Chapter III

Kernels of GCM, RGM and OCM and Their Calculational Methods

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We discuss the calculational procedures of the kernels of GCM, RGM and OCM and some properties of them related to their calculation. The GCM kernels for various types of systems are treated and methods are discussed on the analytical evaluation and on the decomposition in terms of the number of nucleons exchanged between clusters. The RGM kernels are evaluated by the integral transformation of GCM kernels. Various formulas of this transformation are presented including those for the systems of clusters with unequal oscillator widths. The problems related to the RGM norm kernel (RGM-NK) are discussed; firstly on the solution of the eigen-value problem of RGM-NK for various kinds of systems, secondly on the evaluation of kernels or physical quantities obtainable from the knowledge of RGM-NK and finally on the cluster model space for whose character the solution of the eigen-value problem of RGM-NK gives an indispensable information. The projection operator onto the Pauli-allowed states in OCM is obtained directly from the solution of the eigen-value problem of RGM-NK. In this paper we also present another method of construction of this operator of OCM which needs not to solve the eigen-value problem of RGM-NK which is tedious for complex systems even with our present calculational techniques.

Contents

§ 1. Introduction and summary

Recent development[1)~5)] of cluster physics and microscopic treatment of nuclear collisions is, as is discussed in the previous chapters, largely due to the progress in the past few years of the microscopic models, RGM (resonating

group method) and GCM (generator coordinate method), and of the semi-microscopic model OCM (orthogonality condition model), which describe the interaction process between composite particles. The progress of the above-mentioned models owes greatly to the development of the computational procedures, such as the calculation of the exchange (and also direct) integral kernels of the physical quantities and the solution of the model equations (usually integro-differential ones) under the suitable boundary conditions. We can quote some characteristic points of the recent progress of these models as follows:[5] (i) It has been made possible to treat the heavy systems (such as $^{16}O+^{16}O$) in these microscopic and semi-microscopic models, which is in marked contrast to the former situation where the RGM is applied only for the systems lighter than $\alpha+\alpha$. (ii) It has also become possible to treat the complex systems in the framework of these models, which include the channel coupling two-cluster systems where the processes of the internal excitation of clusters and those of the cluster rearrangement take place, and also the systems composed of three and more clusters. (iii) The inter-relation of the model spaces between shell and cluster models has been investigated in many nuclei in this new situation of the enlarged cluster model space mentioned above in (ii), which has revealed many important shell model configurations are contained in the cluster model space and has promoted the studies of the relation between different models, shell and cluster and those of the structure change problem between shell and cluster structures.

The purpose of this chapter is to discuss the calculation of the kernels or the matrix elements of the physical operators in GCM, RGM and OCM, including some review of the recent developments of the calculational methods. Another important problem of the computational procedures concerning how to solve the model equations under the suitable boundary condition is treated in Chap. V. The main cause which has brought about the development of the computational procedures is the introduction of the GCM for the description of the interaction process between clusters, which has become possible by recognizing the transformation relation of the GCM wave function to the RGM one.[6),7)] The GCM adopts the linear combination of the Slater determinants as the model wave function and therefore the usual shell model techniques for the calculation of the matrix elements of the operators by using the many-body wave functions can be utilized, by which we can avoid the hitherto-considered difficulties of the RGM calculations like as (i) the tediousness of the integration with the use of the internal coordinates of clusters and the relative distance coordinates between clusters, and (ii) the difficulty of the treatment of the full antisymmetrization operation within the above internal and relative coordinate system. The computation of the RGM kernels in heavy or complex systems is now therefore done by first calculating the corresponding GCM kernels and then transforming them to the desired

RGM kernels with the use of the transformation relation between wave functions of GCM and RGM. As for the OCM, the calculation of the projection operator onto the Pauli-allowed states needs the solution of the eigen-value problem of the RGM norm kernels, which is obtained now by noting the fact that the corresponding GCM norm kernel plays the role of the generating function of the eigen-values of the RGM norm kernel. The RGM norm kernel determines the character of the cluster model space and the solution of the eigen-value problem of it is indispensable in the discussion of the relation between shell and cluster models.

In this paper, we first discuss in § 2 the calculation of the GCM kernels for various kinds of systems. The transformation process from the GCM kernels to the RGM ones involves the integration of nearly singular character. Although some numerical evaluations of this nearly singular integration are reported[8] to have been executed, it is desirable to treat this transformation in an analytical way. Thus for the sake of the RGM and OCM calculations, we have also discussed this problem of the analytical evaluation of the GCM kernels in this section. What causes the tediousness in the analytical evaluation of the GCM kernels is the non-orthogonality of the single particle wave functions of each Slater determinant of the GCM wave function and the tediousness increases toward the heavier and more complex systems. The systematic methods devised for the computer evaluation which greatly reduce this difficulty are discussed in Chap. IV. What we discuss in this section is about a method which is suitable for a manual evaluation of the analytical form of the GCM kernel. For the understanding of the structure of the GCM kernel, the decomposition of the kernel according to the number of the nucleons exchanged (NNE) between clusters is of great use. We show that NNE governs the range parameters of the GCM kernel.[8)~13)] Usually the GCM kernels have the form of the product of the polynomial function and the Gaussian function of generator coordinates. That the range parameters of these Gaussian parts are determined by NNE is a useful fact also for the analytical evaluation of kernels.

In § 3 we discuss the transformation procedure from the GCM kernels to the RGM ones. We present a few different transformation formulas used by different authors which are of course mutually equivalent. The matrix representation of the RGM kernels in the harmonic oscillator (H.O.) basis of the relative wave functions is often useful as well as the usual coordinate representation. The formulas are also given by which we get directly the matrix elements in this H.O. representation of RGM kernel from the GCM kernel. The GCM with the use of the complex generator coordinates is found to be useful for the transformation from GCM to RGM especially in H.O. representation. The methods for the computer execution of the analytical transformation which are especially desirable in treating the heavier systems like as

$^{16}O+^{16}O$ are given in Chap. IV.

The problems related to the RGM norm kernel are discussed in § 4. First we show how to solve the eigen-value problem of the RGM norm kernel, where the recognition of the following two points is of essential importance;[14)~16)] (i) the eigen-functions have as a quantum number, the definite total number of the H.O. quanta and moreover they are neatly classified by the Elliott SU_3 group, (ii) the corresponding GCM norm kernel is a generating function of the matrix elements of the RGM norm kernel in the H.O. basis of the relative wave functions. Solution of the eigen-value problem of the RGM norm kernel directly accomplishes the construction of the OCM projection operators onto the Pauli-allowed states. Next we discuss the evaluation procedure of the kernels or the physical quantities which are intimately related to the RGM norm kernel, like as the kinetic energy kernel, the reduced width amplitude of cluster-transfer and so on. Finally we discuss the cluster model space which is determined by the RGM norm kernel. The so-called almost-forbidden relative states[17)] are discussed from this viewpoint of the cluster model space. The inter-relation between the cluster model and shell model spaces is briefly reviewed the investigation of which in many nuclei in the new situation of the enlarged cluster model space has contributed much to the studies of the coexistence and structure-change problems between shell and cluster structures.

The final section (§ 5) treats the evaluation of the OCM operators. As for the projection operator onto the Pauli-allowed states, the solution of the eigen-value problem of the RGM norm kernel discussed in § 4 gives, of course, all the necessary quantities. We, however, give another method of construction of the Pauli-allowed states in this section 5. This method avoids solving the eigen-value problem of the RGM norm kernel and therefore is powerful for the complex systems like as the multi-cluster system and the channel coupling system including the cluster rearrangement, for which the eigen-value problem of the RGM norm kernel becomes fairly tedious to solve even with our treatment given in § 4. This method is explained in detail in the case of the three-cluster system. We expect that, in view of the increase of the data in the wide region of light nuclei which need the cluster model analyses, the present article stimulates the further development of the semi-microscopic model OCM which is an easier framework than GCM and RGM, in parallel with GCM and RGM.

§ 2. GCM kernels and their calculation

2.1. GCM wave function and kernel

2.1.a. *Definitions for various cases*

For the sake of notations, we discuss here the form of the wave functions and kernels in the GCM.[18),22),35)] The GCM wave function which we treat in

this paper for the description of the relative motion or collisions between composite particles is a superposition of the generating functions of the form,[18]

$$\Psi(\boldsymbol{R}_1, \cdots, \boldsymbol{R}_n) = n_0 \mathcal{A}\{\psi(C_1, \boldsymbol{R}_1) \cdots \psi(C_n, \boldsymbol{R}_n)\},$$
$$n_0 \equiv \sqrt{\prod_{i=1}^{n} (N_i!)/A!}. \qquad (2\cdot1\cdot1)$$

Here $\psi(C_i, \boldsymbol{R}_i)$ are the harmonic oscillator (H.O.) shell model wave functions of the cluster C_i located around $\boldsymbol{R}_i$, $\mathcal{A}$ is the antisymmetrizer which exchanges the nucleons belonging to different clusters ($\mathcal{A}=1-\sum P_{ij}+\cdots$), N_i is the mass number of the cluster C_i and $A=\sum^n N_i=$total mass number. When it is necessary to denote the spin L_i of the cluster C_i we write like $\psi_{L_i}(C_i, \boldsymbol{R}_i)$ and similarly if the oscillator parameter ν_i of $\psi(C_i, \boldsymbol{R}_i)$ is needed to be explicitly shown, it is denoted by $\psi(C_i, \boldsymbol{R}_i, \nu_i)$.

