Removal of forbidden states in a three-$\alpha$ system

H. Matsumura,$^{1,\dagger}$ M. Orabi,$^{1,\ddagger}$ Y. Suzuki,$^{2,\ddagger}$ and Y. Fujiwara$^{3,§}$

$^1$Graduate School of Science and Technology, Niigata University, Niigata 950-2181, Japan
$^2$Department of Physics, and Graduate School of Science and Technology, Niigata University, Niigata 950-2181, Japan
$^3$Department of Physics, Kyoto University, Kyoto 606-8502, Japan

Abstract

The ground and excited $0^+$ states of $^{12}$C are investigated in a 3$\alpha$ macroscopic model using the deep potential of Buck, Friedrich and Wheatley. The elimination of forbidden states is performed either by constructing the allowed state space explicitly or by using the orthogonalizing pseudopotential. The well-known enigmatic behavior of the latter approach is resolved. It is safe to define the forbidden states referring to the underlying microscopic model.

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*Electronic address: hideki@nt.sc.niigata-u.ac.jp
†Electronic address: orabi@nt.sc.niigata-u.ac.jp
‡Electronic address: suzuki@nt.sc.niigata-u.ac.jp
§Electronic address: fujiwara@ruby.scphys.kyoto-u.ac.jp
I. INTRODUCTION

A microscopic multicluster model is successful for understanding the structure of light nuclei \[^{7-11}\text{Li}\]. One example recently applied to halo nuclei is the description of lithium isotopes \[^{7-11}\text{Li}\] in terms of an \(\alpha + t + xn\) model \[^{2}\] including \((2 + x)\) clusters, where \(x\) denotes the number of neutrons, i.e., \(x = 0, 1, \ldots, 4\) for \(^{7-11}\text{Li}\). With the use of an effective two-nucleon potential, this approach reproduces consistently the ground state energies of these nuclei together with their proton and neutron radii. In particular, a recent experiment \[^{3}\] has confirmed that the isotope dependence of the charge radii is best reproduced by the stochastic variational calculation \[^{4}\] on the basis of this multicluster model.

In the microscopic cluster model, the structures of clusters are described in terms of appropriate wave functions, usually in the simplest configurations of the shell model, and an antisymmetry requirement on the total wave function is taken into account exactly. The multicluster model is thus a microscopic many-body theory based on an effective nucleon-nucleon potential. One must, however, compute fairly complicated matrix elements for those non-orthogonal basis functions used in the multicluster model, which makes it hard to apply to larger nuclei. This motivates another treatment of the multicluster system, that is, a macroscopic cluster model.

In a macroscopic cluster model, the clusters are treated as structureless point particles. In this case, cluster-cluster interactions are usually represented by appropriate local potentials which are, more or less, phenomenologically determined so as to reproduce the relevant data on the cluster-cluster systems. One of the simplest and well-investigated examples is a \(3\alpha\) model for \(^{12}\text{C}\).

Many calculations based on the microscopic \(3\alpha\) model show that it reproduces the general features of the low-lying spectrum and the spectroscopic properties of \(^{12}\text{C}\) \[^{5, 6}\]. Thus we would expect that the macroscopic version of the \(3\alpha\) system could give results of similar quality if it would be a realistic substitute of the microscopic model. Since the \(\alpha\) particle is a tightly bound system, it is natural to conceive that this expectation may come true. Two kinds of local \(\alpha - \alpha\) potential are often employed in the macroscopic \(3\alpha\) model. One is an angular momentum dependent potential such as Ali-Bodmer (AB) potential \[^{7}\], or that proposed in Ref. \[^{8}\]. These potentials are repulsive at the short \(\alpha - \alpha\) distance in the \(s\) and \(d\) waves. The other is a deep, angular momentum independent potential such as Buck-Friedrich-Wheatley (BFW) potential \[^{9, 10}\]. Both potentials reproduce the phase shifts of low-energy \(\alpha - \alpha\) elastic scatterings well, but they differ in the prediction about a \(2\alpha\) bound state. The AB potential produces no bound state, consistently with the fact that the \(2\alpha\) system has no bound states. Contrary to this, the BFW potential is so deep that it produces two bound states (0s and 1s) in the \(s\) wave and one bound state (0d) in the \(d\) wave. These bound states are considered redundant or forbidden states from which a physically acceptable \(\alpha - \alpha\) relative motion function must be free. The removal of unphysical bound states has been done using either the projection technique with an orthogonalizing pseudopotential \(\lambda\Gamma\) \[^{11}\] or a supersymmetric transform of the original potential \[^{12}\]. It was shown in Ref. \[^{12}\] that the supersymmetric partner potential of the BFW potential is similar to the AB potential.

How well does the macroscopic model with the AB or BFW potential reproduce the results of the underlying microscopic calculation for \(^{12}\text{C}\)? In this respect, the macroscopic calculation gives quite poor results \[^{13, 14, 15, 16}\], e.g., the ground state energy appears just below the \(3\alpha\) threshold, which is far from the experimental value, \(-7.27\) MeV. Moreover, the
calculated ground state hardly has the properties suitable for the $^{12}\text{C}$ ground state. It is also confirmed that the projection technique gives highly unstable results which depend on the projection constant $\lambda$ and on how accurately the forbidden states are solved as well [13, 15]. A convergent result is obtained only by letting $\lambda$ sufficiently large. These results are quite embarrassing considering the success of the microscopic $3\alpha$ model.

The purpose of the present study is to clarify the origin of the enigmatic behavior of the projection technique as well as the reason why its ground state obtained in the macroscopic $3\alpha$ model is far from the physical ground state. To answer these questions, we carry out a direct method of removing the forbidden states by diagonalizing the projection operator $\Gamma$. We will show, using an example of the BFW potential, that the enigma can be understood by the existence of particular $3\alpha$ states, which are excluded from the $3\alpha$ function space in the projection technique, but, in our opinion, should be included as allowed states. This is demonstrated by defining both of allowed and forbidden states in translationally invariant harmonic-oscillator basis functions.

In the microscopic $3\alpha$ model, the $\alpha$ particle is usually described in terms of a harmonic-oscillator $(0s)^4$ configuration. Then it is natural to define allowed or forbidden states referring to the Pauli exclusion principle. Such allowed states are obtained explicitly for the $3\alpha$ system through the norm kernel of the microscopic $3\alpha$ wave function [17]. A simpler approximation is to remove the $2\alpha$ Pauli-forbidden states, namely the $0s$, $1s$ and $0d$ harmonic-oscillator states, from any pair of the $\alpha - \alpha$ relative motion [18, 19]. We call the resulting states “Pauli-allowed” states, and distinguish them from those defined according to the redundant bound states in the BFW potential.

In sect. II we discuss the methods of removing the forbidden states in the $3\alpha$ system. We stress the utility of the harmonic-oscillator basis functions, which makes it straightforward to construct the allowed states. In sect. III we discuss the Pauli-allowed states which have direct relationship to the microscopic $3\alpha$ model, where the $\alpha$ particle is described in terms of a harmonic-oscillator $(0s)^4$ configuration. In sect. IV we show how the enigmatic behavior of the projection technique can be understood. In sect. V we discuss such an $\alpha-\alpha$ potential that is suited for the macroscopic calculations. A summary is given in sect. VI. Some of the lowest Pauli-allowed states are given in Appendix.

