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RESEARCH ARTICLE

New microscopic wave function of α-condensation

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We explain how to treat a microscopic wave function of α-condensation taking a 3α-nucleus as a typical example. The wave function has been originally proposed ten years before by Horiuchi, Röpke, Schuck and the present author (Phys. Rev. Lett., 2001, 87: 192501). The microscopic model, which fully takes into account the Pauli principle between all the constituent nucleons, effective inter-nucleon forces and the Coulomb force, can play an important role in reproducing an α-gas nature thanks to α-condensation as an excited state of α-like nuclei. An essential point of the wave function is to describe their ground state simultaneously. We study its typical features by giving an analytical formula of the norm kernel and the kernel concerning the one-body operator for 3α-condensation.

Keywords α-cluster model, analytical formula, α-condensation

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1 Introduction

We have conjectured an excited state of $n\alpha$ nuclei, which is regarded as an α-condensation, on the basis of a new microscopic wave function introduced in our paper ten years ago [1]. The state occurs as a dilute α-gas where the α particles are composite bosons consisting of the fermionic nucleons with maximal occupied spin-isospin states. In order to study the α-condensation with composite bosons, therefore, it is definitely inevitable for us to employ a microscopic model which takes full account of the Pauli exclusion principle between all the constituent nucleons, the effective inter-nucleon force and the Coulomb force without any approximation.

Unlike a fully traditional-microscopic α-cluster model, an ingredient of the wave function is to change the nature of variational parameters in the Hill–Wheeler equation from the relative distances between α particles to their density within the framework of the microscopic model. Obviously, in the traditional α-cluster model, which consists of $n\alpha$-clusters, there are $n-1$ independent parameters corresponding to the number of the internal relative distances, by subtracting the c.m. coordinate. On the other hand, for the new microscopic wave function, we consider only one-parameter contribution for α-condensation apart from entangled parameters coming from relative motion of α-clusters. Successfully applied to $n\alpha$ nuclei consisting of 2- to 5α-clusters, this simple wave function has anticipated that there can be an excited state around the $n\alpha$ break-up energy, which might be regarded as the α-condensation [2]. This is because the wave function has absolutely a long range tail, which could not be artificially cut off and could play an important role in guaranteeing the stability of the α-gas. The more sophisticated development that introduces the quadratic deformation, has been already done by Funaki *et al.* [4, 5]. However, until now, no details to treat the wave function have been given anywhere. In this report, one of the main aims is to show the analytical derivations of the exchange kernels, which are an indispensable tool to solve the Hill–Wheeler equation, by taking 3α-condensation as a typical example. Their various kinds of the behaviors are illustrated for the nuclei from 2α to 6α.

We describe the new wave function and its characteristics in the following section. Section 3 presents the derivation method of the analytical formulae of the norm kernel. In Section 4, the behavior of the norm kernel is discussed. Furthermore, a new treatment for the deformed condensation is proposed in Section 5. Section 6 is devoted to the energy kernel concerning the one-body operator. Section 7 is about the behavior of the one-body kernel in terms of the Taylor expansion. Concluding remarks are given in Section 8.

2 Characteristics of the wave function for α condensation

First of all, we should present the wave function responsible for the $n\alpha$-condensation as follows:

$$|\Psi_{n\alpha}(R_0,b)\rangle = \left\{C_\alpha^\dagger(R_0,b)\right\}^n|0\rangle \tag{1}$$

where $C_\alpha^\dagger(R_0,b)$ is an α-like particle creation operator on a center-of-mass (c.m.) orbit around the origin in the Gaussian constraint, which is defined by

$$C_\alpha^\dagger(R_0,b) = (\pi {R_0}^2)^{-3/2}\int \mathrm{d}\boldsymbol{R}\ \mathrm{e}^{-\boldsymbol{R}^2/{R_0}^2}A_\alpha^\dagger(b) \tag{2}$$

Here, the usual α-cluster creation operator is given by

$$A_\alpha^\dagger(b) = \prod_{k=1}^{4}\int \mathrm{d}\boldsymbol{r}_k\phi_{\boldsymbol{R}}(\boldsymbol{r}_k)a_{\sigma_k\tau_k}^\dagger(\boldsymbol{r}_k) \tag{3}$$

The single nucleon wave function is

$$\phi_{\boldsymbol{R}}(\boldsymbol{r}) = (\sqrt{\pi}b)^{-3/2}\mathrm{e}^{-(\boldsymbol{r}-\boldsymbol{R})^2/(2b^2)} \tag{4}$$

and $a_{\sigma\tau}^\dagger(\boldsymbol{r})$ is the creation operator of a nucleon with spin-isospin $\sigma\tau$ at the position of $\boldsymbol{r}$. The parameter b is the harmonic oscillator strength for a single nucleon wave function in the α-cluster state. Note that auxiliary coordinate is not c.m. coordinate, $\boldsymbol{r}_G = \sum_{k=1}^4 \boldsymbol{r}_k/4$ and will be eliminated as mentioned later. Substituting Eq. (4) into Eq. (2) and integrating over the parameter $\boldsymbol{R}$, we get

$$C_\alpha^\dagger(R_0,b)\,|0\rangle = \left(\frac{b^2}{b^2+2R_0^2}\right)^{3/2}\mathrm{e}^{-2\boldsymbol{r}_G^2/\left(b^2+2R_0^2\right)}\phi_{int} \tag{5}$$

where $\boldsymbol{r}_G$ is the c.m. coordinate for an α-cluster and ϕ_{int} means its internal wave function, which includes only relative coordinates among 4 nucleons concerning the α-cluster. Note that it is very convenient to represent an α-cluster configuration created from a vacuum state with Brink-type model wave function [3], which has been usually employed in the traditional microscopic α cluster models, that is,

$$\begin{aligned}|\Phi_o\rangle &= \left[A_\alpha^\dagger(b)\right]^n|0\rangle\\ &= \sqrt{\frac{1}{4\cdot 3!}}\prod_{k=1}^{4}\begin{vmatrix}\phi_{\boldsymbol{R}_1}(\boldsymbol{r}_1) & \phi_{\boldsymbol{R}_1}(\boldsymbol{r}_2) & \phi_{\boldsymbol{R}_1}(\boldsymbol{r}_3)\\ \phi_{\boldsymbol{R}_2}(\boldsymbol{r}_1) & \phi_{\boldsymbol{R}_2}(\boldsymbol{r}_2) & \phi_{\boldsymbol{R}_2}(\boldsymbol{r}_3)\\ \phi_{\boldsymbol{R}_3}(\boldsymbol{r}_1) & \phi_{\boldsymbol{R}_3}(\boldsymbol{r}_2) & \phi_{\boldsymbol{R}_3}(\boldsymbol{r}_3)\end{vmatrix}_{\sigma_k\tau_k}\end{aligned} \tag{6}$$

Then, we give Eq. (1) for 3α-clusters,

$$|\Psi_{3\alpha}(R_0)\rangle = \left(\frac{b^2}{b^2+2R_0^2}\right)^{9/2}\cdot\mathcal{A}\left[\prod_{k=1}^{3}\mathrm{e}^{-2\boldsymbol{r}_{G(k)}^2/\left(b^2+2R_0^2\right)}\phi_{int(k)}\right] \tag{7}$$

We can easily understand from Eq. (7) that all the α-clusters belong to the same (0s)-orbit with the strength $\sqrt{b^2+2R_0^2}$, and that a necessary condition for α-condensation is satisfied. Therefore, if $R_0\rightarrow 0$, the strength coincides with that of α-cluster, and 3α-nucleus comes to the ground state of ^{12}C. This circumstance is common with that of the traditional-microscopic α-cluster model. The fermionic property of nucleons is in the antisymmetrizer which excludes that 3α-clusters approach each other. We imagine that this condition goes to a dilute α-gas structure. From Eq. (7), we can estimate the c.m. part of the 3α-clusters in the exchange kernels, which should be removed:

$$\left(\frac{6}{\pi b^2}\right)^{3/2}\mathrm{e}^{-6\boldsymbol{r}_G^2/\left(b^2+2R_0^2\right)-6\boldsymbol{r}_G^2/\left(b^2+2R_0'^2\right)} \tag{8}$$

Integrating over $\boldsymbol{r}_G$, we have

$$\left[\frac{\left(b^2+2R_0^2\right)\left(b^2+2R_0'^2\right)}{2b^2\left(b^2+R_0^2+R_0'^2\right)}\right]^{3/2} \tag{9}$$

Next, we introduce a generalized creation operator of Eq. (2) as

$$C_\alpha^\dagger = \int \mathrm{d}\boldsymbol{R}''\prod_j^{x,y,z}(\pi {R_{0j}}^2)^{-1/2}\mathrm{e}^{-\left(R_j''/R_{0j}\right)^2}A_\alpha^\dagger(b) \tag{10}$$

where suffix j stands for one of the 3 spatial components of (x,y,z). The vector $\left(R_x'',\ R_y'',\ R_z''\right)$ is related to a linear transformation M, which is a general rotation:

$$\boldsymbol{R}'' = M\boldsymbol{R}$$

that is,

$$\begin{pmatrix}R_x''\\ R_y''\\ R_z''\end{pmatrix} = \begin{pmatrix}m_{xx} & m_{xy} & m_{xz}\\ m_{yx} & m_{yy} & m_{yz}\\ m_{zx} & m_{zy} & m_{zz}\end{pmatrix}\begin{pmatrix}R_x\\ R_y\\ R_z\end{pmatrix} \tag{11}$$

If we employ the Euler angles (α,β,γ), we can present the matrix M as

$$\begin{pmatrix}\cos\alpha\cos\beta\cos\gamma-\sin\alpha\sin\gamma & \sin\alpha\cos\beta\cos\gamma+\cos\alpha\sin\gamma & -\sin\beta\cos\gamma\\ -\cos\alpha\cos\beta\sin\gamma-\sin\alpha\cos\gamma & -\sin\alpha\cos\beta\sin\gamma+\cos\alpha\cos\gamma & \sin\beta\sin\gamma\\ \cos\alpha\sin\beta & \sin\alpha\sin\beta & \cos\beta\end{pmatrix} \tag{12}$$

Eq. (10) allows us to examine a 3-dimensional deformation of α-condensation. The integral of Eq. (10) with respect to $\boldsymbol{R}$ is carried out directly as follows:

$$M_c^{-1/2}\mathrm{e}^{-2r_G^2/b^2+4/(M_cb^2M_R)} \tag{13}$$

where the constant M_c is defined by

$$M_c = \begin{vmatrix}M_{xx} & M_{xy} & M_{xz}\\ M_{yx} & M_{yy} & M_{yz}\\ M_{zx} & M_{zy} & M_{zz}\end{vmatrix}$$

where

$$M_{xy} = R_{0x}R_{0y}\sum_{j}^{x,y,z}\frac{m_{jx}m_{jy}}{R_{0j}^2} + \frac{2R_{0x}R_{0y}}{b^2}\delta_{xy}, \text{ etc.} \quad (14)$$

and M_R is a function of the c.m. of 3α-clusters

$$M_R = \sum_{ij}^{x,y,z} M_{ij}^c r_{Gi} r_{Gj}$$

where M_{xy}^c is a cofactor of M_{xy}. For Eq. (9), we get a generalized formula for the c.m. part:

$$\left(\frac{6}{b^2}\right)^{3/2}\begin{vmatrix} \mu_{xx} & \mu_{xy} & \mu_{xz} \\ \mu_{yx} & \mu_{yy} & \mu_{yz} \\ \mu_{zx} & \mu_{zy} & \mu_{zz} \end{vmatrix}^{-1/2} \quad (15)$$

where

$$\mu_{xy} = \left(\frac{2}{b^2+2R_0^2} + \frac{2}{b^2}\right)\delta_{xy} + \frac{4M_{xy}'^c}{M_c' b^2}, \quad \text{etc.}$$

Here M_c' means that the parameter R_{0x} in Eq. (14) is substituted with R_{0x}', and so on. In this way, the angular momentum projection is available, and unlike the atomic condensation originated in a big number of particles, we expect another type of condensation coming from an easy deformation thanks to the small number of them.