Since $\psi(C_i, \boldsymbol{R}_i)$ are Slater determinants (or the superposition of the finite number of the Slater determinants), $\psi(\boldsymbol{R}_1, \cdots, \boldsymbol{R}_n)$ is also a Slater determinant (or superposition of Slater determinants). This fact makes the calculation by GCM very practical and easy. Let $\psi(C_i, \boldsymbol{R}_i)$ be

$$\psi(C_i, \boldsymbol{R}_i) = \frac{1}{\sqrt{N_i!}} \det\{\varphi_{\sigma_i,1}(\boldsymbol{X}_1-\boldsymbol{R}_i) \cdots \varphi_{\sigma_i,N_i}(\boldsymbol{X}_{N_i}-\boldsymbol{R}_i)\}, \qquad (2\cdot1\cdot2)$$

which we simply write as $\psi(C_i, \boldsymbol{R}_i) = (1/\sqrt{N_i!}) \det\{\varphi_{\sigma_i,1} \cdots \varphi_{\sigma_i,N_i}\}$, then we get

$$\Psi(\boldsymbol{R}_1, \cdots, \boldsymbol{R}_n) = \frac{1}{\sqrt{A!}} \det\{\varphi_{\sigma_1,1} \cdots \varphi_{\sigma_1,N_1}, \varphi_{\sigma_2,1} \cdots \varphi_{\sigma_2,N_2}, \cdots, \varphi_{\sigma_n,1} \cdots \varphi_{\sigma_n,N_n}\}. \qquad (2\cdot1\cdot3)$$

The H.O. shell model wave function $\psi(C_i, \boldsymbol{R}_i)$ can be written as[7),28)]

$$\psi(C_i, \boldsymbol{R}_i) = \left(\frac{2N_i\nu_i}{\pi}\right)^{3/4} \exp\{-N_i\nu_i(\boldsymbol{X}_i-\boldsymbol{R}_i)^2\} \cdot \phi(C_i), \qquad (2\cdot1\cdot4)$$

where $\boldsymbol{X}_i=$center-of-mass (C.M.) coordinate of C_i and $\phi(C_i)$ is the internal wave function of C_i which does not depend on $\boldsymbol{X}_i$. We therefore have

$$\Psi(\boldsymbol{R}_1, \cdots, \boldsymbol{R}_n) = n_0 \left\{\prod_{i=1}^{n} \left(\frac{2N_i\nu_i}{\pi}\right)^{3/4}\right\} \times \mathcal{A}[\exp\{-\sum_{i=1}^{n} N_i\nu_i(\boldsymbol{X}_i-\boldsymbol{R}_i)^2\} \phi(C_1) \cdots \phi(C_n)]. \qquad (2\cdot1\cdot5)$$

To see the relative motion of clusters it is convenient to use the inter-cluster relative coordinates $\boldsymbol{\xi}_i$ ($i=1\sim n-1$) and the total center-of-mass (C.M.) coordinate $\boldsymbol{X}_G$. An important case is when all the oscillator parameters ν_i are equal $\nu=\nu_1=\cdots=\nu_n$. In this case the dependence on $\boldsymbol{X}_G$ is factored out and therefore $\Psi(\boldsymbol{R}_1, \cdots, \boldsymbol{R}_n)$ is a non-spurious wave function about the center-of-mass (C.M.) motion. If we adopt as $\boldsymbol{\xi}_i$ the Jacobi coordinates, we obtain

$$\nu\sum_i N_i(\boldsymbol{X}_i-\boldsymbol{R}_i)^2=A\nu(\boldsymbol{X}_G-\boldsymbol{R}_G)^2+\frac{N_1N_2}{N_1+N_2}\nu(\boldsymbol{\xi}_1-\boldsymbol{S}_1)^2$$
$$+\frac{(N_1+N_2)N_3}{N_1+N_2+N_3}\nu(\boldsymbol{\xi}_2-\boldsymbol{S}_2)^2+\cdots,$$
$$\boldsymbol{X}_G\equiv(\sum^n N_i\boldsymbol{X}_i)/A,\quad \boldsymbol{\xi}_1\equiv\boldsymbol{X}_2-\boldsymbol{X}_1,\quad \boldsymbol{\xi}_2\equiv\boldsymbol{X}_3-\frac{N_1\boldsymbol{X}_1+N_2\boldsymbol{X}_2}{N_1+N_2},\quad\cdots,$$
$$\boldsymbol{R}_G\equiv(\sum^n N_i\boldsymbol{R}_i)/A,\quad \boldsymbol{S}_1\equiv\boldsymbol{R}_2-\boldsymbol{R}_1,\quad \boldsymbol{S}_2\equiv\boldsymbol{R}_3-\frac{N_1\boldsymbol{R}_1+N_2\boldsymbol{R}_2}{N_1+N_2},\quad\cdots, \tag{2·1·6}$$

and so Ψ is expressed as

$$\Psi(\boldsymbol{R}_1,\cdots,\boldsymbol{R}_n)=\left(\frac{2A\nu}{\pi}\right)^{3/4}\exp\{-A\nu(\boldsymbol{X}_G-\boldsymbol{R}_G)^2\}$$
$$\times n_0\mathcal{A}\{\prod_{i=1}^{n-1}\Gamma(\boldsymbol{\xi}_i,\boldsymbol{S}_i,\gamma_i)\prod_{i=1}^{n}\phi(C_i)\},$$
$$\Gamma(\boldsymbol{\xi},\boldsymbol{S},\gamma)\equiv\left(\frac{2\gamma}{\pi}\right)^{3/4}\exp\{-\gamma(\boldsymbol{\xi}-\boldsymbol{S})^2\},$$
$$\gamma_1\equiv\frac{N_1N_2}{N_1+N_2}\nu,\quad \gamma_2\equiv\frac{(N_1+N_2)N_3}{N_1+N_2+N_3}\nu,\quad\cdots. \tag{2·1·7}$$

When ν_i are different from each other, the C.M. coordinate $\boldsymbol{X}_G$ does not separate and so Ψ necessarily contains the spurious component of the C.M. motion. For example, for two-cluster system

$$N_1\nu_1(\boldsymbol{X}_1-\boldsymbol{R}_1)^2+N_2\nu_2(\boldsymbol{X}_2-\boldsymbol{R}_2)^2=\alpha(\boldsymbol{X}_G-\boldsymbol{R}_G)^2+\beta(\boldsymbol{X}_G-\boldsymbol{R}_G)\cdot(\boldsymbol{r}-\boldsymbol{R})+\gamma(\boldsymbol{r}-\boldsymbol{R})^2,$$
$$\alpha=N_1\nu_1+N_2\nu_2,\quad \beta=\frac{2N_1N_2}{N_1+N_2}(\nu_2-\nu_1),\quad \gamma=\frac{N_1N_2}{(N_1+N_2)^2}(N_2\nu_1+N_1\nu_2),$$
$$\boldsymbol{r}\equiv\boldsymbol{\xi}_1=\boldsymbol{X}_2-\boldsymbol{X}_1,\quad \boldsymbol{R}\equiv\boldsymbol{S}_1=\boldsymbol{R}_2-\boldsymbol{R}_1. \tag{2·1·8}$$

The term $\exp\{\beta(\boldsymbol{X}_G-\boldsymbol{R}_G)(\boldsymbol{r}-\boldsymbol{R})\}$ causes the contamination of the spurious C.M. excitation.

Since we are not interested in the C.M. motion, the GCM wave function Ψ^{GCM} is a superposition of $\Psi(\boldsymbol{R}_1,\cdots,\boldsymbol{R}_n)$ with respect to $\boldsymbol{S}_1,\cdots,\boldsymbol{S}_{n-1}$,

$$\Psi^{\mathrm{GCM}}=\int\prod_{i=1}^{n-1}d\boldsymbol{S}_i f(\boldsymbol{S}_1,\cdots,\boldsymbol{S}_{n-1})\Psi(\boldsymbol{R}_1,\cdots,\boldsymbol{R}_n), \tag{2·1·9}$$

where usually $A\boldsymbol{R}_G=\sum N_i\boldsymbol{R}_i=0$. When the oscillator parameters ν_i are different from each other, Ψ^{GCM} contains the spurious C.M. excitation and so it is desirable to project out the C.M. spurious component of $\Psi(\boldsymbol{R}_1,\cdots,\boldsymbol{R}_n)$. The weight function f of Eq. (2·1·9) is determined by the Griffin-Hill-Wheeler (GHW) equation,[19]

$$\int\prod_{i=1}^{n-1}dS_i'\{H(S_1,\cdots,S_{n-1};S_1',\cdots,S_{n-1}')-EN(S_1,\cdots,S_{n-1};S_1',\cdots,S_{n-1}')\}$$
$$\times f(S_1',\cdots,S_{n-1}')=0\,,$$
$$\begin{Bmatrix}H(S_1,\cdots;S_1',\cdots)\\N(S_1,\cdots;S_1',\cdots)\end{Bmatrix}=\langle\Psi(\boldsymbol{R}_1,\cdots,\boldsymbol{R}_n)|\begin{Bmatrix}H\\1\end{Bmatrix}|\Psi(\boldsymbol{R}_1',\cdots,\boldsymbol{R}_n')\rangle\,,\quad(2\cdot1\cdot10)$$

where H is the Hamiltonian.