II. SOLUTION WITH THE REMOVAL OF FORBIDDEN STATES

The Hamiltonian for the $3\alpha$ system is in the form

$$ H = \sum_{i=1}^{3} \frac{P_i^2}{2m_\alpha} - T_{\text{c.m.}} + \sum_{i=1}^{3} V_i, $$

where $m_\alpha$ is the mass of the $\alpha$ particle and the kinetic energy of the center of mass motion is subtracted. $V_i$ is the $\alpha-\alpha$ potential acting between $(jk)$ pair. Here we use the convention of $(jk) = (23)$ for $i = 1$, $(jk) = (31)$ for $i = 2$, and $(jk) = (12)$ for $i = 3$. We want to solve

$$ H \Psi = E \Psi, $$

with the constraint

$$ \langle \varphi_f(r_i) \mid \Psi \rangle = 0 \quad (i = 1, 2, 3), $$
where \( \varphi_f \) stands for a particular forbidden state. When we have several forbidden states, the above condition must be applied to all of them. The \( \alpha - \alpha \) relative distance vector is given by \( r_i = R_j - R_k \), where \( R_i \) is the center of mass coordinate of the \( i \)th \( \alpha \) particle. Another relative coordinate is denoted by \( \rho_i = (R_j + R_k)/2 - R_i \). The wave function \( \Psi \) must be totally symmetric with respect to the interchange of \( R_i \)'s.

As in the BFW potential, we assume that there exist three forbidden states, \( 0^s \), \( 1^s \) and \( 0^d \). The function \( \varphi_f \) in Eq. (3) thus represents these three states. To solve Eq. (2) with the condition (3), we define an operator

\[
\Gamma = \sum_{i=1}^{3} \Gamma_i, \tag{4}
\]

where

\[
\Gamma_i = \Gamma_i(0^s) + \Gamma_i(1^s) + \Gamma_i(0^d) \tag{5}
\]

with

\[
\Gamma_i(n\ell) = \sum_{m=-\ell}^{\ell} |\varphi_{ntm}(r_i)\rangle \langle \varphi_{ntm}(r_i)|. \tag{6}
\]

The operator \( \Gamma_i \) is a projector onto the forbidden states for the relative motion between the \( \alpha \) particles of \( (jk) \) pair, but we must note that, for \( i \neq j \), it satisfies the relation \( \Gamma_i \Gamma_j \neq \Gamma_j \Gamma_i \neq 0 \).

We consider the eigenvalue problem of \( \Gamma \)

\[
\Gamma \chi_{LM}^{[3]} = \gamma \chi_{LM}^{[3]}, \tag{7}
\]

and obtain those eigenfunctions which are totally symmetric, i.e., \([3]\) symmetry. The eigenvalue \( \gamma \) is non-negative. This is seen as follows:

\[
\begin{align*}
\gamma &= \langle \chi_{LM}^{[3]} | \Gamma | \chi_{LM}^{[3]} \rangle \\
&= 3 \langle \chi_{LM}^{[3]} | \Gamma_i | \chi_{LM}^{[3]} \rangle \quad (i = 1, 2, 3) \\
&= 3 \sum_f \langle \chi_{LM}^{[3]} | \varphi_f(r_i) \rangle \langle \varphi_f(r_i) | \chi_{LM}^{[3]} \rangle. \tag{8}
\end{align*}
\]

Here we used the symmetry of \( \chi_{LM}^{[3]} \) and noted that the matrix element in the last line is non-negative, which follows from the fact that \( \langle \varphi_f(r_i) | \chi_{LM}^{[3]} \rangle \) is a function of \( \rho_i \), say, \( v(\rho_i) \), and thus \( \langle \chi_{LM}^{[3]} | \varphi_f(r_i) \rangle \langle \varphi_f(r_i) | \chi_{LM}^{[3]} \rangle = \langle v | v \rangle \) can not be negative. Clearly \( \gamma = 0 \) is equivalent to \( v = \langle \varphi_f(r_i) | \chi_{LM}^{[3]} \rangle = 0 \) \((i = 1, 2, 3)\), namely, the eigenfunction with \( \gamma = 0 \) contains no forbidden components, so it satisfies the condition \([3]\). We can thus expand the solution of Eq. (2) in terms of the eigenfunctions belonging to \( \gamma = 0 \),

\[
\Psi = \sum_p C_p \chi_{pLM}^{[3]=0}, \tag{9}
\]
where \( p \) is introduced to distinguish the orthonormal eigenfunctions with \( \gamma = 0 \). The coefficients \( C_p \) and the energy \( E \) are determined from the secular equation

\[
\sum_{p'} \langle \chi_{pLM}^{[3]\gamma=0} | H - E | \chi_{p'LM}^{[3]\gamma=0} \rangle C_{p'} = 0. \tag{10}
\]

The procedure explained above is a standard way to obtain a solution which is free from any forbidden components. One, however, has to note that to obtain vanishing eigenvalues of Eq. (7) demands a calculation of high accuracy.

Another method of solution equivalent to the above direct method is to add the orthogonalizing pseudopotential \[11\] to the Hamiltonian

\[
\tilde{H} = H + \lambda \Gamma \tag{11}
\]

and solve the equation for \( \Psi(\lambda) \) of \([3]\) symmetry

\[
\tilde{H} \Psi(\lambda) = E(\lambda) \Psi(\lambda) \tag{12}
\]

as a function of the projection constant \( \lambda \). The solution for \( \Psi(\lambda) \) may be expanded as in Eq. (9) but then all the eigenfunctions with both \( \gamma = 0 \) and \( \gamma \neq 0 \) must be included. The desired solution is such that \( E(\lambda) \) and \( \Psi(\lambda) \) are stable for sufficiently large \( \lambda \). To understand this, we note that the energy \( E(\lambda) \) reads as follows:

\[
E(\lambda) = \langle \Psi(\lambda) | H | \Psi(\lambda) \rangle + \lambda \langle \Psi(\lambda) | \Gamma | \Psi(\lambda) \rangle. \tag{13}
\]

The first term on the right-hand side of Eq. (13) is expected to change moderately as a function of \( \lambda \), but the second term increases rapidly with increasing \( \lambda \) in such a way that \( \Psi(\lambda) \) has a significant overlap with the forbidden states because in that case the probability of finding the forbidden components in \( \Psi(\lambda) \), \( \langle \Psi(\lambda) | \Gamma | \Psi(\lambda) \rangle \), becomes a positive, non-vanishing value. In contrast to this, \( E(\lambda) \) can be stable for sufficiently large \( \lambda \), provided that \( \Psi(\lambda) \) has vanishingly small or no overlap with the forbidden states. The advantage of this pseudopotential method is that one does not need to solve Eq. (7) to construct the allowed space spanned by the solutions with \( \gamma = 0 \), but only needs to diagonalize the Hamiltonian with the pseudopotential. To obtain a stable solution, however, one has to provide a function space large enough to remove the forbidden states.