3 Derivation of the norm kernel

It is extremely difficult to obtain the expected values when we start from Eq. (7) because we need the integration procedure with respect to all the coordinates of nucleons after carrying out the anti-symmetrized operation. Instead, we propose a method in which we integrate over the six parameters in the bracket of the wave functions, $\boldsymbol{R}_1, \boldsymbol{R}_2, \boldsymbol{R}_3, \boldsymbol{R}_1', \boldsymbol{R}_2', \boldsymbol{R}_3'$, after integrating all the real coordinates $\boldsymbol{r}_1, \cdots, \boldsymbol{r}_{12}$. As for the normalization kernel, we should first list the overlapping matrix element between single nucleon wave functions as follows:

$$\left\langle \phi_{\boldsymbol{R}_j}(\boldsymbol{r}) | \phi_{\boldsymbol{R}_k'}(\boldsymbol{r})\right\rangle = \mathrm{e}^{-\left(\boldsymbol{R}_j-\boldsymbol{R}_k'\right)^2/(4b^2)} \equiv G_{jk} \quad (16)$$

Next, using Eq. (16), we get the overlapping between α-cluster configurations corresponding to the norm kernel:

$$\left\langle \Phi_o | \Phi_o \right\rangle = \begin{vmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{vmatrix}^4 \quad (17)$$

We should carry out

$$\langle \Psi_{3\alpha}(R_0) | \Psi_{3\alpha}(R_0')\rangle = \frac{1}{3!}(\pi R_0^2 \pi R_0'^2)^{-9/2} \cdot \int \cdots \cdot \int \prod_{k=1}^{3} \mathrm{d}\boldsymbol{R}_k \mathrm{d}\boldsymbol{R}_k' \, \mathrm{e}^{-\left(\boldsymbol{R}_k^2/R_0^2 + \boldsymbol{R}_k'^2/R_0'^2\right)} \left\langle \Phi_o | \Phi_o \right\rangle \quad (18)$$

The power 4 on the determinant comes from the maximal occupation of the spin-isospin states, and factor 1/(3!) is originated in the symmetric property for the exchange of nucleons. The multi-integral of Eq. (18) is an enormous sum of Gauss functions which have always a quadratic form. For example, the first term without any exchange of nucleons between α-clusters can be written as

$$\begin{aligned} I_1(R_0, R_0') &= (\pi R_0^2 \pi R_0'^2)^{-9/2} \int \cdots \int \prod_{k=1}^{3} \mathrm{d}\boldsymbol{R}_k \mathrm{d}\boldsymbol{R}_k' \\ &\quad \cdot \mathrm{e}^{-\left(\boldsymbol{R}_k^2/R_0^2 + \boldsymbol{R}_k'^2/R_0'^2\right)} G_{kk}^4 \\ &= (\pi R_0^2 \pi R_0'^2)^{-9/2} \int \cdots \int \prod_{k=1}^{3} \mathrm{d}\boldsymbol{R}_k \mathrm{d}\boldsymbol{R}_k' \\ &\quad \cdot \mathrm{e}^{-\left(\boldsymbol{R}_k^2/R_0^2 + \boldsymbol{R}_k'^2/R_0'^2\right) - \left(\boldsymbol{R}_k - \boldsymbol{R}_k'\right)^2/b^2} \end{aligned} \quad (19)$$

The integrand has a quadratic form in an exponent as follows:

$$\left(\, \boldsymbol{R}_1,\ \boldsymbol{R}_2,\ \boldsymbol{R}_3 \,\middle|\, \boldsymbol{R}_1',\ \boldsymbol{R}_2',\ \boldsymbol{R}_3' \,\right) \left(\begin{array}{ccc|ccc} X & 0 & 0 & U & 0 & 0 \\ 0 & X & 0 & 0 & U & 0 \\ 0 & 0 & X & 0 & 0 & U \\ \hline U & 0 & 0 & X' & 0 & 0 \\ 0 & U & 0 & 0 & X' & 0 \\ 0 & 0 & U & 0 & 0 & X' \end{array}\right) \left(\begin{array}{c} \boldsymbol{R}_1 \\ \boldsymbol{R}_2 \\ \boldsymbol{R}_3 \\ \hline \boldsymbol{R}_1' \\ \boldsymbol{R}_2' \\ \boldsymbol{R}_3' \end{array}\right) \quad (20)$$

where

$$X = \frac{1}{R_0^2} + \frac{1}{b^2}, \quad X' = \frac{1}{R_0'^2} + \frac{1}{b^2}, \quad U = -\frac{1}{b^2}$$

Here, the 6×6 coefficients matrix is decomposed by four 3×3 sub-matrices which correspond to $\boldsymbol{R}_i \cdot \boldsymbol{R}_j$ part for the upper-left, $\boldsymbol{R}_i \cdot \boldsymbol{R}_j'$ one for the upper-right, $\boldsymbol{R}_i' \cdot \boldsymbol{R}_j$ one for the lower-left and $\boldsymbol{R}_i' \cdot \boldsymbol{R}_j'$ one for the lower-right, respectively.

The evaluation of integral $I_1(R_0, R_0')$ is easy because of the well-known integral formula:

$$I_1(R_0, R_0') = (\pi R_0^2 \pi R_0'^2)^{-9/2}$$

$$\cdot\left[\pi^3\begin{vmatrix} X & 0 & 0 & U & 0 & 0 \\ 0 & X & 0 & 0 & U & 0 \\ 0 & 0 & X & 0 & 0 & U \\ U & 0 & 0 & X' & 0 & 0 \\ 0 & U & 0 & 0 & X' & 0 \\ 0 & 0 & U & 0 & 0 & X' \end{vmatrix}^{-\frac{1}{2}}\right]^3 \tag{21}$$

where the power 3 over the middle bracket comes from 3-dimensional integral with respect to x, y, z. This is because the same results appear in each direction owing to the sphere constraint. As for the deformed constraint, we are going to talk about it later. The normalization factor $(\pi R_0^2 \pi R_0'^2)^{-9/2}$ can be inserted in the determinant as follows:

$$I_1(R_0, R_0') = \begin{vmatrix} x & 0 & 0 & u & 0 & 0 \\ 0 & x & 0 & 0 & u & 0 \\ 0 & 0 & x & 0 & 0 & u \\ u & 0 & 0 & x' & 0 & 0 \\ 0 & u & 0 & 0 & x' & 0 \\ 0 & 0 & u & 0 & 0 & x' \end{vmatrix}^{-3/2}$$
$$= \begin{vmatrix} xx' - u^2 & 0 & 0 \\ 0 & xx' - u^2 & 0 \\ 0 & 0 & xx' - u^2 \end{vmatrix}^{-3/2} \tag{22}$$

where

$$x = 1 + \frac{R_0^2}{b^2},\ x' = 1 + \frac{R_0'^2}{b^2},\ u = -\frac{R_0 R_0'}{b^2}$$

The general term $I_q(R_0, R_0')$ coming from some permutation is presented by substituting the term $\prod_{k=1}^{3} G_{kk}^4$ in Eq. (19) as

$$\prod_{m=1}^{4} G_{1i_m} G_{2j_m} G_{3k_m}, \quad i_m \neq j_m \neq k_m \tag{23}$$

Eq. (23) with respect to the overlapping matrix is rewritten as

$$G_{11}^{a_{11}} G_{12}^{a_{12}} G_{13}^{a_{13}} G_{21}^{a_{21}} G_{22}^{a_{22}} G_{23}^{a_{23}} G_{31}^{a_{31}} G_{32}^{a_{32}} G_{33}^{a_{33}}$$

which has a symbolic matrix in terms of the power a_{mn} for the function G_{mn} as

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} =$$
$$\begin{bmatrix} \sum_m \delta_{1i_m} & \sum_m \delta_{2i_m} & \sum_m \delta_{3i_m} \\ \sum_m \delta_{1j_m} & \sum_m \delta_{2j_m} & \sum_m \delta_{3j_m} \\ \sum_m \delta_{1k_m} & \sum_m \delta_{2k_m} & \sum_m \delta_{3k_m} \end{bmatrix} \tag{24}$$

Following the expression (24), the first term $\prod_{k=1}^{3} G_{kk}^4$ is written as

$$\begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix} \tag{25}$$

We know from this definition that the coefficient a_{mn} has only 5 integers, that is, 0, 1, 2, 3 and 4. The expression is utilized later in order to account for the character of the integrand.

Let us demonstrate its explicit form of the integral as follows:

$$\begin{aligned} & I_q(R_0, R_0') = \\ & (\pi R_0^2 \pi R_0'^2)^{-9/2} \int \cdots \int \mathrm{d}\boldsymbol{R}_1 \mathrm{d}\boldsymbol{R}_2 \mathrm{d}\boldsymbol{R}_3 \mathrm{d}\boldsymbol{R}_1' \mathrm{d}\boldsymbol{R}_2' \mathrm{d}\boldsymbol{R}_3' \\ & \cdot \mathrm{e}^{-\boldsymbol{R}_1^2/R_0^2 - \boldsymbol{R}_2^2/R_0^2 - \boldsymbol{R}_3^2/R_0^2 - \boldsymbol{R}_1'^2/R_0'^2 - \boldsymbol{R}_2'^2/R_0'^2 - \boldsymbol{R}_3'^2/R_0'^2} \\ & \cdot \mathrm{e}^{-(\boldsymbol{R}_1 - \boldsymbol{R}_{i1}')^2/(4b^2) - (\boldsymbol{R}_2 - \boldsymbol{R}_{j1}')^2/(4b^2) - (\boldsymbol{R}_3 - \boldsymbol{R}_{k1}')^2/(4b^2)} \\ & \cdot \mathrm{e}^{-(\boldsymbol{R}_1 - \boldsymbol{R}_{i2}')^2/(4b^2) - (\boldsymbol{R}_2 - \boldsymbol{R}_{j2}')^2/(4b^2) - (\boldsymbol{R}_3 - \boldsymbol{R}_{k2}')^2/(4b^2)} \\ & \cdot \mathrm{e}^{-(\boldsymbol{R}_1 - \boldsymbol{R}_{i3}')^2/(4b^2) - (\boldsymbol{R}_2 - \boldsymbol{R}_{j3}')^2/(4b^2) - (\boldsymbol{R}_3 - \boldsymbol{R}_{k3}')^2/(4b^2)} \\ & \cdot \mathrm{e}^{-(\boldsymbol{R}_1 - \boldsymbol{R}_{i4}')^2/(4b^2) - (\boldsymbol{R}_2 - \boldsymbol{R}_{j4}')^2/(4b^2) - (\boldsymbol{R}_3 - \boldsymbol{R}_{k4}')^2/(4b^2)} \end{aligned} \tag{26}$$

The exponents with respect to the creation operator give only the diagonal elements in the coefficient matrix where the upper-left sub-matrix has $1/R_0^2$ and the lower-right one has $1/R_0'^2$. The overlapping part G_{pr} can give four elements in the coefficients matrix as follows: $1/(4b^2)$ for the p-th diagonal element in the upper-left submatrix and for the r-th part in the lower-right one, and $-1/(4b^2)$ for pr-element in the upper-right and rp-element in the lower-left one. The contribution from the 12 G_{pr} to the diagonal elements is exactly the same as $1/b^2$. On the other hand, the upper-right and the lower-left parts have their own property due to the permutations. Thus, we can write the coefficients matrix as

$$\left(\begin{array}{ccc|ccc} X & 0 & 0 & a_{11}U' & a_{12}U' & a_{13}U' \\ 0 & X & 0 & a_{21}U' & a_{22}U' & a_{23}U' \\ 0 & 0 & X & a_{31}U' & a_{32}U' & a_{33}U' \\ \hline a_{11}U' & a_{21}U' & a_{31}U' & X' & 0 & 0 \\ a_{12}U' & a_{22}U' & a_{32}U' & 0 & X' & 0 \\ a_{13}U' & a_{23}U' & a_{33}U' & 0 & 0 & X' \end{array}\right) \tag{27}$$

where

$$U' = \frac{1}{4}U \tag{28}$$

The coefficients in the off-diagonal parts have the following two characters:

(1) As mentioned before, all the coefficients a_{ij} have the integers, and $0 \leqslant a_{pr} \leqslant 4$, that is, 0, 1, 2, 3 and 4 are possible numbers.

(2) The following equalities come from 4 times of determinant:

$$\frac{1}{4}\sum_{p=1}^{3} a_{pr} = 1, \quad r = 1,2,3; \quad \frac{1}{4}\sum_{r=1}^{3} a_{pr} = 1, \quad p = 1,2,3 \tag{29}$$

The integral $I_q(R_0, R_0')$ is also evaluated as

$$I_q(R_0, R_0') = \begin{vmatrix} x & 0 & 0 & a_{11}u' & a_{12}u' & a_{13}u' \\ 0 & x & 0 & a_{21}u' & a_{22}u' & a_{23}u' \\ 0 & 0 & x & a_{31}u' & a_{32}u' & a_{33}u' \\ a_{11}u' & a_{21}u' & a_{31}u' & x' & 0 & 0 \\ a_{12}u' & a_{22}u' & a_{32}u' & 0 & x' & 0 \\ a_{13}u' & a_{23}u' & a_{33}u' & 0 & 0 & x' \end{vmatrix}^{-3/2} \tag{30}$$

where

$$u' = \frac{1}{4}u \tag{31}$$

The 6×6 determinant in Eq. (30) can be easily reduced to the 3×3 one by using an ordinary sweep-out method:

(1) Multiply the first row by $a_{11}u'/x$, and subtract them from the fourth row, then we get

$$\begin{vmatrix} x & 0 & 0 & a_{11}u' & a_{12}u' & a_{13}u' \\ 0 & x & 0 & a_{21}u' & a_{22}u' & a_{23}u' \\ 0 & 0 & x & a_{31}u' & a_{32}u' & a_{33}u' \\ 0 & a_{21}u' & a_{31}u' & x' - a_{11}a_{11}u'^2/x & -a_{11}a_{12}u'^2/x & -a_{11}a_{13}u'^2/x \\ a_{12}u' & a_{22}u' & a_{32}u' & 0 & x' & 0 \\ a_{13}u' & a_{23}u' & a_{33}u' & 0 & 0 & x' \end{vmatrix} \tag{32}$$

(2) Multiply the first row by $a_{12}u'/x$, and subtract them from the fifth row, next, multiply the first row by $a_{13}u'/x$, and subtract them from the sixth row, then we get

$$\begin{vmatrix} x & 0 & 0 & a_{11}u' & a_{12}u' & a_{13}u' \\ 0 & x & 0 & a_{21}u' & a_{22}u' & a_{23}u' \\ 0 & 0 & x & a_{31}u' & a_{32}u' & a_{33}u' \\ 0 & a_{21}u' & a_{31}u' & x' - a_{11}a_{11}u'^2/x & -a_{11}a_{12}u'^2/x & -a_{11}a_{13}u'^2/x \\ 0 & a_{22}u' & a_{32}u' & -a_{12}a_{11}u'^2/x & x' - a_{12}a_{12}u'^2/x & -a_{12}a_{13}u'^2/x \\ 0 & a_{23}u' & a_{33}u' & -a_{13}a_{11}u'^2/x & -a_{13}a_{12}u'^2/x & x' - a_{13}a_{13}u'^2/x \end{vmatrix} \tag{33}$$

(3) Multiply the second row by $a_{21}u'/x$, and subtract them from the fourth row, next, multiply the second row by $a_{22}u'/x$, and subtract them from the fifth row, third, multiply the second row by $a_{23}u'/x$, and subtract them from the sixth row.

