilde{T}S\varphi + \sum_{\tau\sim -1} |uf^\tau\rangle \frac{1}{\langle uf^\tau|E - H_0 - V^{\rm BFW}|uf^\tau\rangle} \times \langle uf^\tau|(E - H_0)S|\varphi\rangle. \tag{22}$$

The solutions of this equation are given in Ref. [6], together with the results of the direct variational calculations of Eq. (14), using the translationally invariant h.o. basis.

In summary, we probably cannot obtain the [3](04)-dominant compact ground state without a small admixture of the redundant components, which is related with the model space character that no exact [21]-symmetric solution exists in the model space $|uf^\tau\rangle$, when the BFW bound-state solutions are used for $|u\rangle$. If one insists mathematical rigorousness that the forbidden components should be completely eliminated from the exact solution, we have to say that there is no compact bound state possible in the 3α problem for the BFW $\alpha\alpha$ potential. We, however, keep in mind that the orthogonality condition model is just a model which takes into account the major roles of the Pauli principle among clusters. From the microscopic viewpoint based on the resonating-group method, a small admixture of the redundant components is easily swept away by the effect of antisymmetrization. It is our opinion that the description of the physical ground state of the 3α system with the compact shell-model like structure is far more important than the strict demand to eliminate the redundant components.

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