It is important for our purpose to construct a complete set of \([3]\) symmetry for the \(3\alpha\) system. For example, the eigenvalue problem (7) of the operator \( \Gamma \) can be solved in such a set. The construction of the complete set can be performed using translationally invariant harmonic-oscillator functions

\[
\left[ \psi_{l_1}^{q_1}(\mathbf{r}_1) \psi_{l_2}^{q_2}(\mathbf{r}_2) \right]_{LM}, \tag{14}
\]

where \( \psi_{l,m}^{q} \) is the oscillator function with the number of oscillator quanta \( q \), the orbital angular momentum \( \ell \) and its \( z \) component \( m \). \((q-\ell)\) must be a non-negative even number.) The symbol \([ \cdots ]_{LM} \) indicates the angular momentum coupling. The oscillator parameters of the functions \( \psi_{l_1m_1}^{q_1}(\mathbf{r}_1) \) and \( \psi_{l_2m_2}^{q_2}(\mathbf{p}_1) \) are \( 2\nu \) and \( \frac{5}{2}\nu \), respectively. Here \( \nu = (m_N\omega/2\hbar) \) is the oscillator parameter of the single-nucleon wave function in the harmonic oscillator shell model, where \( m_N \) is the nucleon mass. We choose \( \nu = 0.26 \text{ fm}^{-2} \) because it is an appropriate value to reproduce the charge radius of the \( \alpha \) particle using the \((0s)^4\) wave function \[17\].
One may choose other values of $\nu$, but then the diagonalization of the operator $\Gamma$ and the Hamiltonian, Eqs. (7) and (10), would require larger dimension. Though an elegant method of constructing the states with definite permutational symmetry is given in Ref. [20], we follow a simple procedure of diagonalizing the symmetrizer

$$S = \frac{1}{3} (1 + (1,2,3) + (1,3,2)), \quad (15)$$

where $(1,2,3)$ and $(1,3,2)$ are cyclic permutations. The states with $[3]$ symmetry can be obtained as those with unit eigenvalue of $S$. The symmetrizer $S$ conserves the number of total oscillator quanta $Q = q_1 + q_2$, so the diagonalization of $S$ can be done separately for each $Q$. In this diagonalization one needs the matrix element of the permutation $P((1,2,3)$ and $(1,3,2))$ in the basis (14), which can be easily evaluated using a generalized Talmi-Moshinsky bracket [20, 21].

III. PAULI-ALLOWED STATES IN HARMONIC-OCCILLATOR BASIS

So far we have assumed that the forbidden states $\varphi_f(r)$ are the bound states of the $\alpha-\alpha$ potential, which is considered natural in several studies [11, 13, 15, 16, 18]. A different viewpoint is that the forbidden or redundant states should be defined according to the underlying microscopic model, that is, they are determined solely from the wave function of the $\alpha$ particle, not from the $\alpha-\alpha$ potential employed. For the $\alpha$ particle described with the $(0s)^4$ harmonic-oscillator shell-model with the oscillator constant $\nu$, it is well-known that three Pauli-forbidden states appear for the $\alpha-\alpha$ relative motion. They have the same quantum numbers, $0s, 1s$ and $0d$, as those of the BFW potential, but their wave functions are simply given by the harmonic-oscillator functions $\psi_{\ell m}^q (q=0, 2)$. This approach is in fact a multicluster version of the orthogonality condition model [19, 22]. An $\alpha-\alpha$ potential used in this case is often taken to be close to a double folding potential [23].

It is useful to define an operator $\Gamma^{\text{HO}}$, an analogue to the operator (4), in the harmonic-oscillator basis, where $\Gamma_i(n\ell)$ of Eq. (6) is replaced by

$$\Gamma^{\text{HO}}_i(n\ell) = \sum_{m=-\ell}^\ell | \psi_{\ell m}^q (r_i) \rangle \langle \psi_{\ell m}^q (r_i) | \quad (q = 2n + \ell). \quad (16)$$

The eigenvalue problem for $\Gamma^{\text{HO}}$, the analogue of Eq. (7), can be solved in the basis (14). The eigenfunctions can be classified by $Q$, an SU(3) irreducible representation $(\lambda \mu)$ and an additional quantum number $\kappa$ [19, 18] ($\kappa$ serves to distinguish a multiple occurrence of the same $(\lambda \mu)$ states, and it is otherwise suppressed). That is,

$$\chi_{LM}^{[3]Q(\lambda \mu)\kappa}, \quad (17)$$

and the eigenvalues $\gamma$ are either zero (Pauli-allowed) or non-zero values of order unity (Pauli-forbidden). The SU(3) coupled basis is easily constructed by use of SU(3) coefficients [24]:

$$[\psi_{\ell_1}^{q_1}(r) \psi_{\ell_2}^{q_2}(p)]_{LM}^{(\lambda \mu)} = \sum_{\ell_1 \ell_2} \langle (q_10)\ell_1, (q_20)\ell_2 | (\lambda \mu)L \rangle [\psi_{\ell_1}^{q_1}(r)]_{LM}^{(\lambda \mu)} [\psi_{\ell_2}^{q_2}(p)]_{LM}^{(\lambda \mu)}.$$
Here \((\lambda \mu)\) can in general take the representations of \((q_1 + q_2, 0), (q_1 + q_2 - 2, 1), (q_1 + q_2 - 4, 2), \ldots, (q_\ge - q_\le, q_\ge)\), where \(q_\ge = \max(q_1, q_2)\) and \(q_\le = \min(q_1, q_2)\), but is limited to those which contain the angular momentum \(L\). For \(L = 0\), both \(\lambda\) and \(\mu\) must be even, and a concise expression for the SU(3) coefficients with \(L = 0\) is given in Ref. [25].

For \(Q < 8\), all the \([3]\)-symmetry basis states are Pauli-forbidden. For \(Q = 8\) we have only one Pauli-allowed state with \((\lambda \mu) = (04)\). For \(Q = 10\), two Pauli-allowed states, \((24)\) and \((62)\), appear. We give in Appendix the Pauli-allowed states \(\chi_{10}^{[3]Q(\lambda \mu)\alpha \gamma = 0}\) for \(Q = 8 - 14\) in the SU(3) coupled basis of Eq. (18).

**IV. CASE OF THE BFW POTENTIAL**

The BFW potential reproduces very well the \(\alpha - \alpha\) phase shifts of the \(s, d\) and \(g\) waves for \(E_{c.m.} < 17\) MeV \([3]\). It is a local, angular momentum independent potential given by

\[
V(r) = v_0 \exp(-\rho_0 r^2) + \frac{4e^2}{r} \text{erf}(\beta r),
\]

where \(r\) is the \(\alpha - \alpha\) relative distance vector. The parameters of the BFW potential are \(v_0 = -122.6225\) MeV, \(\rho_0 = 0.22\) fm\(^{-2}\), and \(\beta = 0.75\) fm\(^{-1}\). We choose \(\frac{\hbar^2}{m_\alpha} = 10.4465\) MeV fm\(^2\) and \(e^2 = 1.44\) MeV fm. The three bound states of the BFW potential, \(\varphi_{n\ell m}\), are expanded in terms of the harmonic-oscillator functions \(\psi^{q\ell}(r) = R_{n\ell}(r)Y_{\ell m}(\hat{r})\) \((n' = (q - \ell)/2)\):

\[
\varphi_{n\ell m}(r) = \sum_{n'} U_{nm}^{n'\ell} R_{n'\ell}(r)Y_{\ell m}(\hat{r}).
\]