(4) Multiply the third row by $a_{31}u'/x$, and subtract them from the fourth row, next, multiply the third row by $a_{32}u'/x$, and subtract them from the fifth row, third, multiply the third row by $a_{33}u'/x$, and subtract them from the sixth row, then we get

$$\begin{vmatrix} x & 0 & 0 & a_{11}u' & a_{12}u' & a_{13}u' \\ 0 & x & 0 & a_{21}u' & a_{22}u' & a_{23}u' \\ 0 & 0 & x & a_{31}u' & a_{32}u' & a_{33}u' \\ 0 & 0 & 0 & x' - c_{11}u^2/x & -c_{12}u^2/x & -c_{13}u^2/x \\ 0 & 0 & 0 & -c_{21}u^2/x & x' - c_{22}u^2/x & -c_{23}u^2/x \\ 0 & 0 & 0 & -c_{31}u^2/x & -c_{32}u^2/x & x' - c_{33}u^2/x \end{vmatrix} \tag{34}$$

where

$$c_{pr} = \frac{1}{4\cdot 4}\sum_{k=1}^{3} a_{kp}a_{kr}$$

(5) Multiply three x in the diagonal parts by the fourth row, the fifth row and the sixth row, then we get

$$\begin{vmatrix} xx' - c_{11}u^2 & -c_{12}u^2 & -c_{13}u^2 \\ -c_{21}u^2 & xx' - c_{22}u^2 & -c_{23}u^2 \\ -c_{31}u^2 & -c_{32}u^2 & xx' - c_{33}u^2 \end{vmatrix} \tag{35}$$

Thus, we can get the result of multi-integral:

$$I_q(R_0, R_0') = \begin{vmatrix} xx' - c_{11}u^2 & -c_{12}u^2 & -c_{13}u^2 \\ -c_{21}u^2 & xx' - c_{22}u^2 & -c_{23}u^2 \\ -c_{31}u^2 & -c_{32}u^2 & xx' - c_{33}u^2 \end{vmatrix}^{-3/2} \tag{36}$$

We enumerate the characteristics for the determinant of Eq. (36):

(1) It is the eigen-equation with respect to an unknown parameter xx'/u^2.

(2) All the matrix elements c_{pr} are positive, $c_{pr} \leqslant 1$ and symmetric, then it has positive eigenvalues.

(3) The sum $\sum_{r=1}^{3} c_{pr}$ $(p = 1, 2, 3)$ is unity because

$$\sum_{r=1}^{3} c_{pr} = \frac{1}{4 \cdot 4} \sum_{r=1}^{3} \sum_{k=1}^{3} a_{kp} a_{kr} = \frac{1}{4} \sum_{k=1}^{3} a_{kp} \frac{1}{4} \sum_{r=1}^{3} a_{kr} = \frac{1}{4} \sum_{k=1}^{3} a_{kp} = 1 \tag{37}$$

therefore, at least one of the eigenvalues is absolutely unity. It can be decomposed by

$$I_q\left(R_0, R_0'\right) = \left[\left(xx' - \lambda_1^{(q)} u^2\right)\left(xx' - \lambda_2^{(q)} u^2\right)\left(xx' - u^2\right)\right]^{-3/2} \tag{38}$$

where

$$0 \leqslant \lambda_j^{(q)} \leqslant 1, \quad j = 1, 2$$

(4) We can see that the eigen-equation related to Eq. (35) directly stands for that of the eigen-frequency of a connected complex-spring among the α-clusters. By this meaning, the nucleon-exchanges through the anti-symmetrization may be regarded as springs. The more details will be discussed elsewhere within the framework of a di-nucleon-condensation wave function.

Thanks to a computer software, we can sum up all the same terms which have the same eigenvalues $\lambda_1^{(q)}$ and $\lambda_2^{(q)}$. As a consequence, we can find that there are only 9 independent terms among $(3!)^4$ ones. We demonstrate all the independent terms in Table 1. The second term with $\lambda_2^{(q)} = 1$ corresponds to the case that one nucleon exchange takes place only between two α-clusters, namely, the remaining α-cluster moves freely. The third term also with $\lambda_2^{(q)} = 1$ belongs to the case of two-nucleon exchanges between two α-clusters, and the remaining one is free from the other two. The other six terms show the existence of entangling nucleon exchanges among three α-clusters. It is also useful to show the corresponding symbolic matrices in Table 2, which are basic expressions of general exchange kernel with one-, two- and three-body operators. The number of their diagonal part depends on that of non-exchange nucleon in each α-cluster. On the contrary, their off-diagonal parts concern complicated exchange-parts. Seen from the definition of symbolic matrix (24), there are various symmetric properties which lead to the same value of integral. For example, take the case of $q = 4$, and we know easily the relation of Eq. (39):

$$\begin{bmatrix} 3 & 0 & 1 \\ 1 & 3 & 0 \\ 0 & 1 & 3 \end{bmatrix} = \begin{bmatrix} 3 & 1 & 0 \\ 0 & 3 & 1 \\ 1 & 0 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 3 \\ 3 & 1 & 0 \\ 0 & 3 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 3 & 0 \\ 0 & 1 & 3 \\ 3 & 0 & 1 \end{bmatrix} \tag{39}$$

where the cases with 0 for diagonal elements are reduced to Eq. (39). We show the symbolic matrices in Table 2 corresponding to Table 1, where we can see the relationship of the nucleon exchanges among α-clusters. In particular, we arrange that the number of the diagonal parts in each term exactly correspond to that of the remaining nucleons without any exchange among α-clusters.

Table 1 9 independent terms, where W_q means the weight of terms with the same eigenvalues.

q	W_q	$\lambda_1^{(q)}$	$\lambda_2^{(q)}$	q	W_q	$\lambda_1^{(q)}$	$\lambda_2^{(q)}$
1	1	1	1	6	36	1/16	9/16
2	−12	1/4	1	7	6	1/4	1/4
3	9	0	1	8	−12	1/16	1/16
4	8	7/16	7/16	9	36	0	1/4
5	−72	$(2-\sqrt{3})/8$	$(2+\sqrt{3})/8$				

Table 2 9 independent terms in the expression of sybolic matrix.

q		q		q	
1	$\begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix}$	4	$\begin{bmatrix} 3 & 0 & 1 \\ 1 & 3 & 0 \\ 0 & 1 & 3 \end{bmatrix}$	7	$\begin{bmatrix} 2 & 0 & 2 \\ 2 & 2 & 0 \\ 0 & 2 & 2 \end{bmatrix}$
2	$\begin{bmatrix} 4 & 0 & 0 \\ 0 & 3 & 1 \\ 0 & 1 & 3 \end{bmatrix}$	5	$\begin{bmatrix} 3 & 0 & 1 \\ 1 & 2 & 1 \\ 0 & 2 & 2 \end{bmatrix}$	8	$\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$
3	$\begin{bmatrix} 4 & 0 & 0 \\ 0 & 2 & 2 \\ 0 & 2 & 2 \end{bmatrix}$	6	$\begin{bmatrix} 3 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 3 \end{bmatrix}$	9	$\begin{bmatrix} 2 & 1 & 1 \\ 2 & 1 & 1 \\ 0 & 2 & 2 \end{bmatrix}$

4 Behavior of the norm kernel

Next, we should expand Eq. (18) in terms of $s = u^2/xx'$ that can go from 0 to 1. Namely, we obtain

$$\begin{aligned} \langle \Psi_{3\alpha}(R_0) | \Psi_{3\alpha}(R_0') \rangle &= (xx' - u^2)^{-3/2} \sum_{q=1}^{9} W_q \left[\left(xx' - \lambda_1^{(q)} u^2\right)\left(xx' - \lambda_2^{(q)} u^2\right)\right]^{-3/2} \\ &= (xx')^{-9/2}(1-s)^{-3/2} \sum_{q=1}^{9} W_q \left[\left(1 - \lambda_1^{(q)} s\right)\left(1 - \lambda_2^{(q)} s\right)\right]^{-3/2} \\ &= (xx')^{-9/2}(1-s)^{-3/2} \sum_{k=0}^{\infty} p_k \begin{pmatrix} k+2 \\ k \end{pmatrix} s^k = (xx')^{-9/2}(1-s)^{-3/2} N(s) \end{aligned} \tag{40}$$

where we use the binomial coefficient which is normalization coming from the first term without any nucleon exchanges. This is because

$$N_0(s) = [(1-s)(1-s)]^{-3/2} = \sum_{k=0}^{\infty} \begin{pmatrix} k+2 \\ k \end{pmatrix} s^k \quad (41)$$

From Eq. (40), we get two types of the norm kernel which are concerned with a direct form coming from the multi-integral and its Taylor expansion. The former is utilized in the region of large s going to 1, and the latter is available for the region of small s approaching SU3 shell model limit.

The coefficients p_k are exactly 0 up to $k = 3$ under a quantum condition of ^{12}C. Then the first numerical value is $p_4 = 0.03955\cdots$. Its tendency is shown in Fig. 1 up to $k = 50$. We can see a moderate behavior of p_k which shows very slow convergence to the unity of series for $s \sim 1$. It is noted that when $R_0/b \sim 3$, $s \sim 0.8$. We cannot employ a series of Eq. (40) in analyzing an α-gas state because a large value of s plays an important role. However, we can carry out a precise calculation near $R_0/b \sim 0$ where the ground state should be described. We give the expansion coefficients p_k for the other $n\alpha$-condensation from $n = 2$ to 6 in Table 2. The normalization for p_k is given in

$$N(s) = \sum_{k=0}^{\infty} p_k \begin{pmatrix} k + \frac{1}{2}(3n-5) \\ k \end{pmatrix} s^k \quad (42)$$

because the direct term without any exchange of nucleons is written as

$$N_0(s) = (1-s)^{-3(n-1)/2} = \sum_{k=0}^{\infty} \begin{pmatrix} k + \frac{1}{2}(3n-5) \\ k \end{pmatrix} s^k \quad (43)$$

where the binomial coefficient with half-integer is defined by

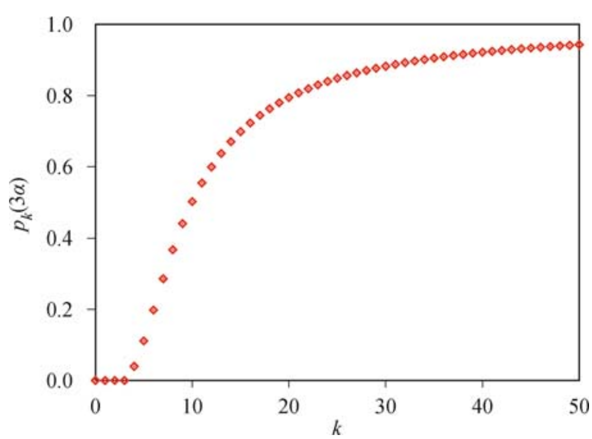

Fig. 1 Expansion coefficients p_k. Reproduced from Ref. [6], Copyright © 2009 World Scientific Publishing Co.

$$\begin{pmatrix} \frac{n}{2} \\ k \end{pmatrix} = \frac{\left(\frac{n}{2}\right)\left(\frac{n}{2}-1\right)\cdots\frac{3}{2}\frac{1}{2}}{\left(\frac{n}{2}-k\right)\left(\frac{n}{2}-k-1\right)\cdots\frac{3}{2}\frac{1}{2}k!} \quad (44)$$

Table 3 tells us the difficulty that we have in giving numerical expansion coefficients for large numbers of α-condensations in the microscopic model. It is also important to note that, in the 2α-condensation, the expansion coefficients exactly coincide with those of the norm kernel which is expanded by the harmonic oscillator for

Table 3 The expansion coefficients p_k for $n\alpha$-condensation. The power $-m$ on the numerical value means $\times 10^{-m}$.

k	$p_k(2\alpha)$	$p_k(3\alpha)$	$p_k(4\alpha)$	$p_k(5\alpha)$	$p_k(6\alpha)$
0	0	0	0	0	0
1	0	0	0	0	0
2	0.7500	0	0	0	0
3	0.9375	0	0	0	0
4	0.9844	0.3955^{-1}	0	0	0
5	0.9961	0.1112	0	0	0
6	0.9990	0.1981	0.6089^{-3}	0	0
7	0.9998	0.2863	0.2753^{-2}	0	0
8	0.9999	0.3678	0.8288^{-2}	0	0
9	1.0000	0.4396	0.1855^{-1}	0	0
10	1.0000	0.5015	0.3389^{-1}	0.3368^{-4}	0
11	1.0000	0.5542	0.5394^{-1}	0.1938^{-3}	0
12	1.0000	0.5990	0.7783^{-1}	0.6341^{-3}	0
13	1.0000	0.6372	0.1047	0.1551^{-2}	0
14	1.0000	0.6700	0.1335	0.3153^{-2}	0.6727^{-6}
15	1.0000	0.6982	0.1634	0.5633^{-2}	0.4909^{-5}
16	1.0000	0.7227	0.1939	0.9145^{-2}	0.1981^{-4}
17	1.0000	0.7441	0.2242	0.1380^{-1}	0.5846^{-4}
18	1.0000	0.7629	0.2542	0.1964^{-1}	0.1410^{-3}
19	1.0000	0.7795	0.2833	0.2668^{-1}	0.2945^{-3}
20	1.0000	0.7942	0.3115	0.3488^{-1}	0.5523^{-3}
21	1.0000	0.8074	0.3387	0.4418^{-1}	0.9524^{-3}
22	1.0000	0.8193	0.3647	0.5448^{-1}	0.1535^{-2}
23	1.0000	0.8300	0.3895	0.6568^{-1}	0.2341^{-2}
24	1.0000	0.8396	0.4132	0.7767^{-1}	0.3409^{-2}
25	1.0000	0.8484	0.4357	0.9034^{-1}	0.4776^{-2}
26	1.0000	0.8564	0.4570	0.1036	0.6473^{-2}
27	1.0000	0.8638	0.4772	0.1173	0.8526^{-2}
28	1.0000	0.8705	0.4964	0.1313	0.1095^{-1}
29	1.0000	0.8767	0.5146	0.1456	0.1377^{-1}
30	1.0000	0.8824	0.5319	0.1601	0.1699^{-1}
31	1.0000	0.8877	0.5483	0.1747	0.2061^{-1}
32	1.0000	0.8926	0.5638	0.1894	0.2463^{-1}
33	1.0000	0.8971	0.5785	0.2040	0.2903^{-1}
34	1.0000	0.9014	0.5925	0.2186	0.3382^{-1}
35	1.0000	0.9053	0.6058	0.2331	0.3898^{-1}
36	1.0000	0.9090	0.6184	0.2474	0.4449^{-1}
37	1.0000	0.9125	0.6304	0.2616	0.5033^{-1}
38	1.0000	0.9158	0.6418	0.2756	0.5648^{-1}
39	1.0000	0.9188	0.6527	0.2894	0.6292^{-1}
40	1.0000	0.9217	0.6631	0.3029	0.6963^{-1}
41	1.0000	0.9244	0.6730	0.3162	0.7659^{-1}
42	1.0000	0.9270	0.6824	0.3292	0.8377^{-1}

the relative coordinate between 2α-clusters. In Fig. 2, we illustrate the tendency of $N(s)/N_0(s)$, which can show the effects of the anti-symmetrization as function of s. We understand its incredible behavior in the small region of s where a strong fall-down of the numerical values takes place. Such a remarkable property strengthens with an increasing number of α-clusters. In particular, the value for 6α-condensation is only 4.708×10^{-30} at $s = 0.01$. We easily understand that a tremendous effort is necessary to remove a serious round-off error in numerical calculations. Otherwise, we could not estimate the ground-state property of $n\alpha$-nuclei. Of course, the feature of the α-gas state strongly depends on the accurate evaluation of the ground state. We think that this is one of the most important points in this wave function.