The matrix element of the operator $\mathcal{O}$ with the GCM wave function of Eq. (2·1·9) is

$$\langle\Psi_1^{\mathrm{GCM}}|\mathcal{O}|\Psi_2^{\mathrm{GCM}}\rangle=\int(\prod_{i=1}^{n-1}dS_i)(\prod_{i=1}^{n-1}dS_i')f_1^*(S_1,\cdots,S_{n-1})$$
$$\times f_2(S_1',\cdots,S_{n-1}')\mathcal{O}(\boldsymbol{R}_G,S_1,\cdots;\boldsymbol{R}_G',S_1',\cdots),$$
$$\mathcal{O}(\boldsymbol{R}_G,S_1,\cdots;\boldsymbol{R}_G',S_1',\cdots)$$
$$\equiv\langle\psi(C_1,\boldsymbol{R}_1)\cdots\psi(C_n,\boldsymbol{R}_n)|\mathcal{O}|\mathcal{A}\{\psi(C_1,\boldsymbol{R}_1')\cdots\psi(C_n,\boldsymbol{R}_n')\}\rangle.\quad(2\cdot1\cdot11)$$

$\mathcal{O}$ is called the GCM (integral) kernel of the operator $\mathcal{O}$. When the G.C. $\boldsymbol{R}_i$ are so chosen as to satisfy $\boldsymbol{R}_G=\sum N_i\boldsymbol{R}_i/A=0$ we use the notation $\mathcal{O}(S_1,\cdots;\boldsymbol{R}_G',S_1',\cdots)$ instead of $\mathcal{O}(\boldsymbol{R}_G=0,S_1,\cdots;\boldsymbol{R}_G',S_1',\cdots)$ and similarly for the case of $\boldsymbol{R}_G'=0$ we use $\mathcal{O}(\boldsymbol{R}_G,S_1,\cdots;S_1',\cdots)$ instead of $\mathcal{O}(\boldsymbol{R}_G,S_1,\cdots;\boldsymbol{R}_G'=0,S_1',\cdots)$. It is convenient for the later discussion to define the kernel M by

$$M(S_1,\cdots,S_{n-1};S_1',\cdots,S_{n-1}')$$
$$\equiv\langle\prod_{i=1}^{n-1}\Gamma(\xi_i,S_i,\gamma_i)\prod_{i=1}^{n}\phi(C_i)|\mathcal{O}|\mathcal{A}\{\prod_{i=1}^{n-1}\Gamma(\xi_i,S_i',\gamma_i)\prod_{i=1}^{n}\phi(C_i)\}\rangle.\quad(2\cdot1\cdot12)$$

The physical operator $\mathcal{O}$ does not contain the C.M. coordinate $\boldsymbol{X}_G$. So for the system with equal oscillator parameters $\nu=\nu_i$ $(i=1\sim n)$ the integration with respect to $\boldsymbol{X}_G$ can be done independently of $\mathcal{O}$ and we obtain

$$\mathcal{O}(\boldsymbol{R}_G,S_1,\cdots;\boldsymbol{R}_G',S_1',\cdots)=\exp\left\{-\frac{1}{2}A\nu(\boldsymbol{R}_G-\boldsymbol{R}_G')^2\right\}M(S_1,\cdots;S_1',\cdots),$$
$$\mathcal{O}(S_1,\cdots;S_1',\cdots)=M(S_1,\cdots;S_1',\cdots)\quad\text{for }\nu_i=\nu\ (i=1\sim n).\quad(2\cdot1\cdot13)$$

For the case of the two-cluster system, $\mathcal{O}(\boldsymbol{R};\boldsymbol{R}')$ and $M(\boldsymbol{R};\boldsymbol{R}')$ are denoted by $\mathcal{O}(\boldsymbol{R},\boldsymbol{R}')$ and $M(\boldsymbol{R},\boldsymbol{R}')$ respectively and if it is necessary to show explicitly the oscillator parameter γ of $\langle\Gamma(\boldsymbol{r},\boldsymbol{R},\gamma)\phi(C_1)\phi(C_2)|\mathcal{O}|\mathcal{A}\{\Gamma(\boldsymbol{r},\boldsymbol{R}',\gamma)\times\phi(C_1)\phi(C_2)\}\rangle(\boldsymbol{r}\equiv\boldsymbol{\xi}_1=\boldsymbol{X}_2-\boldsymbol{X}_1)$ we denote $M(\boldsymbol{R},\boldsymbol{R}')$ by $M_\gamma(\boldsymbol{R},\boldsymbol{R}')$.

The GCM kernels are often divided into the direct and exchange kernels as follows,

$$\mathcal{O}=\mathcal{O}^D+\mathcal{O}^E\,,\quad M=M^D+M^E\,,$$
$$\mathcal{O}^D(\boldsymbol{R}_G,S_1,\cdots;\boldsymbol{R}_G',S_1',\cdots)$$
$$\equiv\langle\psi(C_1,\boldsymbol{R}_1)\cdots\psi(C_n,\boldsymbol{R}_n)|\mathcal{O}|\psi(C_1,\boldsymbol{R}_1')\cdots\psi(C_n,\boldsymbol{R}_n')\rangle,$$

$$M^{D}(\boldsymbol{S}_1, \cdots; \boldsymbol{S}_1', \cdots)$$
$$\equiv\langle\prod_{i=1}^{n-1} \Gamma(\boldsymbol{\xi}_i, \boldsymbol{S}_i, \gamma_i)\prod_{i=1}^{n}\phi(C_i)\,|\mathcal{O}|\prod_{i=1}^{n-1}\Gamma(\boldsymbol{\xi}_i, \boldsymbol{S}_i', \gamma_i)\prod_{i=1}^{n}\phi(C_i)\rangle\,. \quad (2\cdot1\cdot14)$$

When we treat the system with definite angular momentum, we need to project out the definite angular momentum components from $\Psi(\boldsymbol{R}_1, \cdots, \boldsymbol{R}_n)$. Let us consider the non-spurious $\Psi(\boldsymbol{R}_1, \cdots, \boldsymbol{R}_n)$ with $\nu_i=\nu(i=1\sim n)$ of the system of spin-zero clusters. A projection procedure of the angular momentum is given by

$$\int\prod_{i=1}^{n-1} d\hat{S}_i Y_{LM,\alpha}(\hat{S}_1, \cdots, \hat{S}_{n-1})\Psi(\boldsymbol{R}_1, \cdots, \boldsymbol{R}_n)$$
$$=n_0\mathcal{A}\{\prod_{i=1}^{n-1}\Gamma_{L_i}(\xi_i, S_i, \gamma_i)\,h_{LM,\alpha}\}\,\omega_0(\boldsymbol{X}_G),$$

$$h_{LM,\alpha}\equiv Y_{LM,\alpha}(\hat{\xi}_1, \cdots, \hat{\xi}_{n-1})\prod_{i=1}^{n}\phi_0(C_i),$$

$$Y_{LM,\alpha}(\hat{\eta}_1, \cdots, \hat{\eta}_{n-1})\equiv[\cdots[[Y_{L_1}(\hat{\eta}_1)\,Y_{L_2}(\hat{\eta}_2)]_{L_{12}}Y_{L_3}(\hat{\eta}_3)]_{L_{123}}\cdots]_{LM},$$

$$\Gamma_L(\xi, S, \gamma)\equiv\left(\frac{2\gamma}{\pi}\right)^{3/4}4\pi i_L(2\gamma\xi S)\exp\{-\gamma(\xi^2+S^2)\},$$

$$\omega_0(\boldsymbol{X}_G)\equiv\left(\frac{2A\nu}{\pi}\right)^{3/4}\exp\{-A\nu\boldsymbol{X}_G^2\}, \quad (2\cdot1\cdot15)$$

where α stands for the set of quantum numbers $(L_i, L_{12}, L_{123}\cdots)$ and we assumed $\boldsymbol{R}_G=\sum N_i\boldsymbol{R}_i/A=0$. The systems which have non-zero spin clusters are treated similarly. In the simplest case of the two-cluster system with one non-zero spin cluster C_1, the generating wave function is

$$\int d\hat{R}\left[Y_{L_1}(\hat{R})\,\mathcal{A}\left\{\phi_{L_2}\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right)\right\}\right]_{JM}$$
$$=\mathcal{A}\{\Gamma_{L_1}(r, R, \gamma)\,[Y_{L_1}(\hat{r})\,\phi_{L_2}(C_1)]_{JM}\phi_0(C_2)\}\,\omega_0(\boldsymbol{X}_G). \quad (2\cdot1\cdot16)$$

For the system composed of two spin-zero clusters, the projection of relative angular momentum by $\int d\hat{R}Y_{LM}(\hat{R})$ is of course equivalent to the usual projection of the total angular momentum

$$\int d\hat{R}Y_{LM}(\hat{R})\,\Psi\left(\frac{-N_2}{A}\boldsymbol{R}, \frac{N_1}{A}\boldsymbol{R}\right)$$
$$=(\text{constant})\times\int d\Omega D_{M0}^{L*}(\Omega)\,R(\Omega)\,\Psi\left(\frac{-N_2}{A}\boldsymbol{R}, \frac{N_1}{A}\boldsymbol{R}\right),$$

$$R(\Omega)\equiv\exp\{-i\theta_1J_z\}\exp\{-i\theta_2J_y\}\exp\{-i\theta_3J_z\}\,. \quad (2\cdot1\cdot17)$$

The GCM kernels corresponding to these wave functions with definite angular momentum are obtained by the angular momentum projection of the kernels $\mathcal{H}$. For the system with the generating wave function of Eq.