The phase convention of \(R_{n'\ell}(r)\) is such that it is positive for \(r\) greater than the outermost nodal point. Table I lists the expansion coefficients \(U_{nm}^{n'\ell}\). It is seen that the bound state

| \(n'\) | \(U_{10}^{00}\) | \(U_{10}^{10}\) | \(U_{10}^{02}\) |
|---|---|---|---|
| 0 | 0.991259 | 0.122458 | 0.994643 |
| 1 | -0.123881 | 0.984707 | 3.8363 \times 10^{-2} |
| 2 | 4.4209 \times 10^{-2} | 3.6841 \times 10^{-2} | 9.2784 \times 10^{-2} |
| 3 | -9.4402 \times 10^{-3} | 0.114653 | 1.6585 \times 10^{-2} |
| 4 | 3.7620 \times 10^{-3} | 1.8535 \times 10^{-2} | 1.6517 \times 10^{-2} |
| 5 | -9.6104 \times 10^{-4} | 2.0740 \times 10^{-2} | 5.7095 \times 10^{-3} |
| 6 | 4.2760 \times 10^{-4} | 6.5918 \times 10^{-3} | 4.2427 \times 10^{-3} |
| 7 | -1.1796 \times 10^{-4} | 5.1703 \times 10^{-3} | 2.0350 \times 10^{-3} |
| 8 | 5.8853 \times 10^{-5} | 2.3322 \times 10^{-3} | 1.6746 \times 10^{-3} |
| 9 | -1.6647 \times 10^{-5} | 1.6078 \times 10^{-3} | 7.7920 \times 10^{-4} |
| 10 | 9.0250 \times 10^{-6} | 8.7429 \times 10^{-4} | 5.1694 \times 10^{-4} |
| \vdots | \vdots | \vdots | \vdots |
FIG. 1: Plot of \( \log(1/\gamma) \) for \( N = 1 - 174 \) eigenvalues obtained for \( Q_{\text{max}} = 30 \), where \( \gamma \) is the eigenvalue of the operator \( \Gamma \) defined by Eq. (4) using the three forbidden states of the BFW potential (see Eq. (7)). In the inset, the eigenvalues around \( N = 130 \) are compared with those obtained for \( \Gamma_{\text{HO}} \).

Wave functions \( \varphi_{n\ell m}(r) \) are well approximated by the oscillator functions \( \psi_{q\ell m}(r) (q = 2n + \ell) \), but we will see that the small difference between the two functions produces a huge effect on the energy of the \( 3\alpha \) system.

The expansion (20) makes it possible to solve accurately the eigenvalue problem (7) in the translationally invariant harmonic-oscillator functions provided the maximum number of total oscillator quanta \( Q_{\text{max}} \) is sufficiently large. We treat only \( 0^+ \) case in this paper. For \( Q_{\text{max}} = 30 \), there are 444 translationally invariant basis functions, and from them we can construct 174 independent basis functions of [3] symmetry. Figure 1 displays \( \log(1/\gamma) \), where \( \gamma \) is the eigenvalue of \( \Gamma \) obtained for this case. It is clear in the figure that the eigenvalues \( \gamma \) diagonalized in these [3]-symmetry functions are classified into three groups: the first group (Group I) is characterized by \( \gamma = 0 \) and it contains 129 eigenfunctions (the values of \( \gamma \) are actually less than \( 10^{-14} \), which we considered zero within the present numerical accuracy). The elements of this group are allowed states and constitute the basis for diagonalizing the Hamiltonian in Eq. (10). The second group (Group II) contains just two states whose eigenvalues are approximately zero; \( \gamma_1 = 1.35152 \times 10^{-5} \) and \( \gamma_2 = 1.07152 \times 10^{-3} \). The appearance of these states was suggested in a Faddeev treatment of the \( 3\alpha \) system [26, 27, 28]. The third group (Group III) contains 43 elements with eigenvalues of order unity (\( \sim 1 \)). These last states must be discarded because they have a substantial overlap with the forbidden states. Differently, using \( \Gamma_{\text{HO}} \), in which the two-body forbidden states are the harmonic-oscillator functions as defined in Eq. (16), the eigenvalues are divided into two groups only corresponding to I and III, and there is no such a group like II. The inset of the figure compares the eigenvalues of both cases for \( N = 126 - 136 \).

Table II shows the \( Q_{\text{max}} \) dependence of the number of eigenfunctions belonging to each group. There are two noteworthy points; first, the two solutions of Group II always appear
TABLE II: The number of allowed and forbidden states for the 3α system with 0+. The α−α forbidden states are taken as the three bound states of the BFW potential. $Q_{\text{max}}$ is the maximum number of total oscillator quanta, $N_{\text{basis}}$ is the basis dimension of the translationally invariant harmonic-oscillator functions with $Q = 0 - Q_{\text{max}}$, $N^{[3]}$ is the number of totally symmetric functions with $Q = 0 - Q_{\text{max}}$. $N^{\gamma=0}$ is the number of allowed states of Group I, $N^{\gamma\approx0}$ is the number of eigenfunctions of Group II, and $N^{\gamma\sim1}$ is the number of forbidden states of Group III.

| $Q_{\text{max}}$ | $N_{\text{basis}}$ | $N^{[3]}$ | $N^{\gamma=0}$ | $N^{\gamma\approx0}$ | $N^{\gamma\sim1}$ |
|-----------------|-----------------|--------|--------|----------------|----------------|
| 30              | 444             | 174    | 129    | 2              | 43             |
| 40              | 946             | 358    | 298    | 2              | 58             |
| 50              | 1729            | 640    | 565    | 2              | 73             |
| 60              | 2856            | 1041   | 951    | 2              | 88             |

TABLE III: Expansion coefficients of the two states of Group II in terms of the Pauli-allowed states $\chi_{00}^{[3]Q(\lambda\mu)\kappa\gamma=0}$. The index $\kappa$ is suppressed when it is unnecessary. See Appendix for the definition of the two independent states which appear for $Q(\lambda\mu) = 14(64)$.

| $Q$ | $\kappa$ | $\gamma_1$ | $\gamma_2$ |
|-----|----------|------------|------------|
| 8   | (04)     | 0.28139    | 0.85945    |
| 10  | (24)     | 0.38513    | -0.11666   |
| 10  | (62)     | 0.58421    | -0.05242   |
| 12  | (06)     | 0.06598    | -0.02209   |
| 12  | (44)     | -0.03502   | 0.15717    |
| 12  | (82)     | 0.18853    | -0.06749   |
| 12  | (12, 0)  | -0.12627   | 0.42769    |
| 14  | (26)     | -0.07958   | 0.01859    |
| 14  | (64)1    | -0.08228   | 0.03768    |
| 14  | (64)2    | 0.02034    | 0.00586    |
| 14  | (10, 2)  | 0.20863    | -0.02453   |
| 14  | (14, 0)  | -0.42113   | 0.11500    |

for all $Q_{\text{max}}$ values. Moreover, we have confirmed that these solutions (the eigenfunctions and the eigenvalues) are very stable against the increase of $Q_{\text{max}}$, e.g., for $Q_{\text{max}} = 50$, $\gamma_1 = 1.35191 \times 10^{-5}$ and $\gamma_2 = 1.07153 \times 10^{-3}$. Second, the sum of the members of Groups I and II is equal to the number of Pauli-allowed states which occur for the case of $U_{n'\ell}^{n\ell} = \delta_{n'n}$, namely the bound states $\varphi_{n\ell m}$ are replaced with the harmonic-oscillator functions $\psi_{2n+\ell}^{2m+\ell}$.