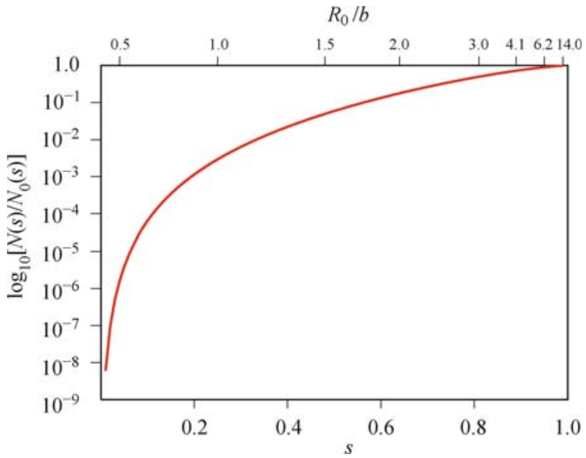

Fig. 2 $N(s)/N_0(s)$, the lower-side scale is s and the upper-side scale is the R_0/b in the case of $R_0 = R'_0$. Reproduced from Ref. [6], Copyright © 2009 World Scientific Publishing Co.

5 Generalization of the norm kernel with deformation of the α-condensation

In the 3α-condensation, the creation operator defined by Eq. (10) gives $(3\times 6)\times(3\times 6)$ determinant for the result of the integral with respect to $\boldsymbol{R}_k$, $\boldsymbol{R}'_k$ as follows:

$$\begin{vmatrix} J^{xx} & J^{xy} & J^{xz} \\ J^{yx} & J^{yy} & J^{yz} \\ J^{zx} & J^{zy} & J^{zz} \end{vmatrix} \tag{45}$$

where J^{xx} and the others are 6×6 matrix. For example, the first diagonal matrix is given by

$$J^{xx} = \begin{pmatrix} x & 0 & 0 & a_{11}u_x & a_{12}u_x & a_{13}u_x \\ 0 & x & 0 & a_{21}u_x & a_{22}u_x & a_{23}u_x \\ 0 & 0 & x & a_{31}u_x & a_{32}u_x & a_{33}u_x \\ a_{11}u_x & a_{21}u_x & a_{31}u_x & x' & 0 & 0 \\ a_{12}u_x & a_{22}u_x & a_{32}u_x & 0 & x' & 0 \\ a_{13}u_x & a_{23}u_x & a_{33}u_x & 0 & 0 & x' \end{pmatrix} \tag{46}$$

and so on. Here the parameter x is common with that in Eq. (22), but x' is given by a little modification of Eq. (14) as

$$x' = R'^2_{0x} \sum_j^{x,y,z} \frac{m^2_{jx}}{R'^2_{0j}} + \frac{R'^2_{0x}}{b^2}$$

The parameter u_x is also the same as Eq. (14),

$$u_x = -\frac{R_{0x}R'_{0x}}{b^2}$$

We define the following relation the same as the preceding section for the later discussion:

$$u'_x = \frac{1}{4}u_x$$

As for the non-diagonal matrices, for instance, we write J^{xy} as follows:

$$J^{xy} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & t_{xy} & 0 & 0 \\ 0 & 0 & 0 & 0 & t_{xy} & 0 \\ 0 & 0 & 0 & 0 & 0 & t_{xy} \end{pmatrix} \tag{47}$$

where t_{xy} is given by adding the primes ($'$) to R_{0x}, R_{0y} in M_{xy} in Eq. (14):

$$t_{xy} = R'_{0x}R'_{0y} \sum_j^{x,y,z} \frac{m_{jx}m_{jy}}{R'^2_{0j}}$$

After the same procedure of the sweep-out as mentioned in the preceding section, we get $(3\times 3)\times(3\times 3)$ determinant:

$$\begin{vmatrix} K^{xx} & K^{xy} & K^{xz} \\ K^{yx} & K^{yy} & K^{yz} \\ K^{zx} & K^{zy} & K^{zz} \end{vmatrix} \tag{48}$$

where K^{xx} and the others are 3×3 matrices as

$$K^{xx} = \begin{pmatrix} xx' - c_{11}u_x^2 & -c_{12}u_x^2 & -c_{13}u_x^2 \\ -c_{21}u_x^2 & xx' - c_{22}u_x^2 & -c_{23}u_x^2 \\ -c_{31}u_x^2 & -c_{32}u_x^2 & xx' - c_{33}u_x^2 \end{pmatrix} \tag{49}$$

for the diagonal matrices, and

$$K^{xy} = \begin{pmatrix} t_{xy} & 0 & 0 \\ 0 & t_{xy} & 0 \\ 0 & 0 & t_{xy} \end{pmatrix} \tag{50}$$

for the off-diagonal matrices. Eq. (48) is rewritten by adequate exchanges of the row and column as follows:

$$\begin{vmatrix} K^{xx} & K^{xy} & K^{xz} \\ K^{yx} & K^{yy} & K^{yz} \\ K^{zx} & K^{zy} & K^{zz} \end{vmatrix} = \begin{vmatrix} L^{11} & L^{12} & L^{13} \\ L^{21} & L^{22} & L^{23} \\ L^{31} & L^{32} & L^{33} \end{vmatrix} \tag{51}$$

where

$$L^{ii} = \begin{pmatrix} xx' - c_{ii}u_x^2 & t_{xy} & t_{xz} \\ t_{yx} & yy' - c_{ii}u_y^2 & t_{yz} \\ t_{zx} & t_{zy} & zz' - c_{ii}u_z^2 \end{pmatrix}$$

$$L^{ij} = c_{ij}\begin{pmatrix} u_x^2 & 0 & 0 \\ 0 & u_y^2 & 0 \\ 0 & 0 & u_z^2 \end{pmatrix}, \quad i \neq j \tag{52}$$

We can use the eigenvalues which are the same as those of the preceding section, then we get

$$\begin{vmatrix} J^{xx} & J^{xy} & J^{xz} \\ J^{yx} & J^{yy} & J^{yz} \\ J^{zx} & J^{zy} & J^{zz} \end{vmatrix} = \begin{vmatrix} L^{11} & L^{12} & L^{13} \\ L^{21} & L^{22} & L^{23} \\ L^{31} & L^{32} & L^{33} \end{vmatrix} =$$

$$\begin{vmatrix} xx' - u_x^2 & t_{xy} & t_{xz} \\ t_{yx} & yy' - u_y^2 & t_{yz} \\ t_{zx} & t_{zy} & zz' - u_z^2 \end{vmatrix}$$

$$\cdot \prod_{j=1}^{2} \begin{vmatrix} xx' - \lambda_j^{(q)}u_x^2 & t_{xy} & t_{xz} \\ t_{yx} & yy' - \lambda_j^{(q)}u_y^2 & t_{yz} \\ t_{zx} & t_{zy} & zz' - \lambda_j^{(q)}u_z^2 \end{vmatrix} \tag{53}$$

We have a simple formula for the norm kernel which are attributed to the eigenvalues coming from the anti-symmetrization. The large numbers of α-condensation are also easily treated in this method even if the deformation is introduced. This formula is transformed by using the eigenvalues related to the geometrical matrix as

$$\begin{vmatrix} \dfrac{xx'}{u_x^2} & \dfrac{t_{xy}}{u_xu_y} & \dfrac{t_{xz}}{u_xu_z} \\ \dfrac{t_{yx}}{u_yu_x} & \dfrac{yy'}{u_y^2} & \dfrac{t_{yz}}{u_yu_z} \\ \dfrac{t_{zx}}{u_zu_z} & \dfrac{t_{zy}}{u_zu_y} & \dfrac{zz'}{u_z^2} \end{vmatrix} = \begin{vmatrix} \nu_1 & 0 & 0 \\ 0 & \nu_2 & 0 \\ 0 & 0 & \nu_3 \end{vmatrix} \tag{54}$$

Eq. (53) is rewritten as

$$(u_x^2u_y^2u_z^2)^3 \begin{vmatrix} \nu_1 - 1 & 0 & 0 \\ 0 & \nu_2 - 1 & 0 \\ 0 & 0 & \nu_3 - 1 \end{vmatrix}$$

$$\cdot \prod_{j=1}^{2} \begin{vmatrix} \nu_1 - \lambda_j^{(q)} & 0 & 0 \\ 0 & \nu_2 - \lambda_j^{(q)} & 0 \\ 0 & 0 & \nu_3 - \lambda_j^{(q)} \end{vmatrix} \tag{55}$$

The norm kernel with the deformation is given by

$$\langle \Psi_{3\alpha}(R_0) | \Psi_{3\alpha}(R_0') \rangle$$

$$= (u_xu_yu_z)^{-3} \begin{vmatrix} \nu_1 - 1 & 0 & 0 \\ 0 & \nu_2 - 1 & 0 \\ 0 & 0 & \nu_3 - 1 \end{vmatrix}^{-1/2}$$

$$\cdot \sum_{q=1}^{9} W_q \prod_{j=1}^{2} \begin{vmatrix} \nu_1 - \lambda_j^{(q)} & 0 & 0 \\ 0 & \nu_2 - \lambda_j^{(q)} & 0 \\ 0 & 0 & \nu_3 - \lambda_j^{(q)} \end{vmatrix}^{-1/2} \tag{56}$$

From Eq. (56), we can understand that the one-dimensional parameter s in Eq. (40) is substituted with the three-dimensional one as $\boldsymbol{s} = (1/\nu_1,\ 1/\nu_2,\ 1/\nu_3)$, and that the Taylor expansion of $N(\boldsymbol{s})$ is also easy, which is,

$$N(\boldsymbol{s}) = \sum_{k_1k_2k_3} p^{(d)}_{k_1k_2k_3} s_1^{k_1} s_2^{k_2} s_3^{k_3} \tag{57}$$

where $p_{k_1k_2k_3}$ is symmetric for the exchange of suffices k_1, k_2, k_3. In the case of 3α-condensation, the binomial coefficients are exactly unity as the normalization seen in Eq. (41). This is because

$$\begin{aligned} N_0(\boldsymbol{s}) &= \left[(1-s_1)^2(1-s_2)^2(1-s_3)^2\right]^{-1/2} \\ &= \sum_{k_1k_2k_3} s_1^{k_1} s_2^{k_2} s_3^{k_3} \end{aligned} \tag{58}$$

In Table 3, we present the coefficients on the 3α-condensation, where we see important quantum conditions coming from the Pauli exclusion principle. For the 3α-condensation, the coefficients $p^{(d)}_{k_1k_2k_3}$ are concerned with the coefficients p_k defined by Eq. (40) as follows:

$$\binom{k+2}{k} p_k = \sum_{k_1,k_2,k_3=0}^{k_1+k_2+k_3=k} p^{(d)}_{k_1k_2k_3} \tag{59}$$

Take $k = 4$, and we obtain

$$\binom{6}{4} 0.3955 \times 10^{-1} = 3 \times 0.1187 + 3 \times 0.7910 \times 10^{-1} \tag{60}$$

The linear terms with $p^{(d)}_{0k_3} = 0$ start at $k_3 = 6$, but their first term is very small as compared with the others with $k_1 + k_2 + k_3 = 6$.

For $n\alpha$-condensation, we can generalize the expression (57) as

$$N(\boldsymbol{s}) = \sum_{k_1k_2k_3} \binom{\frac{1}{2}(n-3)+k_1}{k_1} \binom{\frac{1}{2}(n-3)+k_2}{k_2} \cdot \binom{\frac{1}{2}(n-3)+k_3}{k_3} p^{(d)}_{k_1k_2k_3} s_1^{k_1} s_2^{k_2} s_3^{k_3} \tag{61}$$

At first, we note the remarkable but natural property for the 2α-condensation in Table 5. All the coefficients with the same $k_t = k_1 + k_2 + k_3$ have the same value because the linear, the plane and the cubic properties are not absolutely distinguished in the 2α-condensation. We list the first allowed points for $n\alpha$ with the linear-, the plane- and the cubic-condensations in Table 6. It is obvious that the 3α-condensation has no difference for the plane- and the cubic-ones. Therefore, total difference for the three kinds of condensations exists in more than

4α-nucleus.