(2·1·15),

$$\Theta^{\alpha_1\alpha_2}_{L_1M_1L_2M_2}(S_1,\cdots,S_{n-1};S_1',\cdots,S_{n-1}')$$
$$=\int(\prod_{i=1}^{n-1}d\hat{S}_i)(\prod_{i=1}^{n-1}d\hat{S}_i')Y^*_{L_1M_1,\alpha_1}(\hat{S}_1,\cdots)Y_{L_2M_2,\alpha_2}(\hat{S}_1',\cdots)\Theta(\boldsymbol{S}_1,\cdots;\boldsymbol{S}_1',\cdots). \tag{2·1·18}$$

The angular momentum projection of the kernel for the channel coupling case is treated similarly. We consider the system with the generating wave functions of Eq. (2·1·16). Usually the wave function of the cluster C_1 is expressed by the projection of the angular momentum from a single Slater determinant

$$\psi_{LM}(C_1,\boldsymbol{R}_1=0)=C_L\int d\Omega D^{L*}_{M,0}(\Omega)\psi^\Omega(C_1,\boldsymbol{R}_1=0),$$
$$\psi^\Omega(C_1,\boldsymbol{R}_1=0)\equiv R(\Omega)\psi(C_1,\boldsymbol{R}_1=0), \tag{2·1·19}$$

where we assumed for simplicity the axial symmetry of the intrinsic state $\psi(C_1,\boldsymbol{R}_1=0)$ around z axis. Then the kernel is

$$\Theta^{JMJ'M'}_{i,j}(R,R')=C_{L_2}C_{L_2'}\int d\hat{R}d\hat{R}'d\Omega d\Omega'$$
$$\times[Y_{L_1}(\hat{R})D^{L_2*}_{0,0}(\Omega)]^*_{JM}[Y_{L_1'}(\hat{R}')D^{L_2'*}_{0,0}(\Omega')]_{J'M'}$$
$$\times\left\langle\psi^\Omega\left(C_1,\frac{-N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2,\frac{N_1}{A}\boldsymbol{R}\right)|\mathcal{O}|\mathcal{A}\left\{\psi^{\Omega'}\left(C_1,\frac{-N_2}{A}\boldsymbol{R}'\right)\phi_0\left(C_2,\frac{N_1}{A}\boldsymbol{R}'\right)\right\}\right\rangle, \tag{2·1·20}$$

where $i\equiv(L_1,L_2)$ and $j\equiv(L_1',L_2')$. When the SU_3 shell model wave function[20),21)] is adopted for $\psi_{L_2}(C_1)$, the projection procedure of Eq. (2·1·19) becomes simpler. If the SU_3 symmetry (λ,μ) of $\psi_{L_2}(C_1)$ is $(N,0)$ or $(0,N)$, we have[15),20),21)]

$$\psi(C_1,\boldsymbol{R})=\sum_L A^N_L\psi_{L0}(C_1,\boldsymbol{R}),$$
$$\psi^\Omega(C_1,\boldsymbol{R})=\sum_{LM}A^N_L\sqrt{\frac{4\pi}{2L+1}}Y^*_{LM}(\Omega)\psi_{LM}(C_1,\boldsymbol{R}),$$
$$A^N_L\equiv(-)^{(N-L)/2}\sqrt{\frac{(2L+1)\cdot N!}{(N-L)!!(N+L+1)!!}},\quad \Omega\equiv(\theta_1,\theta_2). \tag{2·1·21}$$

When we treat the system including rearrangement channels, the GCM wave function has the following form:

$$\Psi^{\mathrm{GCM}}=\sum_\alpha\int d\boldsymbol{S}_\alpha f_\alpha(\boldsymbol{S}_\alpha)\frac{1}{\sqrt{\binom{A}{N_{\alpha1}}}}\mathcal{A}_\alpha\left\{\psi\left(C_{\alpha1},\frac{-N_{\alpha2}}{A}\boldsymbol{S}_\alpha\right)\psi\left(C_{\alpha2},\frac{N_{\alpha1}}{A}\boldsymbol{S}_\alpha\right)\right\}, \tag{2·1·22}$$

where the suffices of $\mathcal{A}_\alpha$ are put in order to remark their difference between different channels. ($\mathcal{A}_\alpha$ is composed of $\binom{A}{N_{\alpha 1}}$ terms of the permutation operators.) The GCM kernels necessary for this system are

$$\Theta_{\alpha,\beta}(\boldsymbol{S}_\alpha, \boldsymbol{S}_\beta) \equiv \frac{1}{\sqrt{\binom{A}{N_{\alpha 1}}\binom{A}{N_{\beta 1}}}} \left\langle \mathcal{A}_\alpha \left\{ \psi\left(C_{\alpha 1}, \frac{-N_{\alpha 2}}{A}\boldsymbol{S}_\alpha\right)\psi\left(C_{\alpha 2}, \frac{N_{\alpha 1}}{A}\boldsymbol{S}_\alpha\right)\right\} | \mathcal{O} \right.$$
$$\left. \times | \mathcal{A}_\beta \left\{ \psi\left(C_{\beta 1}, \frac{-N_{\beta 2}}{A}\boldsymbol{S}_\beta\right)\psi\left(C_{\beta 2}, \frac{N_{\beta 1}}{A}\boldsymbol{S}_\beta\right)\right\} \right\rangle. \qquad (2\cdot1\cdot23)$$

The kernels for $\alpha \neq \beta$ are new type of kernels while the diagonal kernels $\Theta_{\alpha,\alpha}(\boldsymbol{S}_\alpha, \boldsymbol{S}_\alpha')$ are of type of Eq. (2·1·11). With these kernels the matrix element of the operator $\mathcal{O}$ by Ψ^{GCM} and $\tilde{\Psi}^{\mathrm{GCM}}$ is given by $\langle \Psi^{\mathrm{GCM}} | \mathcal{O} | \tilde{\Psi}^{\mathrm{GCM}} \rangle = \sum_{\alpha,\beta} \langle f_\alpha | \Theta_{\alpha\beta} | \tilde{f}_\beta \rangle$. When $\psi(C_i, \boldsymbol{R}_i)$ has a form of Eq. (2·1·2) these kernels are rewritten as

$$\Theta_{\alpha,\beta}(\boldsymbol{S}_\alpha, \boldsymbol{S}_\beta) = \langle \varphi_{\sigma_{\alpha 1,1}} \cdots \varphi_{\sigma_{\alpha 2,1}} \cdots | \mathcal{O} | \det\{\varphi_{\sigma_{\beta 1,1}} \cdots \varphi_{\sigma_{\beta 2,1}} \cdots\} \rangle \qquad (2\cdot1\cdot24)$$

because $(1/\sqrt{\binom{A}{N_{\alpha 1}}})\mathcal{A}_\alpha\{\psi(C_{\alpha 1}, (-N_{\alpha 2}/A)\boldsymbol{S}_\alpha)\psi(C_{\alpha 2}, (N_{\alpha 1}/A)\boldsymbol{S}_\alpha)\}$ is written as $(1/\sqrt{A!})\det\{\varphi_{\sigma_{\alpha 1,1}} \cdots \varphi_{\sigma_{\alpha 2,1}} \cdots\}$ as is shown in Eq. (2·1·3). In the case of the common oscillator parameters $\nu = \nu_{\alpha 1} = \nu_{\alpha 2}$, $\Theta_{\alpha,\beta}(\boldsymbol{S}_\alpha, \boldsymbol{S}_\beta) = (1/\sqrt{\binom{A}{N_{\alpha 1}}\binom{A}{N_{\beta 1}}}) \times \langle \mathcal{A}_\alpha\{\Gamma(\boldsymbol{r}_\alpha, \boldsymbol{S}_\alpha, \gamma_\alpha)\phi(C_{\alpha 1})\phi(C_{\alpha 2})\} | \mathcal{O} | \mathcal{A}_\beta\{\Gamma(\boldsymbol{r}_\beta, \boldsymbol{S}_\beta, \gamma_\beta)\phi(C_{\beta 1})\phi(C_{\beta 2})\}\rangle$. The direct part of the kernels $\Theta_{\alpha,\beta}$ which are denoted by $\Theta^D_{\alpha,\beta}$ are defined by Eq. (2·1·23) by dropping $(1/\sqrt{\binom{A}{N_{\alpha 1}}})\mathcal{A}_\alpha$ and $(1/\sqrt{\binom{A}{N_{\beta 1}}})\mathcal{A}_\beta$. The projection problem of the angular momentum can be treated in a similar way to before.

When treating the interaction between clusters it is sometimes necessary to evaluate the GCM kernel of the interaction operator

$$V_r = \sum_{i \in C_1} \sum_{j \in C_2} V_{ij} \qquad (2\cdot1\cdot25)$$

which is not totally symmetric. We define the GCM kernel Θ^r corresponding to this operator as follows:

$$\Theta^r(\boldsymbol{R}_G, \boldsymbol{R}; \boldsymbol{R}_G', \boldsymbol{R}')$$
$$\equiv \langle \psi(C_1, \boldsymbol{R}_1)\psi(C_2, \boldsymbol{R}_2) | V_r | \mathcal{A}\{\psi(C_1, \boldsymbol{R}_1')\psi(C_2, \boldsymbol{R}_2')\}\rangle. \qquad (2\cdot1\cdot26)$$