For later discussion we expand the two states of Group II in terms of the harmonic-oscillator basis functions. Table III lists the overlap of these two states with some of the Pauli-allowed states $\chi_{00}^{[3]Q(\lambda\mu)\kappa\gamma=0}$ (see Appendix for the expressions of these Pauli-allowed states). From the table we can notice that the two states with the eigenvalues $\gamma_1$ and $\gamma_2$ contain predominantly $Q = 10$, 14 and $Q = 8$, 12 components, respectively.
In order to understand the reason why the orthogonalizing pseudopotential approach gives a result quite different from that of the microscopic model, we first diagonalize the Hamiltonian $H$ in the following three different basis sets and compare their energies and properties for the ground and excited $0^+$ states. The three sets are (i) a set spanned by the basis functions of Group I, (ii) a set spanned by the basis functions of Groups I and II, and (iii) a set spanned by the Pauli-allowed states $\chi_0^{[3]Q(\lambda\mu)\gamma=0}$. The calculation has been performed for some $Q_{\text{max}}$ values to check the convergence of the solution. The results obtained with the three sets are listed in Table IV. The energies of set (i) correspond to the eigenvalues of Eq. (10), and will approach the energies $E(\lambda)$ for $\lambda$ sufficiently large as will be shown later. The ground state energy for $Q_{\text{max}} = 60$ is $-0.22$ MeV, which is consistent with the value obtained by the projection technique [15, 16]. The calculated energy is far from the experimental value $-7.27$ MeV and rather close to the $3\alpha$ threshold where the second $0^+$ state is observed. The root mean square (rms) radius $R_{\text{rms}}$ of the $\alpha$ particle distribution for the ground state turns out to be 2.31 fm, which is much larger than 1.92 fm [17].

The result of set (ii) is in a sharp contrast to case (i). The ground state is now very strongly bound and consequently its rms radius is too small compared to the result of the microscopic calculation, whereas the calculated second $0^+$ state appears near the experimental energy and its rms radius is increased to about 2.34 fm, though it is still too small compared to 4.26 fm of the microscopic calculation [17]. It is remarkable that the results calculated with sets (ii) and (iii) are very similar. From this we may conclude that the function space spanned by the members of Groups I and II is nearly the same as that of the Pauli-allowed states.

As demonstrated above, the two states of Group II play a key role in determining the characteristics of the macroscopic $3\alpha$ model. As shown in Table III, they contain a significant amount of the Pauli-allowed states with $Q(\lambda\mu) = 8(04), 10(62), 12(12,0), 14(14,0)$ etc., which should be included from the microscopic point of view. The Hamiltonian matrix elements between these two states are given, in units of MeV, as follows:

\[
\begin{pmatrix}
14.58 & -7.07 \\
-7.07 & -7.78
\end{pmatrix}
\] (21)

We see that the energy of the state with the eigenvalue $\gamma_2$ is already lower than the ground state energy obtained in the calculation with set (i). This is due to the fact that it is dominated by the lowest shell-model configuration of $Q(\lambda\mu) = 8(04)$. The energy obtained by coupling the two states of Group II is $-9.8$ MeV, so they clearly contribute to lowering the energy. Whether these two states are included in the calculation or not, particularly the $\gamma_2$ state, is a crucial factor for producing quite different results.

Next we discuss the origin of the enigmatic behavior of the energy $E(\lambda)$ which is obtained in the projection technique. We plot in Fig. 2 the energies of the ground and excited $0^+$ states as a function of the projection constant $\lambda$ in the case of $Q_{\text{max}} = 50$. Other choice of $Q_{\text{max}}$ gives a similar result. The dependence on $\lambda$ follows the pattern observed in Refs. [13, 15, 16] which use the basis functions different from the harmonic-oscillator basis. No indication of the energy convergence is attained for $\lambda < 10^5$ MeV, but it begins to show a convergence for larger $\lambda$ values. The origin of this behavior is attributed to the particular selection procedure of the states in the projection technique. It is clear that the states of Group III play no active role from the beginning because the eigenvalue $\gamma$ is of order unity and when it is multiplied by a large $\lambda$ value the energy expectation value becomes very high. On
TABLE IV: Comparison of the ground and excited $0^+$ states calculated in the different basis sets: (i) the functions of Group I, (ii) the functions of Groups I and II, and (iii) the Pauli-allowed states obtained in the harmonic-oscillator basis. $E$ is the energy with respect to the $3\alpha$ threshold. $\langle T \rangle$, $\langle V_N \rangle$, and $\langle V_C \rangle$ denote the expectation values of the kinetic energy, the nuclear potential energy, and the Coulomb potential energy, respectively. The $R_{\text{rms}}$ value of Ref. [17] is based on the $\alpha$ boson wave function which is obtained from a mapping of the microscopic $3\alpha$ wave function. All energies are in MeV and the rms radius is in fm.

| Basis  | $Q_{\text{max}}$ | State | $E$  | $\langle T \rangle$ | $\langle V_N \rangle$ | $\langle V_C \rangle$ | $R_{\text{rms}}$ |
|--------|------------------|-------|-----|---------------------|---------------------|---------------------|----------------|
| set (i) | 30               | $0^+_1$ | 0.40 | 74.34              | -80.18              | 6.24               | 2.03           |
|        |                  | $0^+_2$ | 7.27 | 61.91              | -60.21              | 5.56               | 2.28           |
|        |                  | $0^+_3$ | 12.38 | 84.56              | -78.19              | 6.02               | 2.25           |
|        |                  | $0^+_1$ | -0.02 | 65.88              | -71.84              | 5.94               | 2.16           |
| set (i) | 40               | $0^+_2$ | 5.55 | 53.36              | -53.04              | 5.22               | 2.53           |
|        |                  | $0^+_3$ | 8.89 | 61.94              | -58.34              | 5.29               | 2.56           |
|        |                  | $0^+_1$ | -0.16 | 61.77              | -67.71              | 5.78               | 2.25           |
| set (i) | 50               | $0^+_2$ | 4.53 | 48.11              | -48.53              | 4.96               | 2.76           |
|        |                  | $0^+_3$ | 7.29 | 47.84              | -45.33              | 4.78               | 2.80           |
|        |                  | $0^+_1$ | -0.22 | 59.57              | -65.48              | 5.69               | 2.31           |
| set (i) | 60               | $0^+_2$ | 3.85 | 43.49              | -44.34              | 4.70               | 2.99           |
|        |                  | $0^+_3$ | 6.44 | 39.45              | -37.46              | 4.46               | 3.00           |
| set (ii) |                  | $0^+_1$ | -19.90 | 126.69              | -155.08             | 8.50               | 1.31           |
|         | 30               | $0^+_2$ | 0.26 | 69.44              | -75.28              | 6.10               | 2.06           |
|         |                  | $0^+_3$ | 7.58 | 64.61              | -62.63              | 5.60               | 2.31           |
| set (ii) | 40               | $0^+_1$ | -19.90 | 126.69              | -155.08             | 8.50               | 1.31           |
|         |                  | $0^+_2$ | -0.19 | 61.44              | -67.43              | 5.81               | 2.20           |
|         |                  | $0^+_3$ | 5.54 | 54.14              | -53.81              | 5.21               | 2.57           |
| set (ii) | 50               | $0^+_1$ | -19.90 | 126.68              | -155.08             | 8.50               | 1.31           |
|         |                  | $0^+_2$ | -0.34 | 57.60              | -63.59              | 5.65               | 2.28           |
|         |                  | $0^+_3$ | 4.48 | 48.49              | -48.97              | 4.96               | 2.77           |
| set (ii) | 60               | $0^+_1$ | -19.90 | 126.68              | -155.08             | 8.50               | 1.31           |
|         |                  | $0^+_2$ | -0.40 | 55.60              | -61.57              | 5.57               | 2.34           |
|         |                  | $0^+_3$ | 3.82 | 43.77              | -44.67              | 4.72               | 2.98           |
| set (iii) | 30              | $0^+_1$ | -19.25 | 128.33              | -156.10             | 8.53               | 1.31           |
|         |                  | $0^+_2$ | -0.11 | 63.82              | -69.88              | 5.95               | 2.09           |
|         |                  | $0^+_3$ | 7.03 | 60.11              | -58.57              | 5.49               | 2.34           |
| set (iii) | 40              | $0^+_1$ | -19.25 | 128.32              | -156.09             | 8.53               | 1.31           |
|         |                  | $0^+_2$ | -0.59 | 55.55              | -61.78              | 5.64               | 2.23           |
|         |                  | $0^+_3$ | 5.02 | 50.22              | -50.34              | 5.13               | 2.57           |
| set (iii) | 50              | $0^+_1$ | -19.25 | 128.32              | -156.09             | 8.53               | 1.31           |
|         |                  | $0^+_2$ | -0.75 | 51.75              | -57.98              | 5.49               | 2.32           |
|         |                  | $0^+_3$ | 4.04 | 45.28              | -46.15              | 4.91               | 2.76           |
| set (iii) | 60              | $0^+_1$ | -19.25 | 128.32              | -156.09             | 8.53               | 1.31           |
|         |                  | $0^+_2$ | -0.81 | 49.86              | -56.07              | 5.41               | 2.36           |
|         |                  | $0^+_3$ | 3.44 | 41.15              | -42.40              | 4.69               | 2.88           |
| Microscopic | 30 | $0^+_1$ | -7.72 | 1.92               |                     |                    |                |
| (Ref. [17]) |                  | $0^+_2$ | 0.71 | 4.26               |                     |                    |                |
FIG. 2: Convergence of the energy with respect to the $3\alpha$ threshold as a function of the projection constant $\lambda$. $Q_{\text{max}} = 50$.