Table 4 The expansion coefficients $p^{(d)}_{k_1k_2k_3}$ for 3α-condensation, where $k_t = k_1 + k_2 + k_3$. The numerical values are symmetric for the exchange of suffices.

k_t	k_1	k_2	k_3	$p^{(d)}_{k_1k_2k_3}(3\alpha)$	k_t	k_1	k_2	k_3	$p^{(d)}_{k_1k_2k_3}(3\alpha)$
0	0	0	0	0	7	0	0	7	0.3549^{-1}
						0	1	6	0.9603^{-1}
1	0	0	1	0		0	2	5	0.2841
						0	3	4	0.3595
2	0	0	2	0		1	1	5	0.2450
	0	1	1	0		1	2	4	0.3852
						1	3	3	0.4247
3	0	0	3	0		2	2	3	0.4801
	0	1	2	0					
	1	1	1	0	8	0	0	8	0.6742^{-1}
						0	1	7	0.1401
4	0	0	4	0		0	2	6	0.3276
	0	1	3	0		0	3	5	0.4120
	0	2	2	0.1187		0	4	4	0.4356
	1	1	2	0.7910^{-1}		1	1	6	0.2928
						1	2	5	0.4356
5	0	0	5	0		1	3	4	0.4911
	0	1	4	0.1978^{-1}		2	2	4	0.5392
	0	2	3	0.1854		2	3	3	0.5683
	1	1	3	0.1384					
	1	2	2	0.2299	9	0	0	9	0.1029
						0	1	8	0.1829
6	0	0	6	0.1159^{-1}		0	2	7	0.3672
	0	1	5	0.5407^{-1}		0	3	6	0.4549
	0	2	4	0.2372		0	4	5	0.4894
	0	3	3	0.2905		1	1	7	0.3358
	1	1	4	0.1931		1	2	6	0.4771
	1	2	3	0.3210		1	3	5	0.5391
	2	2	2	0.3889		1	4	4	0.5564
						2	2	5	0.5821
						2	3	4	0.6230
						3	3	3	0.6467

Table 5 The expansion coefficients $p^{(d)}_{k_1k_2k_3}$ for 2α-condensation, where $k_t = k_1 + k_2 + k_3$. The numerical values are symmetric for the exchange of suffices.

k_t	k_1	k_2	k_3	$p^{(d)}_{k_1k_2k_3}(2\alpha)$	k_t	k_1	k_2	k_3	$p^{(d)}_{k_1k_2k_3}(2\alpha)$
0	0	0	0	0	4	0	0	4	0.9844
						0	1	3	0.9844
1	0	0	1	0		0	2	2	0.9844
						1	1	2	0.9844
2	0	0	2	0.7500					
	0	1	1	0.7500	5	0	0	5	0.9961
						0	1	4	0.9961
3	0	0	3	0.9375		0	2	3	0.9961
	0	1	2	0.9375		1	1	3	0.9961
	1	1	1	0.9375		1	2	2	0.9961

Table 6 The first allowed k_t for linear-, the plane- and the cubic-condensations.

	2α k_t	3α k_t	4α k_t	5α k_t	6α k_t
linear: $k_t = 0 + 0 + k_3$	2	6	12	20	30
plane: $k_t = 0 + k_2 + k_3$	2	4	8	12	16
cubic: $k_t = k_1 + k_2 + k_3$	2	4	6	10	14

Finally, it might be important to avoid a confusion by pointing out the case of 4α-condensation as

$$\begin{vmatrix} K^{xx} & K^{xy} & K^{xz} \\ K^{yx} & K^{yy} & K^{yz} \\ K^{zx} & K^{zy} & K^{zz} \end{vmatrix} = \begin{vmatrix} L^{11} & L^{12} & L^{13} & L^{14} \\ L^{21} & L^{22} & L^{23} & L^{24} \\ L^{31} & L^{32} & L^{33} & L^{34} \\ L^{41} & L^{42} & L^{43} & L^{44} \end{vmatrix}$$

$$= \left(u_x^2 u_y^2 u_z^2\right)^4 \times \begin{vmatrix} \nu_1 - 1 & 0 & 0 \\ 0 & \nu_2 - 1 & 0 \\ 0 & 0 & \nu_3 - 1 \end{vmatrix}$$

$$\cdot \prod_{j=1}^{3} \begin{vmatrix} \nu_1 - \lambda_j^{(q)} & 0 & 0 \\ 0 & \nu_2 - \lambda_j^{(q)} & 0 \\ 0 & 0 & \nu_3 - \lambda_j^{(q)} \end{vmatrix} \tag{62}$$

Namely, the dimension of the matrices K^{xx} and so on depends on the number of the α-clusters, but that of matrices L^{ij} is always 3 because of the spatial dimension.

6 Derivation of the energy kernel on the one-body operator

We now come back to the ordinary problem without the deformation of the α-condensation. We address ourselves to the energy kernel on the one-body operator where the kinetic energy operator and the r^2-operator, which is necessary for obtaining the r.m.s radius of the wave function, are included. We begin with the matrix elements of the α-cluster configuration:

$$\begin{aligned} &\left\langle \Phi_o \right| \mathcal{O} \left| \Phi_o \right\rangle \\ &\quad = 4\left\langle \Phi_o \middle| \Phi_o \right\rangle \sum_{i,j}^{3} \left\langle \phi_{\boldsymbol{R}_i}(\boldsymbol{r}) \middle| \hat{O}_j^{(1)} \middle| \phi_{\boldsymbol{R}'_j}(\boldsymbol{r}) \right\rangle G_{ji}^{-1} \\ &\quad = 4 \sum_{j}^{3} f_j^{(1)}\left(\boldsymbol{R}_1, \cdots, \boldsymbol{R}'_3\right) \end{aligned} \tag{63}$$

Eq. (63) can be rewritten in an explicit form of determinants. For example, the parts with $j = 1$ have

$$f_1^{(1)}\left(\boldsymbol{R}_1, \cdots, \boldsymbol{R}'_3\right) = \begin{vmatrix} O_{11}^{(1)} & G_{12} & G_{13} \\ O_{21}^{(1)} & G_{22} & G_{23} \\ O_{31}^{(1)} & G_{23} & G_{33} \end{vmatrix} \cdot \begin{vmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{23} & G_{33} \end{vmatrix}^3 \tag{64}$$

where the factor 4 is omitted for simplicity. The one-body matrix elements $O_{ij}^{(1)}$ are defined by

$$O_{ij}^{(1)} = \langle \phi_{\boldsymbol{R}_i}(\boldsymbol{r}) | \, \hat{O}_j^{(1)} \, | \phi_{\boldsymbol{R}'_j}(\boldsymbol{r}) \rangle \tag{65}$$

Their explicit forms are given by each operator. If we employ the operator r.m.s radius r_j^2,

$$\begin{aligned} O_{ij}^{(1)} &= \langle \phi_{\boldsymbol{R}_i}(\boldsymbol{r}) | \, r_j^2 \, | \phi_{\boldsymbol{R}'_j}(\boldsymbol{r}) \rangle \\ &= \left[\frac{3}{4} b^2 + \frac{1}{4} \left(\boldsymbol{R}_i + \boldsymbol{R}'_j \right)^2 \right] G_{ij} \end{aligned} \tag{66}$$

As for the kinetic energy operator, we give

$$\begin{aligned} O_{ij}^{(1)} &= \langle \phi_{\boldsymbol{R}_i}(\boldsymbol{r}) | \, -\frac{\hbar^2}{2M} \nabla_j^2 \, | \phi_{\boldsymbol{R}'_j}(\boldsymbol{r}) \rangle \\ &= \hbar\omega \left[\frac{3}{4} - \frac{1}{8b^2} \left(\boldsymbol{R}_i - \boldsymbol{R}'_j \right)^2 \right] G_{ij} \end{aligned} \tag{67}$$

where M is the nucleon mass, and $\hbar\omega = \hbar^2/(Mb^2)$. The matrix elements for the last two operators have a divided form where the constant term is the first and the quadric form on $\boldsymbol{R}_i \pm \boldsymbol{R}'_j$ is the second. For the case of Gaussian operator, the matrix element is

$$\begin{aligned} O_{ij}^{(1)} &= \langle \phi_{\boldsymbol{R}_i}(\boldsymbol{r}) | \, \mathrm{e}^{-\beta r_j^2} \, | \phi_{\boldsymbol{R}'_j}(\boldsymbol{r}) \rangle \\ &= \left(\frac{1}{1+\beta b^2} \right)^{3/2} \mathrm{e}^{-\beta/4 \left(\boldsymbol{R}_i + \boldsymbol{R}'_j \right)^2} G_{ij} \end{aligned} \tag{68}$$

In Eqs. (66) and (67), the contribution from the first term is attributed to the norm kernel by multiplying some constant. On the other hand, the second term can be written by the differential with respect to a coefficient γ as

$$\left(\boldsymbol{R}_i \pm \boldsymbol{R}'_j \right)^2 = -\lim_{\gamma \to 0} \frac{\partial}{\partial \gamma} \mathrm{e}^{-\gamma \left(\boldsymbol{R}_i \pm \boldsymbol{R}'_j \right)^2} \tag{69}$$

We expect that, together with Eq. (68), all the matrix elements for $O_{ij}^{(1)}$ have absolutely the common factor as

$$O_{ij}^{(1)} \propto \mathrm{e}^{-\gamma \left(\boldsymbol{R}_i \pm \boldsymbol{R}'_j \right)^2} G_{ij} \tag{70}$$

so that Eq. (64) is given by

$$\begin{aligned} f_1^{(1)}(\boldsymbol{R}_1, \cdots, \boldsymbol{R}'_3) \propto &\begin{vmatrix} \mathrm{e}^{-\gamma \left(\boldsymbol{R}_1 \pm \boldsymbol{R}'_1 \right)^2} G_{11} & G_{12} & G_{13} \\ \mathrm{e}^{-\gamma \left(\boldsymbol{R}_2 \pm \boldsymbol{R}'_1 \right)^2} G_{21} & G_{22} & G_{23} \\ \mathrm{e}^{-\gamma \left(\boldsymbol{R}_3 \pm \boldsymbol{R}'_1 \right)^2} G_{31} & G_{23} & G_{33} \end{vmatrix} \\ &\cdot \begin{vmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{23} & G_{33} \end{vmatrix}^3 \end{aligned} \tag{71}$$

Next we should consider the same multi-integral as Eq. (18):

$$\begin{aligned} I^{(1)}(R_0, R'_0, \gamma) = &(\pi R_0^2 \pi R_0'^2)^{-9/2} \cdot \int \cdots \\ &\cdot \int \prod_{k=1}^{3} \mathrm{d}\boldsymbol{R}_k \mathrm{d}\boldsymbol{R}'_k \, \mathrm{e}^{-\left(\boldsymbol{R}_k^2/R_0^2 + \boldsymbol{R}_k'^2/R_0'^2 \right)} f_1^{(1)}(\boldsymbol{R}_1, \cdots, \boldsymbol{R}'_3) \end{aligned} \tag{72}$$

where the integrand is a lot of summations of Gaussian function. Before examining general terms coming from the integrand, the same as Eq. (19), we write out the first term without any exchange of nucleons between α-clusters,

$$\begin{aligned} I_1^{(1)}(R_0, R'_0, \gamma) = &(\pi R_0^2 \pi R_0'^2)^{-9/2} \cdot \int \cdots \\ &\cdot \int \prod_{k=1}^{3} \mathrm{d}\boldsymbol{R}_k \mathrm{d}\boldsymbol{R}'_k \, \mathrm{e}^{-\left(\boldsymbol{R}_k^2/R_0^2 + \boldsymbol{R}_k'^2/R_0'^2 \right)} G_{kk}^4 \mathrm{e}^{-\gamma \left(\boldsymbol{R}_1 \pm \boldsymbol{R}'_1 \right)^2} \\ = &(\pi R_0^2 \pi R_0'^2)^{-9/2} \cdot \int \cdots \int \prod_{k=1}^{3} \mathrm{d}\boldsymbol{R}_k \mathrm{d}\boldsymbol{R}'_k \\ &\cdot \mathrm{e}^{-\left(\boldsymbol{R}_k^2/R_0^2 + \boldsymbol{R}_k'^2/R_0'^2 \right) - \left(\boldsymbol{R}_k - \boldsymbol{R}'_k \right)^2/b^2 - \gamma \left(\boldsymbol{R}_1 \pm \boldsymbol{R}'_1 \right)^2} \end{aligned} \tag{73}$$

The same with Eq. (19), the integrand has a quadric form in an exponent as follows:

$$\left(\boldsymbol{R}_1, \ \boldsymbol{R}_2, \ \boldsymbol{R}_3 \, \middle| \, \boldsymbol{R}'_1, \ \boldsymbol{R}'_2, \ \boldsymbol{R}'_3 \right) \left(\begin{array}{ccc|ccc} X+\gamma & 0 & 0 & U \pm \gamma & 0 & 0 \\ 0 & X & 0 & 0 & U & 0 \\ 0 & 0 & X & 0 & 0 & U \\ \hline U \pm \gamma & 0 & 0 & X'+\gamma & 0 & 0 \\ 0 & U & 0 & 0 & X' & 0 \\ 0 & 0 & U & 0 & 0 & X' \end{array} \right) \left(\begin{array}{c} \boldsymbol{R}_1 \\ \boldsymbol{R}_2 \\ \boldsymbol{R}_3 \\ \hline \boldsymbol{R}'_1 \\ \boldsymbol{R}'_2 \\ \boldsymbol{R}'_3 \end{array} \right) \tag{74}$$

Therefore, the result of the integral Eq. (73) is obtained the same as Eqs. (21) and (22):

$$\begin{aligned} I_1^{(1)}(R_0, R'_0, \gamma) &= D_1^{-3/2} \\ &= \begin{vmatrix} x+\gamma_{xx} & 0 & 0 & u \mp \gamma_{xx'} & 0 & 0 \\ 0 & x & 0 & 0 & u & 0 \\ 0 & 0 & x & 0 & 0 & u \\ u \mp \gamma_{xx'} & 0 & 0 & x'+\gamma_{x'x'} & 0 & 0 \\ 0 & u & 0 & 0 & x' & 0 \\ 0 & 0 & u & 0 & 0 & x' \end{vmatrix}^{-3/2} \\ &= \begin{vmatrix} (x+\gamma_{xx})(x'+\gamma_{x'x'}) - (u \mp \gamma_{xx'})^2 & 0 & 0 \\ 0 & xx'-u^2 & 0 \\ 0 & 0 & xx'-u^2 \end{vmatrix}^{-3/2} \end{aligned} \tag{75}$$

where

$$\begin{aligned} \gamma_{xx} &= R_0^2 \gamma = b^2 \gamma (x-1) \\ \gamma_{x'x'} &= R_0'^2 \gamma = b^2 \gamma (x'-1) \\ \gamma_{xx'} &= R_0 R'_0 \gamma = b^2 \gamma u \end{aligned}$$

The determinant in Eq. (75) can be written as

$$\begin{aligned} D_1 &= \left(xx' - u^2\right)^3 \\ &\quad + \left(\gamma_{x'x'} x + \gamma_{xx} x' \pm 2\gamma_{xx'} u\right)\left(xx' - u^2\right)^2 \\ &= \left(xx' - u^2\right)^3 + b^2 \gamma \left[-\left(x + x'\right) \right. \\ &\quad \left. + 2\left(xx' \pm u^2\right)\right]\left(xx' - u^2\right)^2 \end{aligned} \tag{76}$$

which shows a linear formula with respect to γ. This property conserves through all the terms in the kernel for one-body operator as will be mentioned soon.