2.1.b. *Complex GCM*

In the above the generator coordinates (GC) $\boldsymbol{R}_i$ or $\boldsymbol{S}_i$, $\boldsymbol{R}_G$ are assumed to be real numbers. As is well known, the GCM with real number GC (which we call real-GCM or R-GCM) has difficulties[22] such as the violent behaviour of the weight function f of Eq. (2·1·9) obtained by solving the Griffin-Hill-Wheeler (GHW) equation of Eq. (2·1·10). The extension of the GC to the complex number[16),22)~27)] resolves these difficulties of R-GCM. For the sake of simplicity we consider the two-cluster system. The oscillator parameters are taken to be the same, $\nu_1 = \nu_2 = \nu$, in order to avoid the C.M. spurious problem. In the R-GCM,

$$\Psi^{\text{R-GCM}}=\frac{1}{\sqrt{\binom{A}{N_1}}}\int d\boldsymbol{R} f(\boldsymbol{R})\mathcal{A}\{\Gamma(\boldsymbol{r},\boldsymbol{R},\gamma)\phi(C_1)\phi(C_2)\}\omega_0(\boldsymbol{X}_G), \quad (2\cdot1\cdot27)$$

while in C-GCM we adopt the following form,[16]

$$\Psi^{\text{C-GCM}}=\frac{1}{\sqrt{\binom{A}{N_1}}}\int d\mu(\boldsymbol{z}) f(\boldsymbol{z})\mathcal{A}\{A_\gamma^*(\boldsymbol{r},\boldsymbol{z})\phi(C_1)\phi(C_2)\}\omega_0(\boldsymbol{X}_G), \quad (2\cdot1\cdot28)$$

where[29]

$$A_\gamma(\boldsymbol{r},\boldsymbol{z})\equiv\left(\frac{2\gamma}{\pi}\right)^{3/4}\exp\left\{-\gamma\left(\boldsymbol{r}-\frac{\boldsymbol{z}}{\sqrt{\gamma}}\right)^2+\frac{1}{2}\boldsymbol{z}^2\right\}$$
$$=\exp\left\{\frac{1}{2}\boldsymbol{z}^2\right\}\Gamma\left(\boldsymbol{r},\frac{\boldsymbol{z}}{\sqrt{\gamma}},\gamma\right),$$
$$d\mu(\boldsymbol{z})\equiv\prod_{i=1}^{3}\frac{1}{\pi}e^{-|z_i|^2}d[\mathrm{Re}(z_i)]d[\mathrm{Im}(z_i)]. \quad (2\cdot1\cdot29)$$

The kernels in C-GCM are obtained simply by replacing the real GC $\boldsymbol{R}$ by complex GC $\boldsymbol{z}^*/\sqrt{\gamma}$. $A_\gamma(\boldsymbol{r},\boldsymbol{z})$ is the so-called coherent[30),31)] state and can be expressed as follows:

$$A_\gamma(\boldsymbol{r},\boldsymbol{z})=e^{\boldsymbol{z}\cdot\boldsymbol{a}^\dagger}W_0(\boldsymbol{r}),$$
$$W_0(\boldsymbol{r})\equiv\left(\frac{2\gamma}{\pi}\right)^{3/4}e^{-\gamma r^2}, \quad \boldsymbol{a}^\dagger\equiv\sqrt{\gamma}\left(\boldsymbol{r}-\frac{i}{2\hbar\gamma}\boldsymbol{p}\right),$$
$$\boldsymbol{p}\equiv-i\hbar\frac{\partial}{\partial\boldsymbol{r}}. \quad (2\cdot1\cdot30)$$

Using the identity $\exp(\boldsymbol{z}\cdot\boldsymbol{a}^\dagger)\exp(-\boldsymbol{z}^*\cdot\boldsymbol{a})=\exp(\boldsymbol{z}\cdot\boldsymbol{z}^*/2)\exp(\boldsymbol{z}\cdot\boldsymbol{a}^\dagger-\boldsymbol{z}^*\boldsymbol{a})$, we obtain

$$A_\gamma(\boldsymbol{r},\boldsymbol{z})=\exp\left\{\frac{1}{2}\boldsymbol{z}\cdot\boldsymbol{z}^*\right\}\exp\{\boldsymbol{z}\cdot\boldsymbol{a}^\dagger-\boldsymbol{z}^*\cdot\boldsymbol{a}\}W_0(\boldsymbol{r}). \quad (2\cdot1\cdot31)$$

By expressing $\boldsymbol{z}$ as a sum of real and imaginary parts as follows,

$$\boldsymbol{z}=\sqrt{\gamma}\left(\boldsymbol{R}+\frac{i}{2\hbar\gamma}\boldsymbol{P}\right),$$
$$\mathrm{Re}(\boldsymbol{z})=\sqrt{\gamma}\,\boldsymbol{R}, \quad \mathrm{Im}(\boldsymbol{z})=\frac{1}{2\hbar\sqrt{\gamma}}\boldsymbol{P}, \quad (2\cdot1\cdot32)$$

we get[27)]

$$A_\gamma(\boldsymbol{r},\boldsymbol{z})=\exp\left\{\frac{1}{2}\boldsymbol{z}\cdot\boldsymbol{z}^*\right\}\exp\left\{\frac{i}{\hbar}(\boldsymbol{P}\cdot\boldsymbol{r}-\boldsymbol{R}\cdot\boldsymbol{p})\right\}W_0(\boldsymbol{r})$$

$$=\left(\frac{2\gamma}{\pi}\right)^{3/4}\exp\left\{-\gamma(\boldsymbol{r}-\boldsymbol{R})^2+\frac{i}{\hbar}\boldsymbol{P}\cdot(\boldsymbol{r}-\boldsymbol{R})\right\}\cdot\exp\left\{\frac{P^2}{4\hbar^2\gamma}+\frac{1}{2}\boldsymbol{z}^2\right\},$$

$$d\mu(\boldsymbol{z})=\left(\frac{1}{2\pi\hbar}\right)^3 e^{-\boldsymbol{z}\cdot\boldsymbol{z}^*}d\boldsymbol{R}d\boldsymbol{P}. \qquad (2\cdot1\cdot33)$$

Noting the normalization of A_γ given by $\langle A_\gamma|A_\gamma\rangle\equiv\int d\boldsymbol{r}A_\gamma(\boldsymbol{r},\boldsymbol{z})A_\gamma^*(\boldsymbol{r},\boldsymbol{z})=\exp(\boldsymbol{z}\cdot\boldsymbol{z}^*)$, we obtain

$$\frac{\langle A_\gamma|\boldsymbol{r}|A_\gamma\rangle}{\langle A_\gamma|A_\gamma\rangle}=\boldsymbol{R},\quad \frac{\langle A_\gamma|\boldsymbol{p}|A_\gamma\rangle}{\langle A_\gamma|A_\gamma\rangle}=\boldsymbol{P}. \qquad (2\cdot1\cdot34)$$

Equations (2·1·32)$\sim$(2·1·34) show that the extension of the real GC to the complex GC means the extension of the wave packet at rest $\Gamma(\boldsymbol{r},\boldsymbol{R},\gamma)$ to the moving wave packet $A_\gamma(\boldsymbol{r},\boldsymbol{z})$.

2.2. Calculation of GCM kernels

2.2.a. *General prescription*

We treat the calculation of the GCM kernel when $\psi(C_i,\boldsymbol{R}_i)$ is expressed by Eq. (2·1·2). When we use the fully antisymmetrized wave function, the GCM kernel is a matrix element of an operator $\mathcal{O}$ by two Slater determinants. The GCM kernel $\mathcal{H}$ of Eq. (2·1·11) is written, by Eq. (2·1·3), as

$$\mathcal{H}(\boldsymbol{R}_G,\boldsymbol{S}_1,\cdots;\boldsymbol{R}_G',\boldsymbol{S}_1',\cdots)=\langle\varphi_{\sigma_1,1}\cdots\varphi_{\sigma_2,1}\cdots\varphi_{\sigma_n,N_n}|\mathcal{O}|\det\{\varphi'_{\sigma_1,1}\cdots\varphi'_{\sigma_2,1}\cdots\varphi'_{\sigma_n,N_n}\}\rangle, \qquad (2\cdot2\cdot1)$$

where $\varphi_{\sigma_i,J}\equiv\varphi_{\sigma_i}(\boldsymbol{x}_j-\boldsymbol{R}_i)$, $\varphi'_{\sigma_i,J}\equiv\varphi_{\sigma_i}(\boldsymbol{x}_j-\boldsymbol{R}_i')$. The coupling kernels between rearranged channels have the similar form as above as is shown in Eq. (2·1·21).

The evaluation of the matrix element of an operator with the use of Slater determinants composed of the non-orthogonal single particle orbitals is a well investigated problem.[18] For the sake of the discussion in this section, we first remind the reader of the Laplace expansion of a general determinant,

$$\det\{a_{ij}\}=\sum(-)^{\sum_{i=1}^{r}(k_i+l_i)}A\begin{pmatrix}k_1,k_2,\cdots,k_r\\ l_1,l_2,\cdots,l_r\end{pmatrix}B\begin{pmatrix}k_1,k_2,\cdots,k_r\\ l_1,l_2,\cdots,l_r\end{pmatrix},$$

$$\sum=\sum_{(k_1,k_2,\cdots,k_r)}\quad\text{or}\quad\sum_{(l_1,l_2,\cdots,l_r)}, \qquad (2\cdot2\cdot2)$$

where $(k_1,k_2,\cdots,k_r)$ and $(l_1,l_2,\cdots,l_r)$ are any sets of r numbers chosen from $(1,2,\cdots,n)$ satisfying $k_1<k_2\cdots<k_r$, $l_1<l_2<\cdots<l_r$, and $A\binom{k_1,k_2,\cdots,k_r}{l_1,l_2,\cdots,l_r}$ is a minor determinant composed by adopting k_1, k_2, $\cdots k_r$ rows and l_1, l_2, $\cdots$, l_r columns from the original matrix a_{ij},

$$A\begin{pmatrix}k_1,k_2,\cdots,k_r\\ l_1,l_2,\cdots,l_r\end{pmatrix}\equiv\begin{vmatrix}a_{k_1l_1}a_{k_1l_2}\cdots\cdots a_{k_1l_r}\\ \vdots\qquad\qquad\vdots\\ a_{k_rl_1}\cdots\cdots\cdots a_{k_rl_r}\end{vmatrix}, \qquad (2\cdot2\cdot3)$$

while $B\binom{k_1,k_2,\cdots,k_r}{l_1,l_2,\cdots,l_r}$ is a complementary minor determinant composed of remaining