the contrary, the states of Group I are always active in the diagonalization of the pseudo Hamiltonian $\tilde{H}$ as their eigenvalues are zero. The two states of Group II, especially the state with the eigenvalue $\gamma_2 = 1.07153 \times 10^{-3}$, are in a subtle situation. The expectation value of $\tilde{H}$ for this state is

$$-7.78 + \lambda \gamma_2,$$

so the state is expected to contribute to the ground state significantly as long as $\lambda \gamma_2$ is smaller than, say 8 MeV, that is, for $\lambda < 10^4$ MeV, but it will be excluded in the end for sufficiently large $\lambda$. This is confirmed in Table V which displays the probability of finding the state with $\gamma_2$ in the wave functions of the three $0^+$ states. The probability found in the ground state is 0.64 for $\lambda = 10^4$ MeV and it decreases rapidly for $\lambda \geq 10^5$ MeV.

TABLE V: $\lambda$ dependence of the probability of finding the state with the eigenvalue $\gamma_2$ in the ground and excited $0^+$ states in $^{12}\text{C}$. The calculations are performed for $Q_{\text{max}} = 50$.

| $^{12}\text{C}$ | $10^2$   | $10^3$   | $10^4$   | $10^5$   | $10^6$   | $10^7$   | $10^8$   |
|----------------|--------|--------|--------|--------|--------|--------|--------|
| $0_1^+$        | 7.16×10^{-1} | 7.46×10^{-1} | 6.44×10^{-1} | 9.62×10^{-4} | 1.74×10^{-6} | 3.03×10^{-9} | 1.76×10^{-11} |
| $0_2^+$        | 1.87×10^{-2} | 6.05×10^{-3} | 1.04×10^{-2} | 1.07×10^{-3} | 6.20×10^{-7} | 9.76×10^{-10} | 6.17×10^{-12} |
| $0_3^+$        | 4.83×10^{-3} | 1.07×10^{-3} | 1.64×10^{-3} | 9.83×10^{-3} | 1.67×10^{-5} | 1.04×10^{-7} | 9.81×10^{-10} |
V.  $\alpha-\alpha$ POTENTIAL

In the previous section we have argued that the two-body forbidden states for the $\alpha-\alpha$ relative motion have to be defined referring to the microscopic wave function of the $\alpha$ particle, not from the bound states of the $\alpha-\alpha$ potential. Based on this viewpoint, we have shown that the BFW potential is so attractive that the ground state energy of $^{12}$C is strongly bound. Here we discuss an $\alpha-\alpha$ potential which is more suitable for the macroscopic calculation. In doing so, we impose the condition that the $\alpha-\alpha$ relative motion should be orthogonal to the $2\alpha$ Pauli-forbidden states, that is, the harmonic-oscillator functions $\psi^{q}_{\alpha}$ with $q = 0, 2$.

First we modify the strength of the BFW potential so as to reproduce the $0^+$ resonance energy of the $2\alpha$ system under the above orthogonality constraint. The resulting potential, which we call MBFW, has a strength parameter of $v_0 = -121.888$ MeV. Note, however, that this modified potential does not reproduce the $2^+$ resonance energy. Table VII lists the energies and $R_{\text{rms}}$ values calculated with this potential in the basis functions of set (iii) with $Q_{\text{max}} = 50$. They are almost the same as those obtained with the BFW potential. Compare these with the result of set (iii) in Table IV. Since no improvement is attained by the MBFW potential, we conclude that the change of $v_0$ of the BFW potential does not lead to an $\alpha-\alpha$ potential suitable for the macroscopic calculation.

It seems that the range of the BFW potential has no direct connection to the underlying nucleon-nucleon potential or to the wave function of the $\alpha$ particle. Another potential we consider here is similar to the $\alpha-\alpha$ folding potential used in Ref. [23]. We assume the same form as the BFW potential, and choose the potential parameters as follows:

$$v_0 = -107.9 \text{ MeV}, \quad \rho_0 = 0.20 \text{ fm}^{-2}, \quad \beta = 0.589 \text{ fm}^{-1}.$$

Again, this potential reproduces the $0^+$ resonance of $^8\text{Be}$, but predicts the $2^+$ resonance to be about 1.9 MeV, which appears too low compared to the experimental value, $E = 3.13$ MeV. The range of this potential is longer than that of the BFW potential, and consequently its strength is made considerably weaker. The energies and $R_{\text{rms}}$ values of the ground and excited $0^+$ states are obtained with this new potential in the Pauli-allowed space of set (iii) and they are listed in Table VII. The energy of the ground state is now pretty much improved, though it is still too strongly bound by about 4 MeV.

The truncation with $Q_{\text{max}} = 50$ may not be good enough to obtain convergent results for the excited states. To check this, we diagonalize the Hamiltonian in $\alpha$-boson functions $g$ which are obtained from correlated Gaussians $G$ through the following fermion→boson mapping:

$$g(a, r_1, \rho_1) = \langle \phi(\alpha_1)\phi(\alpha_2)\phi(\alpha_3) \mid A \{ \phi(\alpha_1)\phi(\alpha_2)\phi(\alpha_3)G(a, R) \} \rangle,$$

with

$$G(a, R) = \exp\left\{-a_{12}(R_1 - R_2)^2 - a_{13}(R_1 - R_3)^2 - a_{23}(R_2 - R_3)^2\right\},$$

where $\phi(\alpha)$ is the intrinsic wave function of the $\alpha$ particle, and $A$ is an operator which antisymmetrizes the $3\alpha$ microscopic wave function built on the 12-nucleon coordinates. A parameter $a = (a_{12}, a_{13}, a_{23})$ specifies the correlated Gaussian. By choosing the parameter $a$ appropriately, one can express a variety of different shapes of the three-body system. The function $g$ obviously has [3] symmetry, i.e., $g(a, r_1, \rho_1) = g(a, r_2, \rho_2) = g(a, r_3, \rho_3)$ and $g(a, -r_1, \rho_1) = g(a, r_1, \rho_2)$ etc. Furthermore, it is orthogonal to the Pauli-forbidden states
TABLE VI: Comparison of the ground and excited $0^+$ states calculated with the different $\alpha-\alpha$ potentials. The basis states are either harmonic-oscillator functions of set (iii) with $Q_{\text{max}} = 50$, or the $\alpha$ boson wave functions defined in Eq. (24). See the caption of Table IV.