The determinant of the general term $I_q^{(1)}\left(R_0, R_0', \gamma\right)$ has the expression with an extra parameter γ for Eq. (30):

$$\begin{vmatrix} x + \gamma_{xx} & 0 & 0 & a_{11}u' \mp \gamma_{xx'} & a_{12}u' & a_{13}u' \\ 0 & x & 0 & a_{21}u' & a_{22}u' & a_{23}u' \\ 0 & 0 & x & a_{31}u' & a_{32}u' & a_{33}u' \\ a_{11}u' \mp \gamma_{xx'} & a_{21}u' & a_{31}u' & x' + \gamma_{x'x'} & 0 & 0 \\ a_{12}u' & a_{22}u' & a_{32}u' & 0 & x' & 0 \\ a_{13}u' & a_{23}u' & a_{33}u' & 0 & 0 & x' \end{vmatrix} \tag{77}$$

The determinant Eq. (77) is decomposed by four determinants according to a primitive rule on the determinants:

$$\begin{aligned} &\begin{vmatrix} x & 0 & 0 & a_{11}u' & a_{12}u' & a_{13}u' \\ 0 & x & 0 & a_{21}u' & a_{22}u' & a_{23}u' \\ 0 & 0 & x & a_{31}u' & a_{32}u' & a_{33}u' \\ a_{11}u' & a_{21}u' & a_{31}u' & x' & 0 & 0 \\ a_{12}u' & a_{22}u' & a_{32}u' & 0 & x' & 0 \\ a_{13}u' & a_{23}u' & a_{33}u' & 0 & 0 & x' \end{vmatrix} \\ &+ \begin{vmatrix} \gamma_{xx} & 0 & 0 & a_{11}u' & a_{12}u' & a_{13}u' \\ 0 & x & 0 & a_{21}u' & a_{22}u' & a_{23}u' \\ 0 & 0 & x & a_{31}u' & a_{32}u' & a_{33}u' \\ \mp\gamma_{xx'} & a_{21}u' & a_{31}u' & x' & 0 & 0 \\ 0 & a_{22}u' & a_{32}u' & 0 & x' & 0 \\ 0 & a_{23}u' & a_{33}u' & 0 & 0 & x' \end{vmatrix} \\ &+ \begin{vmatrix} x & 0 & 0 & \mp\gamma_{xx'} & a_{12}u' & a_{13}u' \\ 0 & x & 0 & 0 & a_{22}u' & a_{23}u' \\ 0 & 0 & x & 0 & a_{32}u' & a_{33}u' \\ a_{11}u' & a_{21}u' & a_{31}u' & \gamma_{x'x'} & 0 & 0 \\ a_{12}u' & a_{22}u' & a_{32}u' & 0 & x' & 0 \\ a_{13}u' & a_{23}u' & a_{33}u' & 0 & 0 & x' \end{vmatrix} \\ &+ \begin{vmatrix} \gamma_{xx} & 0 & 0 & \mp\gamma_{xx'} & a_{12}u' & a_{13}u' \\ 0 & x & 0 & 0 & a_{22}u' & a_{23}u' \\ 0 & 0 & x & 0 & a_{32}u' & a_{33}u' \\ \mp\gamma_{xx'} & a_{21}u' & a_{31}u' & \gamma_{x'x'} & 0 & 0 \\ 0 & a_{22}u' & a_{32}u' & 0 & x' & 0 \\ 0 & a_{23}u' & a_{33}u' & 0 & 0 & x' \end{vmatrix} \end{aligned} \tag{78}$$

The first term in Eq. (78) is exactly the same with that of the norm kernel, and the final one is identically equal to 0, which explains the reason why the determinant in the general term of the integral is not quadric but linear with respect to the parameter γ. This property is also kept for the integral on the two-body operator. The second and the third terms are concerned with the parameter γ, where the linear dependence is shown. Thus, let us consider the properties of the second and the third determinants in Eq. (78). At first, we should reduce the 6×6 determinant to a 3×3 one using the sweep-out method as follows:

$$\begin{aligned} &\begin{vmatrix} \gamma_{xx} & 0 & 0 & a_{11}u' & a_{12}u' & a_{13}u' \\ 0 & x & 0 & a_{21}u' & a_{22}u' & a_{23}u' \\ 0 & 0 & x & a_{31}u' & a_{32}u' & a_{33}u' \\ \mp\gamma_{xx'} & a_{21}u' & a_{31}u' & x' & 0 & 0 \\ 0 & a_{22}u' & a_{32}u' & 0 & x' & 0 \\ 0 & a_{23}u' & a_{33}u' & 0 & 0 & x' \end{vmatrix} \\ &= \begin{vmatrix} \gamma_{xx}x' \pm \gamma_{xx'}a_{11}u' & -c_{12}'u^2 & -c_{13}'u^2 \\ \pm\gamma_{xx'}a_{21}u' & xx' - c_{22}'u^2 & -c_{23}'u^2 \\ \pm\gamma_{xx'}a_{31}u' & -c_{32}'u^2 & xx' - c_{33}'u^2 \end{vmatrix} \end{aligned} \tag{79}$$

and

$$\begin{aligned} &\begin{vmatrix} x & 0 & 0 & \mp\gamma_{xx'} & a_{12}u' & a_{13}u' \\ 0 & x & 0 & 0 & a_{22}u' & a_{23}u' \\ 0 & 0 & x & 0 & a_{32}u' & a_{33}u' \\ a_{11}u' & a_{21}u' & a_{31}u' & \gamma_{x'x'} & 0 & 0 \\ a_{12}u' & a_{22}u' & a_{32}u' & 0 & x' & 0 \\ a_{13}u' & a_{23}u' & a_{33}u' & 0 & 0 & x' \end{vmatrix} \\ &= \begin{vmatrix} \gamma_{x'x'}x \pm \gamma_{xx'}a_{11}u' & -c_{12}u^2 & -c_{13}u^2 \\ \pm\gamma_{xx'}a_{12}u' & xx' - c_{22}u^2 & -c_{23}u^2 \\ \pm\gamma_{xx'}a_{13}u' & -c_{32}u^2 & xx' - c_{33}u^2 \end{vmatrix} \end{aligned} \tag{80}$$

where

$$c_{pr} = \frac{1}{4 \cdot 4}\sum_{k=1}^{3} a_{kp}a_{kr}, \quad c_{pr}' = \frac{1}{4 \cdot 4}\sum_{k=1}^{3} a_{pk}a_{rk}$$

Here, c_{pr} is exactly the same as that in Eq. (35). Eqs. (79) and (80) are also decomposed by the two determinants of each other:

$$\begin{aligned} &\begin{vmatrix} \gamma_{xx}x' \pm \gamma_{xx'}a_{11}u' & -c_{12}'u^2 & -c_{13}'u^2 \\ \pm\gamma_{xx'}a_{21}u' & xx' - c_{22}'u^2 & -c_{23}'u^2 \\ \pm\gamma_{xx'}a_{31}u' & -c_{32}'u^2 & xx' - c_{33}'u^2 \end{vmatrix} \\ &= b^2\gamma \begin{vmatrix} -x' + xx' \pm a_{11}u'^2 & -c_{12}'u^2 & -c_{13}'u^2 \\ \pm a_{21}u'^2 & xx' - c_{22}'u^2 & -c_{23}'u^2 \\ \pm a_{31}u'^2 & -c_{32}'u^2 & xx' - c_{33}'u^2 \end{vmatrix} \\ &= b^2\gamma \left[\Bigg[\begin{vmatrix} -x' & -c_{12}'u^2 & -c_{13}'u^2 \\ 0 & xx' - c_{22}'u^2 & -c_{23}'u^2 \\ 0 & -c_{32}'u^2 & xx' - c_{33}'u^2 \end{vmatrix} \right. \end{aligned}$$

$$
+\left|\begin{array}{ccc} xx'\pm a_{11}u'^2 & -c'_{12}u^2 & -c'_{13}u^2 \\ \pm a_{21}u'^2 & xx'-c'_{22}u^2 & -c'_{23}u^2 \\ \pm a_{31}u'^2 & -c'_{32}u^2 & xx'-c'_{33}u^2 \end{array}\right|\Bigg]\Bigg]
$$

$$
=b^2\gamma\left[-x'\left|\begin{array}{cc} xx'-c'_{22}u^2 & -c'_{23}u^2 \\ -c'_{32}u^2 & xx'-c'_{33}u^2 \end{array}\right|\right.
$$

$$
\left.+\left|\begin{array}{ccc} xx'\pm a_{11}u'^2 & -c'_{12}u^2 & -c'_{13}u^2 \\ \pm a_{21}u'^2 & xx'-c'_{22}u^2 & -c'_{23}u^2 \\ \pm a_{31}u'^2 & -c'_{32}u^2 & xx'-c'_{33}u^2 \end{array}\right|\right]
$$

$$
=b^2\gamma\left[-x'\prod_{k=1}^{2}\left(xx'-\lambda_{a'k}u^2\right)+\prod_{k=1}^{3}\left(xx'-\lambda^{(\pm)}_{b'k}u^2\right)\right] \tag{81}
$$

and

$$
\left|\begin{array}{ccc} \gamma_{x'x'}x\pm\gamma_{xx'}a_{11}u' & -c_{12}u^2 & -c_{13}u^2 \\ \pm\gamma_{xx'}a_{12}u' & xx'-c_{22}u^2 & -c_{23}u^2 \\ \pm\gamma_{xx'}a_{13}u' & -c_{32}u^2 & xx'-c_{33}u^2 \end{array}\right|
$$

$$
=b^2\gamma\left|\begin{array}{ccc} -x+xx'\pm a_{11}u'^2 & -c_{12}u^2 & -c_{13}u^2 \\ \pm a_{12}u'^2 & xx'-c_{22}u^2 & -c_{23}u^2 \\ \pm a_{31}u'^2 & -c_{32}u^2 & xx'-c_{33}u^2 \end{array}\right|
$$

$$
=b^2\gamma\left[\left[\left|\begin{array}{ccc} -x & -c_{12}u^2 & -c_{13}u^2 \\ 0 & xx'-c_{22}u^2 & -c_{23}u^2 \\ 0 & -c_{32}u^2 & xx'-c_{33}u^2 \end{array}\right|\right.\right.
$$

$$
\left.\left.+\left|\begin{array}{ccc} xx'\pm a_{11}u'^2 & -c_{12}u^2 & -c_{13}u^2 \\ \pm a_{12}u'^2 & xx'-c_{22}u^2 & -c_{23}u^2 \\ \pm a_{13}u'^2 & -c_{32}u^2 & xx'-c_{33}u^2 \end{array}\right|\right]\right]
$$

$$
=b^2\gamma\left[-x\left|\begin{array}{cc} xx'-c_{22}u^2 & -c_{23}u^2 \\ -c_{32}u^2 & xx'-c_{33}u^2 \end{array}\right|\right.
$$

$$
\left.+\left|\begin{array}{ccc} xx'\pm a_{11}u'^2 & -c_{12}u^2 & -c_{13}u^2 \\ \pm a_{12}u'^2 & xx'-c_{22}u^2 & -c_{23}u^2 \\ \pm a_{13}u'^2 & -c_{32}u^2 & xx'-c_{33}u^2 \end{array}\right|\right]
$$

$$
=b^2\gamma\left[-x\prod_{k=1}^{2}\left(xx'-\lambda_{ak}u^2\right)+\prod_{k=1}^{3}\left(xx'-\lambda^{(\pm)}_{bk}u^2\right)\right] \tag{82}
$$