rows and columns of a_{ij} other than used in A. When $r=1$,

$$\det\cdot a=\det\{a_{ij}\}=\sum_k a_{kl}C_{kl}=\sum_l a_{kl}C_{kl}\,,$$

$$C_{kl}\equiv(-)^{k+l}B\binom{k}{l}, \tag{2·2·4}$$

and C_{kl} satisfies

$$\sum_k a_{kl}C_{kl'}=(\det\cdot a)\,\delta_{l,l'}\,, \tag{2·2·5}$$

since if we use the notation $\det\{a_{ij}\}=\det\{\boldsymbol{a}_1,\boldsymbol{a}_2,\cdots,\boldsymbol{a}_n\}$ with $\boldsymbol{a}_i=(a_{1i},a_{2i},\cdots,a_{ni})$, $\sum_k a_{kl}C_{kl'}$ with $l\neq l'$ is just equal to $\det\{\boldsymbol{a}_1,\cdots,\boldsymbol{a}_n\}$ where $\boldsymbol{a}_{l'}$ is replaced by $\boldsymbol{a}_l$ and therefore vanishes. Equation (2·2·5) means for $\det\{a_{ij}\}\neq 0$

$$C_{kl}=(\det\cdot a)\,(a^{-1})_{lk}\,,$$

$$B\binom{k}{l}=(\det\cdot a)\,(-)^{l+k}(a^{-1})_{lk}\,, \tag{2·2·6}$$

where $(a^{-1})_{lk}$ are components of the inverse matrix of the matrix $\{a_{ij}\}$. Generally we can express $B\binom{k_1,k_2,\cdots,k_r}{l_1,l_2,\cdots,l_r}$ *in terms of* a^{-1} as follows:

$$B\begin{pmatrix}k_1,k_2,\cdots,k_r\\ l_1,l_2,\cdots,l_r\end{pmatrix}=(\det\cdot a)\,(-)^{\sum_{i=1}^{r}(k_i+l_i)}\begin{vmatrix}(a^{-1})_{l_1k_1}&\cdots\cdots&(a^{-1})_{l_1k_r}\\ \vdots&&\vdots\\ (a^{-1})_{l_rk_1}&\cdots\cdots&(a^{-1})_{l_rk_r}\end{vmatrix}, \tag{2·2·7}$$

which is known as the Jacobi formula and is proved in Appendix A. 1. The Laplace expansion for $r=2$, therefore, becomes

$$\det\{a_{ij}\}=\sum\begin{vmatrix}a_{k_1l_1}a_{k_1l_2}\\ a_{k_2l_1}a_{k_2l_2}\end{vmatrix}C(k_1k_2,l_1l_2),$$

$$\sum=\sum_{k_1<k_2}\quad\text{or}\quad\sum_{l_1<l_2}\,,$$

$$C(k_1k_2,l_1l_2)=(\det\cdot a)\begin{vmatrix}(a^{-1})_{l_1k_1}&(a^{-1})_{l_1k_2}\\ (a^{-1})_{l_2k_1}&(a^{-1})_{l_2k_2}\end{vmatrix}. \tag{2·2·8}$$

It is easy to see that Eq. (2·2·8) is rewritten as follows:

$$\begin{aligned}\det\{a_{ij}\}&=2\sum_{l_1<l_2}a_{k_1l_1}a_{k_2l_2}C(k_1k_2,l_1l_2)\\ &=\sum_{l_1,l_2}a_{k_1l_1}a_{k_2l_2}C(k_1k_2,l_1l_2).\end{aligned} \tag{2·2·9}$$

Let Φ and Ψ be Slater determinants expressed by $\Phi=(1/\sqrt{A!})\times\det\{\varphi_1(\boldsymbol{x}_1)\cdots\varphi_A(\boldsymbol{x}_A)\}$, $\Psi=(1/\sqrt{A!})\det\{\psi_1(\boldsymbol{x}_1)\cdots\psi_A(\boldsymbol{x}_A)\}$, respectively. Then the overlap between them is

$$\begin{aligned}\langle\Phi|\Psi\rangle&=\langle\varphi_1(\boldsymbol{x}_1)\cdots\varphi_A(\boldsymbol{x}_A)\,|\det\{\psi_1(\boldsymbol{x}_1)\cdots\psi_A(\boldsymbol{x}_A)\}\rangle\\ &=\sum_P\varepsilon(P)\langle\varphi_1|\psi_{P_1}\rangle\langle\varphi_2|\psi_{P_2}\rangle\cdots\langle\varphi_A|\psi_{P_A}\rangle\end{aligned}$$

$$=\det\{\langle\varphi_i|\psi_j\rangle\}. \tag{2·2·10}$$

The matrix element of the one-body operator is

$$\begin{aligned}
\langle\Phi|\sum_{i=1}^{A}\mathcal{O}_i|\Psi\rangle &= \sum_{i=1}^{A}\langle\varphi_1(\boldsymbol{x}_1)\cdots\varphi_A(\boldsymbol{x}_A)|\mathcal{O}_i|\det\{\psi_1(\boldsymbol{x}_1)\cdots\psi_A(\boldsymbol{x}_A)\}\rangle \\
&= \sum_{i=1}^{A}\langle\varphi_1(\boldsymbol{x}_1)\cdots(\mathcal{O}_i^{\dagger}\varphi_i(\boldsymbol{x}_i))\cdots\varphi_A(\boldsymbol{x}_A)|\det\{\psi_1(\boldsymbol{x}_1)\cdots\psi_A(\boldsymbol{x}_A)\}\rangle \\
&= \sum_{i=1}^{A}\begin{vmatrix} \langle\varphi_1|\psi_1\rangle & \cdots\cdots & \langle\varphi_1|\psi_A\rangle \\ \vdots & & \vdots \\ \langle\varphi_i|\mathcal{O}|\psi_1\rangle & \cdots\cdots & \langle\varphi_i|\mathcal{O}|\psi_A\rangle \\ \vdots & & \vdots \\ \langle\varphi_A|\psi_1\rangle & \cdots\cdots & \langle\varphi_A|\psi_A\rangle \end{vmatrix} \\
&= \sum_{i=1}^{A}\sum_{j=1}^{A}\langle\varphi_i|\mathcal{O}|\psi_j\rangle(\det\cdot B)\,(B^{-1})_{ji} \\
&= \langle\Phi|\Psi\rangle\sum_{i,j}^{A}\langle\varphi_i|\mathcal{O}|\psi_j\rangle(B^{-1})_{ji},
\end{aligned} \tag{2·2·11}$$

where

$$B_{ij}\equiv\langle\varphi_i|\psi_j\rangle, \tag{2·2·12}$$

and use is made of Eqs. (2·2·4) and (2·2·6). In order to simplify the treatment of the two-body operator $(1/2)\sum_{i\neq j}\mathcal{O}_{ij}$, we expand $\mathcal{O}_{12}$ as $\mathcal{O}_{12}=\sum_{m_1n_1m_2n_2}\langle m_1m_2|\mathcal{O}|n_1n_2\rangle\mathcal{O}_{m_1n_1}(\boldsymbol{x}_1)\mathcal{O}_{m_2n_2}(\boldsymbol{x}_2)$ where $\mathcal{O}_{mn}(\boldsymbol{x})=|m(\boldsymbol{x})\rangle\langle n(\boldsymbol{x})|$. Now we get

$$\begin{aligned}
\langle\Phi|\sum_{i\neq j}^{A}\mathcal{O}_{ij}|\Psi\rangle &= \sum_{i\neq j}^{A}\langle\varphi_1(\boldsymbol{x}_1)\cdots\varphi_A(\boldsymbol{x}_A)|\mathcal{O}_{ij}|\det\{\psi_1(\boldsymbol{x}_1)\cdots\psi_A(\boldsymbol{x}_A)\}\rangle \\
&= \sum_{m_1n_1m_2n_2}\langle m_1m_2|\mathcal{O}|n_1n_2\rangle\sum_{i\neq j}^{A}\langle\varphi_1(\boldsymbol{x}_1)\cdots(\mathcal{O}^{\dagger}_{m_1n_1}(\boldsymbol{x}_i)\varphi_i(\boldsymbol{x}_i)) \\
&\qquad\cdots(\mathcal{O}^{\dagger}_{m_2n_2}(\boldsymbol{x}_j)\varphi_j(\boldsymbol{x}_j))\cdots\varphi_A(\boldsymbol{x}_A)|\det\{\psi_1(\boldsymbol{x}_1)\cdots\psi_A(\boldsymbol{x}_A)\}\rangle \\
&= \sum_{m_1n_1m_2n_2}\langle m_1m_2|\mathcal{O}|n_1n_2\rangle\sum_{i\neq j}^{A}\begin{vmatrix} \langle\varphi_1|\psi_1\rangle & \cdots\cdots & \langle\varphi_1|\psi_A\rangle \\ \vdots & & \vdots \\ \langle\varphi_i|\mathcal{O}_{m_1n_1}|\psi_1\rangle & \cdots\cdots & \langle\varphi_i|\mathcal{O}_{m_1n_1}|\psi_A\rangle \\ \vdots & & \vdots \\ \langle\varphi_j|\mathcal{O}_{m_2n_2}|\psi_1\rangle & \cdots\cdots & \langle\varphi_j|\mathcal{O}_{m_2n_2}|\psi_A\rangle \\ \vdots & & \vdots \\ \langle\varphi_A|\psi_1\rangle & \cdots\cdots & \langle\varphi_A|\psi_A\rangle \end{vmatrix} \\
&= \langle\Phi|\Psi\rangle\sum_{ijkl}\langle\varphi_i\varphi_j|\mathcal{O}|\psi_k\psi_l\rangle\{(B^{-1})_{ki}(B^{-1})_{lj}-(B^{-1})_{kj}(B^{-1})_{li}\},
\end{aligned} \tag{2·2·13}$$

where Eqs. (2·2·8) and (2·2·9) are utilized. Equations (2·2·10)$\sim$(2·2·13) are well known[18] and furnish the calculational procedure for the GCM kernels of the type of Eqs. (2·1·24) and Eq. (2·2·1). We can, of course, similarly treat the three-body operator like as the Skyrme force as in the above way, where Eq. (2·2·7) gives the necessary coefficients $B\binom{k_1k_2k_3}{l_1l_2l_3}$.