| Potential | Basis | State | $E$  | $\langle T \rangle$ | $\langle V_N \rangle$ | $\langle V_C \rangle$ | $R_{\text{rms}}$ |
|-----------|-------|-------|------|----------------------|-----------------------|-----------------------|------------------|
| MBFW      | set (iii) | $0^+_1$ | $-18.32$ | $126.58$ | $-153.37$ | $8.48$ | $1.32$ |
|           |       | $0^+_2$ | $-0.41$   | $49.44$   | $-55.25$ | $5.40$ | $2.36$ |
|           |       | $0^+_3$ | $4.31$    | $44.92$   | $-45.50$ | $4.90$ | $2.76$ |
| Eq. (23)  | set (iii) | $0^+_1$ | $-11.68$ | $95.66$   | $-114.33$ | $6.99$ | $1.52$ |
|           |       | $0^+_2$ | $0.63$    | $35.18$   | $-39.18$ | $4.63$ | $2.61$ |
|           |       | $0^+_3$ | $5.00$    | $37.94$   | $-37.46$ | $4.52$ | $2.79$ |
| Eq. (23)  | $\alpha$-boson | $0^+_1$ | $-11.69$ | $95.87$   | $-114.56$ | $6.99$ | $1.52$ |
|           |       | $0^+_2$ | $0.21$    | $25.98$   | $-29.92$ | $4.15$ | $3.17$ |

$\psi_{\ell m}^q (q = 0, 2)$ if $\phi(\alpha)$ is constructed from the $(0s)^4$ harmonic-oscillator function (with its center of mass part being eliminated). Thus the function $g$, for arbitrary $a$, satisfies all the conditions necessary for the allowed states as discussed in sect. IIII. Moreover, it should be noted that the boson function $g$ contains not only the two-body Pauli effects but also full three-body exchange effects. The method of calculating $g$ is given in Ref. [17].

The $3\alpha$ wave function $\Psi$ is now approximated with a combination of $g$. The parameters of $g$ are selected by the stochastic variational method [4]. The results of this calculation are also given in Table VI. It is seen that the harmonic-oscillator expansion converges very slowly except for the ground state. The $R_{\text{rms}}$ value for the $0^+_1$ state increases to $3.17$ fm, which is still smaller than the value calculated in the microscopic model. As noted above, the calculation using $g$ includes not only the two-body Pauli effects but also the three-body exchange effects, whereas the calculation of set (iii) includes only the two-body Pauli effects. The fact that they give virtually the same result for the ground state indicates that the three-body exchange effects are negligibly small. Thus we do not agree with the discussion of Ref. [13], which was made for a possible reason of the sensitivity of the projection technique.

Though a considerable improvement is obtained with the new potential, the ground state energy is still too low by about $4$ MeV. One possible reason for this is that the potential is too attractive for the $d$ wave (and probably for the $g$ wave as well). Then the lowest Pauli-allowed state of $Q(\lambda\mu) = 8(04)$ with $\ell = 0$, for example, gains too much energy, because the dominating partial waves of this state are $d$ and $g$ waves, as understood from the SU(3) coefficients $\langle 4(0)\ell, 4(0)\ell || (04)0 \rangle^2$, which are $0.28, 0.36$, and $0.36$ for $\ell = 0, 2$, and $4$, respectively.

The above consideration suggests that a more suitable $\alpha-\alpha$ potential should have an $\ell$-dependence. In this respect, it is interesting to recall a series of recent publications [26, 29, 30], where the utility of a $2\alpha$ resonating group method (RGM) kernel has been investigated for the $3\alpha$ system. The RGM kernel is non-local and energy-dependent, and therefore a solution of the system with such a potential requires some sort of self consistency procedure. The ground state energy of $^{12}$C turns out to be quite acceptable, that is, it is not strongly bound and is predicted to be around the value obtained by the microscopic calculation. Since a non-local potential could be converted to an equivalent local potential with $\ell$ dependence,
an $\alpha-\alpha$ potential suitable for a macroscopic calculation may be found in $\ell$-dependent form.

VI. SUMMARY

We studied the ground and excited $0^+$ states of $^{12}$C in the $3\alpha$ model, using the deep BFW potential. The three redundant states with $0s$, $1s$, and $0d$ of this potential were eliminated from the function space of the $3\alpha$ system. Two methods of elimination were tested. One is to diagonalize $\Gamma$ in a complete set of translationally invariant harmonic-oscillator functions with $[3]$ symmetry in order to separate the allowed states from the forbidden ones. The other is to use the orthogonalizing pseudopotential $\lambda \Gamma$ and to obtain the energy which converges for $\lambda$ large enough to kill the contribution of the forbidden states. These methods, though equivalent, were tested in order to clarify not only the origin of the enigmatic $\lambda$-behavior of the second method, but also to give a reason why the ground state energy is very high.

We found two eigenstates of $\Gamma$ with almost zero eigenvalues. One of them especially plays a key role. This one has a dominant configuration corresponding to the lowest shell-model state of $Q(\lambda\mu) = 8(04)$, and in spite of its small eigenvalue, of order $10^{-3}$, it was eliminated as a forbidden state in the orthogonalizing pseudopotential approach. The energy expectation value of this state alone is already close to the ground state of $^{12}$C. With the exclusion of this state, there is no hope to get a ground state energy close to the experiment. In addition, we showed that the peculiar dependence of the energy on $\lambda$ can be understood from the admixture of this state in the solution: for $\lambda < 10^4$ MeV, this state can have the effect of lowering the energy, but for $\lambda > 10^5$ MeV it can no longer keep this effect in the ground state energy.

The existence of the states with almost zero eigenvalue of $\Gamma$ is not a characteristic of the BFW potential, but also applies to other $\alpha-\alpha$ potentials provided their bound states are well approximated with the three harmonic-oscillator functions $\psi_{\ell m}^q$ $(q = 0, 2)$. We find that the potential of Eq. (23) produces two almost Pauli-allowed states with $\gamma_1 = 1.59640 \times 10^{-5}$ and $\gamma_2 = 1.17812 \times 10^{-5}$ for $Q_{\text{max}} = 50$.

In our opinion the eigenstates with almost zero eigenvalue should be included in the $3\alpha$ allowed space as they correspond to the most important shell-model configurations, otherwise, the $3\alpha$ macroscopic model loses a link to the microscopic $3\alpha$ model. To include these states automatically, it is safe to define the operator $\Gamma$ in terms of the harmonic-oscillator functions. With this definition of $\Gamma$ we demonstrated that the BFW potential is too attractive and an appropriate $\alpha-\alpha$ potential has to be determined referring to the underlying microscopic model.