It is noted that the second eigen-equation in each part is not symmetric, which may lead to complex eigenvalue. Eqs. (81) and (82) make the determinant in the general form of the integral $I_q^{(1)}\left(R_0,R'_0,\gamma\right)$ together with Eq. (38):

$$
D_q=\left(xx'-u^2\right)\prod_{k=1}^{2}\left(xx'-\lambda_k^{(q)}u^2\right)
$$

$$
-b^2\gamma\left[x\prod_{k=1}^{2}\left(xx'-\lambda_{ak}^{(q)}u^2\right)+x'\prod_{k=1}^{2}\left(xx'-\lambda_{a'k}^{(q)}u^2\right)\right]
$$

$$
+b^2\gamma\left[\prod_{k=1}^{3}\left(xx'-\lambda_{bk}^{(q\pm)}u^2\right)+\prod_{k=1}^{3}\left(xx'-\lambda_{b'k}^{(q\pm)}u^2\right)\right] \tag{83}
$$

This is also regarded as a generalization of Eq. (83). Thus, we have 5 kinds of indices which distinguish the integral; that is, $\lambda,\lambda_a,\lambda_b,\lambda_{a'}$, and $\lambda_{b'}$. We sum up the terms of which the indices are the same with each other with an aid of the computer software. As a consequence, we have only 25 independent terms as shown in Table 7, where we rewrite the final middle-bracket with the polynomials in order to avoid showing the complex numbers and the irrational numbers in Table 7,

$$
\prod_{k=1}^{2}\left(xx'-\lambda_{ak}^{(q)}u^2\right)=\left(xx'\right)^2\left(1+d_{x1}^{(q)}s+d_{x0}^{(q)}s^2\right)
$$

$$
=\left(xx'\right)^2P_x^{(q)}(s)
$$

$$
\prod_{k=1}^{2}\left(xx'-\lambda_{a'k}^{(q)}u^2\right)=\left(xx'\right)^2\left(1+d_{x'1}^{(q)}s+d_{x'0}^{(q)}s^2\right)
$$

$$
=\left(xx'\right)^2P_{x'}^{(q)}(s)
$$

and

$$
\prod_{k=1}^{3}\left(xx'-\lambda_{bk}^{(q\pm)}u^2\right)+\prod_{k=1}^{3}\left(xx'-\lambda_{b'k}^{(q\pm)}u^2\right)
$$

$$
=\left(xx'\right)^3\left(2+d_2^{(q\pm)}s+d_1^{(q\pm)}s^2+d_0^{(q\pm)}s^3\right)
$$

$$
=\left(xx'\right)^3P_0^{(q)}(s) \tag{84}
$$

Table 7 is also restricted to the case of $\mathrm{e}^{-\gamma\left(\boldsymbol{R}_i-\boldsymbol{R}'_j\right)^2}$ in Eq. (70), directly related to the dependent terms on x and x' in the kinetic energy kernel. The column of q_n corresponds to that of q in Table 7 where 9 independent terms are shown in the norm kernel. Therefore, the eigenvalues of $\lambda_k^{(q)}$ are omitted in Table 7. We can know how the terms with the same eigenvalues of $\lambda_k^{(q)}$ are divided from each other. Take the case of $q_n=4$ as an example, and we show the difference of the two terms. As for the term of $q=7$, the integrand is as follows:

$$
\mathrm{e}^{-\gamma\left(\boldsymbol{R}_1-\boldsymbol{R}'_1\right)^2}G_{11}^3G_{13}G_{21}G_{22}^3G_{32}G_{33}^3 \tag{85}
$$

On the other hand, the term of $q=8$ has the integrand of

$$
\mathrm{e}^{-\gamma\left(\boldsymbol{R}_1-\boldsymbol{R}'_1\right)^2}G_{11}G_{13}^3G_{21}^3G_{22}G_{32}^3G_{33} \tag{86}
$$

which is equivalent to

$$
\mathrm{e}^{-\gamma\left(\boldsymbol{R}_1-\boldsymbol{R}'_3\right)^2}G_{11}^3G_{13}G_{21}G_{22}^3G_{32}G_{33}^3 \tag{87}
$$

Namely, if the one-body operator puts on a nucleon which does not concern the exchange between α-clusters, the result of the integral leads to the case of $q=7$. On the contrary, $q=8$ if the one-body operater operates on a nucleon related to the chain-like exchange among three

Table 7 25 independent terms, where $W_q^{(1)}$ means the weight of terms with the same eigenvalues, where the label * in the columns of $d_{x'1}^{(q)}$ and $d_{x'0}^{(q)}$ means the case of $d_{x1}^{(q)} = d_{x'1}^{(q)}$ and $d_{x0}^{(q)} = d_{x'0}^{(q)}$.

q	q_n	$W_q^{(1)}$	$d_{x1}^{(q)}$	$d_{x0}^{(q)}$	$d_{x'1}^{(q)}$	$d_{x'0}^{(q)}$	$d_2^{(q-)}$	$d_1^{(q-)}$	$d_0^{(q-)}$
1	1	1	−2	1	*	*	−6	6	−2
2	2	−4	−5/4	1/4	*	*	−9/2	3	−1/2
3		−6	−13/8	5/8	*	*	−19/4	7/2	−3/4
4		−2	−13/8	5/8	*	*	−15/4	3/2	1/4
5	3	3	−1	0	*	*	−4	2	0
6		6	−3/2	1/2	*	*	−4	2	0
7	4	6	−5/4	91/256	*	*	−4	319/128	−63/128
8		2	−5/4	91/256	*	*	−3	135/128	−7/128
9	5	−18	−7/8	3/64	*	*	−13/4	41/32	−1/32
10		−12	−9/8	19/64	−1	11/64	−25/8	39/32	−3/32
11		−12	−1	11/64	−9/8	19/64	−25/8	39/32	−3/32
12		−12	−1	11/64	*	*	−3	31/32	1/32
13		−6	−9/8	19/64	−7/8	3/64	−5/2	17/32	−1/32
14		−6	−7/8	3/64	−9/8	19/64	−5/2	17/32	−1/32
15		−6	−9/8	19/64	*	*	−11/4	21/32	3/32
16	6	18	−1	35/256	*	*	−7/2	207/128	−15/128
17		6	−5/4	99/256	*	*	−7/2	219/128	−27/128
18		6	−5/4	99/256	−1	35/256	−11/4	87/128	9/128
19		6	−1	35/256	−5/4	99/256	−11/4	87/128	9/128
20	7	6	−1	3/16	*	*	−3	9/8	−1/8
21	8	−6	−3/4	11/256	*	*	−5/2	67/128	−3/128
22		−6	−3/4	11/256	*	*	−2	−1/128	1/128
23	9	12	−7/8	1/8	−3/4	0	−21/8	1/8	0
24		12	−3/4	0	−7/8	1/8	−21/8	1/8	0
25		12	−7/8	1/8	*	*	−9/4	1/4	0

α-clusters. We also show in Table 8 that the 8 terms have their conjugate in between each other with respect to x and x' as follows:

$$D_{10}(x,x') = D_{11}(x',x)$$
$$D_{13}(x,x') = D_{14}(x',x)$$
$$D_{18}(x,x') = D_{19}(x',x)$$

and

$$D_{23}(x,x') = D_{24}(x',x) \tag{88}$$

The other 17 terms are self-conjugate as

$$D_q(x,x') = D_q(x',x) \tag{89}$$

These characteristics can be shown in Table 8 by using the symbolic matrix defined by Eq. (24). We explain the relation of conjugate by focusing on the arrangement of the row and column. At first, we point out that the pair of the conjugates naturally belongs to the same q_n, which leads to the same term of the norm kernel. The cases of $q = 10$ and $q = 11$ belong to $q_n = 5$. For $q = 10$, we show the row and column which have a pivot as the element labeled by circle,

$$\begin{bmatrix} 1 & \circ 2 & 1 \end{bmatrix} \qquad \begin{bmatrix} 0 \\ \circ 2 \\ 2 \end{bmatrix} \tag{90}$$

On the other hand, for $q = 11$, the row and column are as follows:

$$\begin{bmatrix} 0 & 2 & \circ 2 \end{bmatrix} \qquad \begin{bmatrix} 1 \\ 1 \\ \circ 2 \end{bmatrix} \tag{91}$$

The exchange characters for the row and column are inverted for $q = 10$ and $q = 11$.

7 Behavior of the one-body kernel

The one-body kernel is written by

$$\begin{aligned} \langle \Psi_{3\alpha}(R_0)|\, \mathcal{O}\, |\Psi_{3\alpha}(R_0')\rangle &= 4\cdot 3\sum_{q=1}^{25} W_q^{(1)} I_q \\ &= 4\cdot 3\sum_{q=1}^{25} W_q^{(1)} D_q^{-3/2} \end{aligned} \tag{92}$$

where D_q is the function of the dimensionless parameter $b^2\gamma$ which is related to the width of one-body operator. As an analysis, we should expand Eq. (92) with the parameter $b^2\gamma$. This is because the first order of it just corresponds to the second term of the matrix element in the kinetic energy kernel in Eq. (67). Using Eqs. (82) and (84), we write out an explicit form of D_q:

$$
\begin{aligned}
D_q &= (xx')^3 (1-s) \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right) \\
&\quad -b^2\gamma \Big[x (xx')^2 P_x^{(q)}(s) \\
&\quad + x' (xx')^2 P_{x'}^{(q)}(s) - (xx')^3 P_0^{(q)}(s) \Big] \\
&= (xx')^3 \left\{ (1-s) \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right) \right. \\
&\quad \left. - b^2\gamma \left[\frac{1}{x'} P_x^{(q)}(s) + \frac{1}{x} P_{x'}^{(q)}(s) - P_0^{(q)}(s) \right] \right\} \qquad (93)
\end{aligned}
$$

The integral $I_q^{(1)}(R_0, R_0', \gamma)$ is given by the Taylor expansion with respect to $b^2\gamma$:

$$
\begin{aligned}
I_q^{(1)}(R_0, R_0', \gamma) &= D_q^{-3/2} \\
&= (xx')^{-9/2} \left\{ (1-s) \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right) \right. \\
&\quad \left. - b^2\gamma \left[\frac{1}{x'} P_x^{(q)}(s) + \frac{1}{x} P_{x'}^{(q)}(s) - P_0^{(q)}(s) \right] \right\}^{-3/2} \\
&= (xx')^{-9/2} (1-s)^{-3/2} \left\{ \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-3/2} \right. \\
&\quad + \frac{3}{2} b^2\gamma \left[\frac{1}{x'} P_x^{(q)}(s) + \frac{1}{x} P_{x'}^{(q)}(s) - P_0^{(q)}(s) \right] \\
&\quad \left. \cdot \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-5/2} + \cdots \right\} \qquad (94)
\end{aligned}
$$

Table 8 The 25 independent terms by the expression of symbolic matrix, where the symbol $\circ$ puts on the position of the one-body operator.

q	q_n		q	q_n		q	q_n	
1	1	$\begin{bmatrix} \circ 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix}$	10	5	$\begin{bmatrix} 3 & 0 & 1 \\ 1 & \circ 2 & 1 \\ 0 & 2 & 2 \end{bmatrix}$	19	6	$\begin{bmatrix} 3 & 1 & 0 \\ 1 & 2 & \circ 1 \\ 0 & 1 & 3 \end{bmatrix}$
2	2	$\begin{bmatrix} \circ 4 & 0 & 0 \\ 0 & 3 & 1 \\ 0 & 1 & 3 \end{bmatrix}$	11	5	$\begin{bmatrix} 3 & 0 & 1 \\ 1 & 2 & 1 \\ 0 & 2 & \circ 2 \end{bmatrix}$	20	7	$\begin{bmatrix} \circ 2 & 0 & 2 \\ 2 & 2 & 2 \\ 0 & 2 & 0 \end{bmatrix}$
3	2	$\begin{bmatrix} 4 & 0 & 0 \\ 0 & \circ 3 & 1 \\ 0 & 1 & 3 \end{bmatrix}$	12	5	$\begin{bmatrix} 3 & 0 & 1 \\ 1 & 2 & 1 \\ 0 & \circ 2 & 2 \end{bmatrix}$	21	8	$\begin{bmatrix} \circ 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$
4	2	$\begin{bmatrix} 4 & 0 & 0 \\ 0 & 3 & \circ 1 \\ 0 & 1 & 3 \end{bmatrix}$	13	5	$\begin{bmatrix} 3 & 0 & 1 \\ \circ 1 & 2 & 1 \\ 0 & 2 & 2 \end{bmatrix}$	22	8	$\begin{bmatrix} 2 & \circ 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$
5	3	$\begin{bmatrix} \circ 4 & 0 & 0 \\ 0 & 2 & 2 \\ 0 & 2 & 2 \end{bmatrix}$	14	5	$\begin{bmatrix} 3 & 0 & \circ 1 \\ 1 & 2 & 1 \\ 0 & 2 & 2 \end{bmatrix}$	23	9	$\begin{bmatrix} \circ 2 & 1 & 1 \\ 2 & 1 & 1 \\ 0 & 2 & 2 \end{bmatrix}$
6	3	$\begin{bmatrix} 4 & 0 & 0 \\ 0 & \circ 2 & 2 \\ 0 & 2 & 2 \end{bmatrix}$	15	5	$\begin{bmatrix} 3 & 0 & 1 \\ 1 & 2 & \circ 1 \\ 0 & 2 & 2 \end{bmatrix}$	24	9	$\begin{bmatrix} 2 & 1 & 1 \\ 2 & 1 & 1 \\ 0 & 2 & \circ 2 \end{bmatrix}$
7	4	$\begin{bmatrix} \circ 3 & 0 & 1 \\ 1 & 3 & 0 \\ 0 & 1 & 3 \end{bmatrix}$	16	6	$\begin{bmatrix} \circ 3 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 3 \end{bmatrix}$	25	9	$\begin{bmatrix} 2 & \circ 1 & 1 \\ 2 & 1 & 1 \\ 0 & 2 & 2 \end{bmatrix}$
8	4	$\begin{bmatrix} 3 & 0 & 1 \\ \circ 1 & 3 & 0 \\ 0 & 1 & 3 \end{bmatrix}$	17	6	$\begin{bmatrix} 3 & 1 & 0 \\ 1 & \circ 2 & 1 \\ 0 & 1 & 3 \end{bmatrix}$			
9	5	$\begin{bmatrix} \circ 3 & 0 & 1 \\ 1 & 2 & 1 \\ 0 & 2 & 2 \end{bmatrix}$	18	6	$\begin{bmatrix} 3 & \circ 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 3 \end{bmatrix}$			