The calculation of the GCM kernel of the type of $\mathcal{H}^r$ of Eq. (2·1·26) is evident from the derivation process of Eq. (2·2·13) and we get

$$\begin{aligned}
&\mathcal{H}^r(\boldsymbol{R}_G, \boldsymbol{R}; \boldsymbol{R}_G', \boldsymbol{R}') \\
&\quad = \langle \psi(C_1, \boldsymbol{R}_1)\psi(C_2, \boldsymbol{R}_2) | \sum_{i=1}^{N_1}\sum_{j=1}^{N_2} V_{ij} | \mathcal{A}\{\psi(C_1, \boldsymbol{R}_1')\psi(C_2, \boldsymbol{R}_2')\}\rangle \\
&\quad = \langle \varphi_{C_1,1}\cdots\varphi_{C_2,1}\cdots | \sum_{i=1}^{N_1}\sum_{j=1}^{N_2} V_{ij} | \det\{\varphi'_{C_1,1}\cdots\varphi'_{C_2,1}\cdots\}\rangle \\
&\quad = \det\{B_{kl}\} \sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\sum_{k,l}^{A} \langle \varphi_{C_1,i}\varphi_{C_2,j} | V | \varphi_k'\varphi_l'\rangle \\
&\qquad\qquad \times \{(B^{-1})_{k,C_1i}(B^{-1})_{l,C_2j} - (B^{-1})_{k,C_2j}(B^{-1})_{l,C_1i}\}, \\
&B_{kl} = \langle \varphi_k | \varphi_l'\rangle, \qquad (2\cdot2\cdot14)
\end{aligned}$$

where φ_k is an element of the set $\{\varphi_{C_1,1}, \cdots\varphi_{C_2,1}, \cdots\}$ and φ_l' belongs to $\{\varphi'_{C_1,1}, \cdots\varphi'_{C_2,1}, \cdots\}$.

Now we consider the calculation of the direct kernel. First we treat the two-cluster system as an illustrative case without rearrangement. The overlap is evidently

$$\begin{aligned}
&\langle \psi(C_1, \boldsymbol{R}_1)\psi(C_2, \boldsymbol{R}_2) | \psi(C_1, \boldsymbol{R}_1')\psi(C_2, \boldsymbol{R}_2')\rangle \\
&\quad = \langle \psi(C_1, \boldsymbol{R}_1) | \psi(C_1, \boldsymbol{R}_1')\rangle \langle \psi(C_2, \boldsymbol{R}_2) | \psi(C_2, \boldsymbol{R}_2')\rangle, \\
&\langle \psi(C_1, \boldsymbol{R}_1) | \psi(C_1, \boldsymbol{R}_1')\rangle = \det\cdot B^{\mathrm{I}} = \exp\left\{-\frac{1}{2}N_1\nu_1(\boldsymbol{R}_1 - \boldsymbol{R}_1')^2\right\}, \\
&\langle \psi(C_2, \boldsymbol{R}_1) | \psi(C_2, \boldsymbol{R}_2')\rangle = \det\cdot B^{\mathrm{II}} = \exp\left\{-\frac{1}{2}N_2\nu_2(\boldsymbol{R}_2 - \boldsymbol{R}_2')^2\right\}, \\
&(B^{\mathrm{I}})_{ij} \equiv \langle \varphi_{C_1,i} | \varphi'_{C_1,j}\rangle, \quad (B^{\mathrm{II}})_{ij} \equiv \langle \varphi_{C_2,i} | \varphi'_{C_2,j}\rangle. \qquad (2\cdot2\cdot15)
\end{aligned}$$

For the one-body operator, also evidently

$$\begin{aligned}
&\langle \psi(C_1, \boldsymbol{R}_1)\psi(C_2, \boldsymbol{R}_2) | \sum_{i=1}^{A} \mathcal{O}_i | \psi(C_1, \boldsymbol{R}_1')\psi(C_2, \boldsymbol{R}_2')\rangle \\
&\quad = \langle \psi(C_1, \boldsymbol{R}_1) | \sum_{i=1}^{N_1} \mathcal{O}_i | \psi(C_1, \boldsymbol{R}_1')\rangle \langle \psi(C_2, \boldsymbol{R}_2) | \psi(C_2, \boldsymbol{R}_2')\rangle \\
&\qquad + \langle \psi(C_1, \boldsymbol{R}_1) | \psi(C_1, \boldsymbol{R}_1')\rangle \langle \psi(C_2, \boldsymbol{R}_2) | \sum_{i=N_1+1}^{A} \mathcal{O}_i | \psi(C_2, \boldsymbol{R}_2')\rangle \\
&\quad = (\det\cdot B^{\mathrm{I}})(\det\cdot B^{\mathrm{II}}) \{\sum_{i,j}^{N_1} \langle \varphi_{C_1,i} | \mathcal{O} | \varphi'_{C_1,j}\rangle (B^{\mathrm{I}-1})_{ji} \\
&\qquad + \sum_{i,j}^{N_2} \langle \varphi_{C_2,i} | \mathcal{O} | \varphi'_{C_2,j}\rangle (B^{\mathrm{II}-1})_{ji}\}. \qquad (2\cdot2\cdot16)
\end{aligned}$$

For the two-body operator we get

$$\langle\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)|\sum_{i\neq j}^{A}\mathcal{O}_{ij}|\psi(C_1,\boldsymbol{R}_1')\psi(C_2,\boldsymbol{R}_2')\rangle$$

$$=(\det\cdot B^{\mathrm{I}})\,(\det\cdot B^{\mathrm{II}})\Big[\sum_{ijkl}^{N_1}\langle\varphi_{\sigma_1,i}\varphi_{\sigma_1,j}|\mathcal{O}|\varphi'_{\sigma_1,k}\varphi'_{\sigma_1,l}\rangle$$

$$\times\{(B^{\mathrm{I}-1})_{ki}(B^{\mathrm{I}-1})_{lj}-(B^{\mathrm{I}-1})_{kj}(B^{\mathrm{I}-1})_{li}\}+\sum_{ijkl}^{N_2}\langle\varphi_{\sigma_2,i}\varphi_{\sigma_2,j}|\mathcal{O}|\varphi'_{\sigma_2,k}\varphi'_{\sigma_2,l}\rangle$$

$$\times\{(B^{\mathrm{II}-1})_{ki}(B^{\mathrm{II}-1})_{lj}-(B^{\mathrm{II}-1})_{kj}(B^{\mathrm{II}-1})_{li}\}$$

$$+2\sum_{ik}^{N_1}\sum_{jl}^{N_2}\langle\varphi_{\sigma_1,i}\varphi_{\sigma_2,j}|\mathcal{O}|\varphi'_{\sigma_1,k}\varphi'_{\sigma_2,l}\rangle(B^{\mathrm{I}-1})_{ki}(B^{\mathrm{II}-1})_{lj}\Big]. \qquad (2\cdot2\cdot17)$$

This is because

$$\langle\psi(C_2,\boldsymbol{R}_2)|\sum_{j=1}^{N_2}\mathcal{O}_{ij}|\psi(C_2,\boldsymbol{R}_2')\rangle$$

$$=(\det\cdot B^{\mathrm{II}})\sum_{j,l}^{N_2}\langle\varphi_{\sigma_2,j}|\mathcal{O}_{i2}|\varphi'_{\sigma_2,l}\rangle(B^{\mathrm{II}-1})_{lj}\,,$$

$$\langle\varphi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)|\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\mathcal{O}_{ij}|\psi(C_1,\boldsymbol{R}_1')\psi(C_2,\boldsymbol{R}_2')\rangle$$

$$=(\det\cdot B^{\mathrm{I}})\,(\det\cdot B^{\mathrm{II}})\sum_{i,k}^{N_1}\sum_{j,l}^{N_2}\langle\varphi_{\sigma_1,i}\varphi_{\sigma_2,j}|\mathcal{O}|\varphi'_{\sigma_1,k}\varphi'_{\sigma_2,l}\rangle(B^{\mathrm{I}-1})_{ki}(B^{\mathrm{II}-1})_{lj}\,. \qquad (2\cdot2\cdot18)$$

We can easily see that all the expressions of Eqs. (2·2·15), (2·2·16) and (2·2·17) are obtainable from Eqs. (2·2·10), (2·2·11) and (2·2·13), respectively, simply by the following replacements:

$$B=\begin{pmatrix}B^{\mathrm{I}} & B^{\mathrm{I\,II}}\\ B^{\mathrm{II\,I}} & B^{\mathrm{II}}\end{pmatrix}\to\begin{pmatrix}B^{\mathrm{I}} & 0\\ 0 & B^{\mathrm{II}}\end{pmatrix},$$

$$\text{therefore}\quad B^{-1}\to\begin{pmatrix}(B^{\mathrm{I}})^{-1} & 0\\ 0 & (B^{\mathrm{II}})^{-1}\end{pmatrix}. \qquad (2\cdot2\cdot19)$$