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Appendix: Pauli-allowed states in SU(3) coupled basis

We give the Pauli-allowed states, $\chi_{00}^{[3]Q(\lambda\mu)\kappa\gamma=0}$, for $Q = 8 - 14$ in terms of the SU(3) coupled basis. The index $\kappa$ is suppressed when it is unnecessary.
• $Q = 8$

\[
\chi_{00}^{[3]8(04)\gamma=0} = [\psi^4(\mathbf{r}_1)\psi^4(\mathbf{\rho}_1)]_{00}^{(04)}.
\]  

(26)

• $Q = 10$

\[
\chi_{00}^{[3]10(24)\gamma=0} = \frac{1}{\sqrt{2}}[\psi^4(\mathbf{r}_1)\psi^6(\mathbf{\rho}_1)]_{00}^{(24)} + \frac{1}{\sqrt{2}}[\psi^6(\mathbf{r}_1)\psi^4(\mathbf{\rho}_1)]_{00}^{(24)};
\]
\[
\chi_{00}^{[3]10(62)\gamma=0} = \frac{3\sqrt{3}}{2\sqrt{11}}[\psi^4(\mathbf{r}_1)\psi^6(\mathbf{\rho}_1)]_{00}^{(62)} - \frac{\sqrt{3}}{\sqrt{11}}[\psi^6(\mathbf{r}_1)\psi^4(\mathbf{\rho}_1)]_{00}^{(62)}
\]
\[+ \frac{\sqrt{5}}{2\sqrt{11}}[\psi^8(\mathbf{r}_1)\psi^2(\mathbf{\rho}_1)]_{00}^{(62)}.
\]  

(27)

• $Q = 12$

\[
\chi_{00}^{[3]12(06)\gamma=0} = [\psi^6(\mathbf{r}_1)\psi^6(\mathbf{\rho}_1)]_{00}^{(06)},
\]
\[
\chi_{00}^{[3]12(44)\gamma=0} = \frac{\sqrt{3}}{2\sqrt{2}}[\psi^4(\mathbf{r}_1)\psi^8(\mathbf{\rho}_1)]_{00}^{(44)} + \frac{1}{2}[\psi^6(\mathbf{r}_1)\psi^6(\mathbf{\rho}_1)]_{00}^{(44)}
\]
\[+ \frac{\sqrt{3}}{2\sqrt{2}}[\psi^8(\mathbf{r}_1)\psi^4(\mathbf{\rho}_1)]_{00}^{(44)},
\]
\[
\chi_{00}^{[3]12(82)\gamma=0} = \frac{9\sqrt{5}}{4\sqrt{43}}[\psi^4(\mathbf{r}_1)\psi^8(\mathbf{\rho}_1)]_{00}^{(82)} + \frac{3}{2\sqrt{86}}[\psi^6(\mathbf{r}_1)\psi^6(\mathbf{\rho}_1)]_{00}^{(82)}
\]
\[\frac{5\sqrt{5}}{4\sqrt{43}}[\psi^8(\mathbf{r}_1)\psi^4(\mathbf{\rho}_1)]_{00}^{(82)} + \frac{\sqrt{35}}{2\sqrt{43}}[\psi^{10}(\mathbf{r}_1)\psi^2(\mathbf{\rho}_1)]_{00}^{(82)},
\]
\[
\chi_{00}^{[3]12(12,0)\gamma=0} = \frac{27\sqrt{7}}{116}[\psi^4(\mathbf{r}_1)\psi^8(\mathbf{\rho}_1)]_{00}^{(12,0)} - \frac{9\sqrt{15}}{58}[\psi^6(\mathbf{r}_1)\psi^6(\mathbf{\rho}_1)]_{00}^{(12,0)}
\]
\[+ \frac{9\sqrt{7}}{58}[\psi^8(\mathbf{r}_1)\psi^4(\mathbf{\rho}_1)]_{00}^{(12,0)} - \frac{\sqrt{105}}{29\sqrt{2}}[\psi^{10}(\mathbf{r}_1)\psi^2(\mathbf{\rho}_1)]_{00}^{(12,0)}
\]
\[+ \frac{\sqrt{385}}{116}[\psi^{12}(\mathbf{r}_1)\psi^0(\mathbf{\rho}_1)]_{00}^{(12,0)}.
\]  

(28)

We have two Pauli-allowed states for $Q(\lambda\mu) = 14(64)$, so there is a freedom to fix them. Here they are defined in such a way that one of them ($\kappa = 2$) contains no $[\psi^{10}(\mathbf{r}_1)\psi^4(\mathbf{\rho}_1)]_{00}^{(64)}$ component.
\( Q = 14 \)

\[
\begin{align*}
\chi_{00}^{[3]14(26)\gamma=0} &= \frac{1}{\sqrt{2}}[\psi^6(r_1)\psi^8(\rho_1)]^{(26)}_{00} + \frac{1}{\sqrt{2}}[\psi^8(r_1)\psi^6(\rho_1)]^{(26)}_{00}, \\
\chi_{00}^{[3]14(64)\kappa=1\gamma=0} &= 0.479702[\psi^4(r_1)\psi^{10}(\rho_1)]^{(64)}_{00} + 0.619292[\psi^6(r_1)\psi^8(\rho_1)]^{(64)}_{00} \\
&\quad + 0.206431[\psi^8(r_1)\psi^6(\rho_1)]^{(64)}_{00} + 0.586302[\psi^{10}(r_1)\psi^4(\rho_1)]^{(64)}_{00}, \\
\chi_{00}^{[3]14(64)\kappa=2\gamma=0} &= 0.337100[\psi^4(r_1)\psi^{10}(\rho_1)]^{(64)}_{00} - 0.522233[\psi^6(r_1)\psi^8(\rho_1)]^{(64)}_{00} \\
&\quad + 0.783349[\psi^8(r_1)\psi^6(\rho_1)]^{(64)}_{00}, \\
\chi_{00}^{[3]14(10,2)\gamma=0} &= \frac{9\sqrt{7}}{8\sqrt{19}}[\psi^4(r_1)\psi^{10}(\rho_1)]^{(10,2)}_{00} + \frac{3\sqrt{3}}{2\sqrt{38}}[\psi^6(r_1)\psi^8(\rho_1)]^{(10,2)}_{00} \\
&\quad - \frac{\sqrt{3}}{4\sqrt{38}}[\psi^8(r_1)\psi^6(\rho_1)]^{(10,2)}_{00} - \frac{\sqrt{7}}{2\sqrt{19}}[\psi^{10}(r_1)\psi^4(\rho_1)]^{(10,2)}_{00} \\
&\quad - \frac{3\sqrt{35}}{8\sqrt{19}}[\psi^{12}(r_1)\psi^2(\rho_1)]^{(10,2)}_{00}, \\
\chi_{00}^{[3]14(14,0)\gamma=0} &= \frac{81}{4\sqrt{742}}[\psi^4(r_1)\psi^{10}(\rho_1)]^{(14,0)}_{00} - \frac{9\sqrt{3}}{4\sqrt{742}}[\psi^6(r_1)\psi^8(\rho_1)]^{(14,0)}_{00} \\
&\quad - \frac{9\sqrt{3}}{2\sqrt{742}}[\psi^8(r_1)\psi^6(\rho_1)]^{(14,0)}_{00} + \frac{21}{2\sqrt{742}}[\psi^{10}(r_1)\psi^4(\rho_1)]^{(14,0)}_{00} \\
&\quad - \frac{11\sqrt{11}}{4\sqrt{742}}[\psi^{12}(r_1)\psi^2(\rho_1)]^{(14,0)}_{00} + \frac{\sqrt{143}}{4\sqrt{106}}[\psi^{14}(r_1)\psi^0(\rho_1)]^{(14,0)}_{00}.
\end{align*}
\]
[1] see, for example, K. Ikeda et al., Prog. Theor. Phys. Suppl. 68 (1980) 1.
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