Therefore, the one-body kernel is given by an expansion formula in terms of $b^2\gamma$:

$$
\begin{aligned}
&\langle \varPsi_{3\alpha}(R_0) | \mathcal{O} | \varPsi_{3\alpha}(R_0') \rangle = 4 \cdot 3 (xx')^{-9/2} \\
&\quad \cdot (1-s)^{-3/2} \left\{ \sum_{q=1}^{25} W_q^{(1)} \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-3/2} \right. \\
&\quad + \frac{3}{2} b^2\gamma \left[\frac{1}{x'} \sum_{q=1}^{25} W_q^{(1)} P_x^{(q)}(s) \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-5/2} \right. \\
&\quad + \frac{1}{x} \sum_{q=1}^{25} W_q^{(1)} P_{x'}^{(q)}(s) \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-5/2} \\
&\quad \left. \left. - \sum_{q=1}^{25} W_q^{(1)} P_0^{(q)}(s) \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-5/2} \right] + \cdots \right\} \qquad (95)
\end{aligned}
$$

There are four kinds of summations in Eq. (95). The first one is just that of the norm kernel defined by Eq. (40):

$$
\sum_{q=1}^{25} W_q^{(1)} \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-3/2} = N(s) \qquad (96)
$$

The second and the third one lead to the same result due to the symmetric property with respect to x and x'. We define it as the function of $K^{(x)}$:

$$
\begin{aligned}
K^{(x)}(s) &= \sum_{q=1}^{25} W_q^{(1)} P_x^{(q)}(s) \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-5/2} \\
&= \sum_{q=1}^{25} W_q^{(1)} P_{x'}^{(q)}(s) \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-5/2} \qquad (97)
\end{aligned}
$$

The final summation is defined as $K^{(0)}$:

$$
K^{(0)}(s) = \sum_{q=1}^{25} W_q^{(1)} P_0^{(q)}(s) \prod_{k=1}^{2} \left(1-\lambda_k^{(q)} s\right)^{-5/2} \qquad (98)
$$

We regard the one-body kernel as a generating function of $K^{(x)}$ and $K^{(0)}$, and rewrite Eq. (95) into

$$
\begin{aligned}
&\langle \varPsi_{3\alpha}(R_0) | \mathcal{O} | \varPsi_{3\alpha}(R_0') \rangle \\
&\quad = 4 \cdot 3 (xx')^{-9/2} (1-s)^{-3/2} \left\{ N(s) + \frac{3}{2} b^2\gamma \right. \\
&\quad \left. \cdot \left[\left(\frac{1}{x'} + \frac{1}{x} \right) K^{(x)}(s) - K^{(0)}(s) \right] + \cdots \right\} \qquad (99)
\end{aligned}
$$

Next, we try to expand the functions $K^{(x)}$ and $K^{(0)}$

with respect to s. Before doing so, we should see the structure of $D_1^{-3/2}$ with the case of $(-)$ defined in Eq. (83), namely,

$$\begin{aligned} D_1 &= \left(xx' - u^2\right)^3 + b^2\gamma[-(x + x') \\ &\quad +2\left(xx' - u^2\right)]\left(xx' - u^2\right)^2 \\ &= (xx')^3 \left\{(1-s)^3 - b^2\gamma\left[\left(\frac{1}{x'} + \frac{1}{x}\right)\right.\right. \\ &\quad \left.\left.\cdot (1-s)^2 - 2(1-s)^3\right]\right\} \end{aligned} \tag{100}$$

The power $(-3/2)$ for D_1 is given by taking account of commensurableness $(1-s)$ through all the terms:

$$\begin{aligned} D_1^{-3/2} &= (xx')^{-9/2}(1-s)^{-3/2} \times \left\{(1-s)^2\right. \\ &\quad \left. -b^2\gamma\left[\left(\frac{1}{x'} + \frac{1}{x}\right)(1-s) - 2(1-s)^2\right]\right\}^{-3/2} \\ &= (xx')^{-9/2}(1-s)^{-3/2} \times \left\{(1-s)^{-3} + \frac{3}{2}b^2\gamma\right. \\ &\quad \left.\cdot\left[\left(\frac{1}{x'} + \frac{1}{x}\right)(1-s)^{-4} - 2(1-s)^{-3}\right] + \cdots\right\} \end{aligned} \tag{101}$$

From Eqs. (42), (43) and (101), we obtain an appropriate expressions of the expansion formulae:

$$\begin{aligned} K^{(x)}(s) &= \sum_k p_k^{(x)} \begin{pmatrix} k+3 \\ k \end{pmatrix} s^k \\ K^{(0)}(s) &= 2\sum_k p_k^{(0)} \begin{pmatrix} k+2 \\ k \end{pmatrix} s^k \end{aligned} \tag{102}$$

For $n\alpha$-condensation, we give

$$\begin{aligned} K^{(x)}(s) &= \sum_k p_k^{(x)} \begin{pmatrix} k+\frac{3}{2}(n-1) \\ k \end{pmatrix} s^k \\ K^{(0)}(s) &= 2\sum_k p_k^{(0)} \begin{pmatrix} k+\frac{1}{2}(3n-5) \\ k \end{pmatrix} s^k \end{aligned} \tag{103}$$

The coefficients $p_k^{(x)}$ and $p_k^{(0)}$ are listed in the following Tables 9 and 10. We enumerate their features.

- Except for 2α-condensation, the coefficients monotonously increase and approach unity.
- The starting points of k with non-zero component are the same with those of the norm kernel $N(s)$. This is because the quantum condition of $n\alpha$-condensation is also satisfied for the functions $K^{(x)}(s)$ and $K^{(0)}(s)$.

8 Concluding remarks

We present a mathematical formula for the microscopic wave function of α-condensation, taking 3α-clusters as an example. We give one of the methods deriving the norm kernel and the one-body energy kernel in an analytical way. This method is powerful only if we can use a computer memory analytically. Nevertheless, for the case of large number of α-condensation, it is extremely difficult to have an expansion formula in terms of the density of α-clusters because of a serious round-off error coming from the tremendous large numbers of permutations.

Table 9 The expansion coefficients $p_k^{(x)}$ for $n\alpha$-condensation. The power $-m$ on the numerical value means $\times 10^{-m}$.

k	$p_k^{(x)}(2\alpha)$	$p_k^{(x)}(3\alpha)$	$p_k^{(x)}(4\alpha)$	$p_k^{(x)}(5\alpha)$	$p_k^{(x)}(6\alpha)$
0	0	0	0	0	0
1	0	0	0	0	0
2	1.2500	0	0	0	0
3	1.1250	0	0	0	0
4	1.0469	0.7471^{-1}	0	0	0
5	1.0156	0.1909	0	0	0
6	1.0049	0.3140	0.1218^{-2}	0	0
7	1.0015	0.4233	0.5254^{-2}	0	0
8	1.0004	0.5127	0.1567^{-1}	0	0
9	1.0001	0.5833	0.3393^{-1}	0	0
10	1.0000	0.6389	0.5946^{-1}	0.7858^{-4}	0
11	1.0000	0.6831	0.9065^{-1}	0.4285^{-3}	0
12	1.0000	0.7186	0.1257	0.1339^{-2}	0
13	1.0000	0.7476	0.1628	0.3140^{-2}	0
14	1.0000	0.7718	0.2007	0.6143^{-2}	0.1719^{-5}
15	1.0000	0.7923	0.2383	0.1059^{-1}	0.1197^{-4}
16	1.0000	0.8097	0.2750	0.1664^{-1}	0.4630^{-4}
17	1.0000	0.8248	0.3103	0.2434^{-1}	0.1315^{-3}
18	1.0000	0.8380	0.3439	0.3366^{-1}	0.3060^{-3}
19	1.0000	0.8496	0.3757	0.4452^{-1}	0.6186^{-3}
20	1.0000	0.8599	0.4056	0.5676^{-1}	0.1125^{-2}
21	1.0000	0.8690	0.4337	0.7021^{-1}	0.1886^{-2}
22	1.0000	0.8772	0.4601	0.8470^{-1}	0.2959^{-2}
23	1.0000	0.8845	0.4847	0.1000	0.4400^{-2}
24	1.0000	0.8912	0.5077	0.1160	0.6259^{-2}
25	1.0000	0.8972	0.5293	0.1326	0.8573^{-2}
26	1.0000	0.9027	0.5495	0.1494	0.1138^{-1}
27	1.0000	0.9077	0.5683	0.1665	0.1468^{-1}
28	1.0000	0.9124	0.5860	0.1837	0.1851^{-1}
29	1.0000	0.9166	0.6026	0.2010	0.2286^{-1}
30	1.0000	0.9205	0.6182	0.2181	0.2771^{-1}
31	1.0000	0.9241	0.6328	0.2351	0.3307^{-1}
32	1.0000	0.9274	0.6466	0.2519	0.3891^{-1}
33	1.0000	0.9305	0.6595	0.2685	0.4520^{-1}
34	1.0000	0.9334	0.6718	0.2847	0.5192^{-1}
35	1.0000	0.9361	0.6833	0.3007	0.5903^{-1}
36	1.0000	0.9387	0.6942	0.3163	0.6652^{-1}
37	1.0000	0.9410	0.7045	0.3315	0.7433^{-1}
38	1.0000	0.9432	0.7142	0.3464	0.8245^{-1}
39	1.0000	0.9453	0.7235	0.3609	0.9084^{-1}
40	1.0000	0.9472	0.7322	0.3751	0.9946^{-1}
41	1.0000	0.9491	0.7406	0.3888	0.1083
42	1.0000	0.9508	0.7485	0.4022	0.1173

Table 10 The expansion coefficients $p_k^{(0)}$ for $n\alpha$-condensation. The power $-m$ on the numerical value means $\times 10^{-m}$.

k	$p_k^{(0)}(2\alpha)$	$p_k^{(0)}(3\alpha)$	$p_k^{(0)}(4\alpha)$	$p_k^{(0)}(5\alpha)$	$p_k^{(0)}(6\alpha)$	k	$p_k^{(0)}(2\alpha)$	$p_k^{(0)}(3\alpha)$	$p_k^{(0)}(4\alpha)$	$p_k^{(0)}(5\alpha)$	$p_k^{(0)}(6\alpha)$
0	0	0	0	0	0	22	1.0000	0.8740	0.4550	0.8316^{-1}	0.2889^{-2}
1	0	0	0	0	0	23	1.0000	0.8817	0.4799	0.9835^{-1}	0.4302^{-2}
2	0.9722	0	0	0	0	24	1.0000	0.8886	0.5031	0.1142	0.6128^{-2}
3	1.0529	0	0	0	0	25	1.0000	0.8949	0.5249	0.1306	0.8405^{-2}
4	1.0285	0.6592^{-1}	0	0	0	26	1.0000	0.9006	0.5453	0.1474	0.1117^{-1}
5	1.0110	0.1743	0	0	0	27	1.0000	0.9058	0.5644	0.1644	0.1443^{-1}
6	1.0037	0.2933	0.1120^{-2}	0	0	28	1.0000	0.9105	0.5823	0.1816	0.1821^{-1}
7	1.0012	0.4019	0.4897^{-2}	0	0	29	1.0000	0.9149	0.5990	0.1988	0.2250^{-1}
8	1.0004	0.4925	0.1472^{-1}	0	0	30	1.0000	0.9190	0.6148	0.2159	0.2731^{-1}
9	1.0001	0.5654	0.3214^{-1}	0	0	31	1.0000	0.9227	0.6296	0.2328	0.3262^{-1}
10	1.0000	0.6233	0.5674^{-1}	0.7409^{-4}	0	32	1.0000	0.9261	0.6435	0.2496	0.3840^{-1}
11	1.0000	0.6696	0.8705^{-1}	0.4068^{-3}	0	33	1.0000	0.9293	0.6566	0.2662	0.4464^{-1}
12	1.0000	0.7071	0.1213	0.1278^{-2}	0	34	1.0000	0.9323	0.6690	0.2824	0.5131^{-1}
13	1.0000	0.7370	0.1579	0.3012^{-2}	0	35	1.0000	0.9351	0.6806	0.2984	0.5838^{-1}
14	1.0000	0.7634	0.1953	0.5916^{-2}	0.1643^{-5}	36	1.0000	0.9377	0.6917	0.3140	0.6581^{-1}
15	1.0000	0.7849	0.2327	0.1024^{-1}	0.1149^{-4}	37	1.0000	0.9401	0.7021	0.3293	0.7359^{-1}
16	1.0000	0.8033	0.2693	0.1613^{-1}	0.4458^{-4}	38	1.0000	0.9423	0.7120	0.3442	0.8166^{-1}
17	1.0000	0.8192	0.3046	0.2366^{-1}	0.1270^{-3}	39	1.0000	0.9445	0.7213	0.3588	0.9001^{-1}
18	1.0000	0.8331	0.3382	0.3281^{-1}	0.2963^{-3}	40	1.0000	0.9465	0.7302	0.3730	0.9860^{-1}
19	1.0000	0.8452	0.3702	0.4348^{-1}	0.6004^{-3}	41	1.0000	0.9483	0.7386	0.3868	0.1074
20	1.0000	0.8560	0.4002	0.5554^{-1}	0.1095^{-2}	42	1.0000	0.9501	0.7466	0.4002	0.1164
21	1.0000	0.8655	0.4285	0.6883^{-1}	0.1838^{-2}						

Finally, we point out that all the terms coming from permutations are attributed to the problem concerned with eigen-frequency. By this meaning, the antisymmetrization in terms of this wave function would be regarded as a superposition of compound spring systems.

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