Next we consider the direct rearrangement kernel for the process $C_1+C_2\to C_3+C_4$. We assume that $N_1>N_3$ (and therefore $N_2<N_4$) and that N_3 nucleons of C_1 constitute C_3 and the remaining (N_1-N_3) nucleons in C_1 are absorbed together with N_2 nucleons of C_2 into C_4. The overlap kernel is

$$\langle\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)|\psi(C_3,\boldsymbol{R}_3)\psi(C_4,\boldsymbol{R}_4)\rangle$$

$$=\frac{1}{\sqrt{\prod_{i=1}^{4}(N_i!)}}\langle\det\{\varphi_{\sigma_1,1}\cdots\varphi_{\sigma_1,N_1}\}\det\{\varphi_{\sigma_2,1}\cdots\varphi_{\sigma_2,N_2}\}|$$

$$\det\{\varphi_{\sigma_3,1}\cdots\varphi_{\sigma_3,N_3}\}\det\{\varphi_{\sigma_4,1}\cdots\varphi_{\sigma_4,N_4}\}\rangle$$

$$=\sqrt{\frac{N_2!}{N_1!\,N_3!\,N_4!}}\sum_{\sigma}\varepsilon\begin{pmatrix}1\cdots N_1\\ \sigma_1\cdots\sigma_{N_1}\end{pmatrix}\langle\varphi_{\sigma_1\sigma_1}\cdots\varphi_{\sigma_1\sigma_{N_1}}\varphi_{\sigma_2,1}\cdots\varphi_{\sigma_2N_2}|$$

$$\det\{\varphi_{\sigma_3,1}\cdots\varphi_{\sigma_3,N_3}\}\det\{\varphi_{\sigma_4,1}\cdots\varphi_{\sigma_4,N_4}\}\rangle$$

$$
\begin{aligned}
&=\sqrt{\frac{N_2!}{N_1!\,N_3!\,N_4!}}\sum_{\sigma}\varepsilon\begin{pmatrix}1\cdots N_1\\ \sigma_1\cdots\sigma_{N_1}\end{pmatrix}\\
&\quad\times\begin{vmatrix}\langle\varphi^1_{\sigma_1}|\varphi_1{}^3\rangle & \cdots\cdots & \langle\varphi^1_{\sigma_1}|\varphi^3_{N_3}\rangle\\ \vdots & & \vdots\\ \langle\varphi^1_{\sigma_{N_3}}|\varphi_1{}^3\rangle & \cdots\cdots & \langle\varphi^1_{\sigma_{N_3}}|\varphi^3_{N_3}\rangle\end{vmatrix}\\
&\quad\times\begin{vmatrix}\langle\varphi^1_{\sigma_{N_3+1}}|\varphi_1{}^4\rangle & \cdots\cdots & \langle\varphi^1_{\sigma_{N_3+1}}|\varphi^4_{N_4}\rangle\\ \vdots & & \vdots\\ \langle\varphi^1_{\sigma_{N_1}}|\varphi_1{}^4\rangle & \cdots\cdots & \langle\varphi^1_{\sigma_{N_1}}|\varphi^4_{N_4}\rangle\\ \langle\varphi_1{}^2|\varphi_1{}^4\rangle & \cdots\cdots\cdots & \langle\varphi_1{}^2|\varphi^4_{N_4}\rangle\\ \vdots & & \vdots\\ \langle\varphi^2_{N_2}|\varphi_1{}^4\rangle & \cdots\cdots\cdots & \langle\varphi^2_{N_2}|\varphi^4_{N_4}\rangle\end{vmatrix},
\end{aligned}
\tag{2·2·20}
$$

where we used the abbreviation $\varphi^i\equiv\varphi_{C_i}$. By using the following relation,

$$
\begin{aligned}
&\sum_{\sigma}\varepsilon\begin{pmatrix}1\cdots N_1\\ \sigma_1\cdots\sigma_{N_1}\end{pmatrix}P\begin{pmatrix}1\cdots N_1\\ \sigma_1\cdots\sigma_{N_1}\end{pmatrix}\\
&\quad=\sum_{k_1<k_2<\cdots<k_{N_3}}\varepsilon\begin{pmatrix}1\cdots N_3 & N_3+1\cdots & N_1\\ k_1\cdots k_{N_3} & p_1\ \cdots p_{N_1-N_3}\end{pmatrix}\\
&\qquad\times\sum_{\alpha,\beta}\varepsilon\begin{pmatrix}k_1 & \cdots & k_{N_3}\\ \alpha(k_1)\cdots\alpha(k_{N_3})\end{pmatrix}\varepsilon\begin{pmatrix}p_1 & \cdots & p_{N_1-N_3}\\ \beta(p_1)\cdots\beta(p_{N_1-N_3})\end{pmatrix}\\
&\qquad\times P\begin{pmatrix}1 & \cdots & N_3 & N_3+1\cdots & N_1\\ \alpha(k_1)\cdots\alpha(k_{N_3}) & & \beta(p_1) & \cdots\beta(p_{N_1-N_3})\end{pmatrix},
\end{aligned}
\tag{2·2·21}
$$

where $(p_1,\cdots p_{N_1-N_3})$ are the numbers which are left after subtracting the numbers $(k_1,\cdots,k_{N_3})$ from $(1,2,\cdots,N_1)$ and satisfy $p_1<p_2<\cdots<p_{N_1-N_3}$, we obtain

$$
\begin{aligned}
&\langle\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)\,|\psi(C_3,\boldsymbol{R}_3)\psi(C_4,\boldsymbol{R}_4)\rangle\\
&\quad=\sqrt{\frac{N_2!\,N_3!}{N_1!\,N_4!}}(N_1-N_3)!\sum_{(k_1<k_2<\cdots<k_{N_3})}\varepsilon\begin{pmatrix}1\cdots N_3 & N_3+1\cdots & N_1\\ k_1\cdots k_{N_3} & p_1\ \cdots p_{N_1-N_3}\end{pmatrix}\\
&\qquad\times\begin{vmatrix}\langle\varphi^1_{k_1}|\varphi_1{}^3\rangle & \cdots\cdots & \langle\varphi^1_{k_1}|\varphi^3_{N_3}\rangle\\ \vdots & & \vdots\\ \langle\varphi^1_{k_{N_3}}|\varphi_1{}^3\rangle & \cdots\cdots & \langle\varphi^1_{k_{N_3}}|\varphi^3_{N_3}\rangle\end{vmatrix}\\
&\qquad\times\begin{vmatrix}\langle\varphi^1_{p_1}|\varphi_1{}^4\rangle & \cdots\cdots\cdots & \langle\varphi^1_{p_1}|\varphi^4_{N_4}\rangle\\ \vdots & & \\ \langle\varphi^1_{p_{N_1-N_3}}|\varphi_1{}^4\rangle & \cdots\cdots & \langle\varphi^1_{p_{N_1-N_3}}|\varphi^4_{N_4}\rangle\\ \langle\varphi_1{}^2|\varphi_1{}^4\rangle & \cdots\cdots\cdots & \langle\varphi_1{}^2|\varphi^4_{N_4}\rangle\\ \vdots & & \vdots\\ \langle\varphi^2_{N_2}|\varphi_1{}^4\rangle & \cdots\cdots\cdots & \langle\varphi^2_{N_2}|\varphi^4_{N_4}\rangle\end{vmatrix}.
\end{aligned}
\tag{2·2·22}
$$

Since, as is proved in Appendix A·2,

$$
\varepsilon\begin{pmatrix}1\cdots N_3 & N_3+1\cdots & N_1\\ k_1\cdots k_{N_3} & p_1\ \cdots p_{N_1-N_3}\end{pmatrix}=(-)^{\sum_{i=1}^{N_3}(i+k_i)},
\tag{2·2·23}
$$

we know that Eq. (2·2·22) is nothing but the Laplace expansion of the following overlap determinant:

$$\langle\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)\,|\psi(C_3,\boldsymbol{R}_3)\psi(C_4,\boldsymbol{R}_4)\rangle$$
$$=\sqrt{\frac{N_2!\,N_3!}{N_1!\,N_4!}}(N_1-N_3)!\cdot(\det\cdot\tilde{B}),$$
$$\tilde{B}\equiv\begin{pmatrix}\langle\varphi_1^1|\varphi_1^3\rangle & \cdots & \langle\varphi_1^1|\varphi_{N_3}^3\rangle & \langle\varphi_1^1|\varphi_1^4\rangle & \cdots & \langle\varphi_1^1|\varphi_{N_4}^4\rangle\\ \vdots & & \vdots & \vdots & & \vdots\\ \langle\varphi_{N_1}^1|\varphi_1^3\rangle & \cdots & \langle\varphi_{N_1}^1|\varphi_{N_3}^3\rangle & \langle\varphi_{N_1}^1|\varphi_1^4\rangle & \cdots & \langle\varphi_{N_1}^1|\varphi_{N_4}^4\rangle\\ & & & \langle\varphi_1^2|\varphi_1^4\rangle & \cdots & \langle\varphi_1^2|\varphi_{N_4}^4\rangle\\ & 0 & & \vdots & & \vdots\\ & & & \langle\varphi_{N_2}^2|\varphi_1^4\rangle & \cdots & \langle\varphi_{N_2}^2|\varphi_{N_4}^4\rangle\end{pmatrix}. \qquad (2\cdot2\cdot24)$$

For the one-body operator, we get

$$\langle\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)\,|\sum_{i=1}^{A}\mathcal{O}_i|\psi(C_3,\boldsymbol{R}_3)\psi(C_4,\boldsymbol{R}_4)\rangle$$
$$=\sqrt{\frac{N_2}{N_1!\,N_3!\,N_4!}}\sum_{\sigma}\varepsilon\begin{pmatrix}1\cdots N_1\\ \sigma_1\cdots\sigma_{N_1}\end{pmatrix}$$
$$\times\Bigg[\sum_{i=1}^{N_3}\begin{vmatrix}\langle\varphi_{\sigma_1}^1|\varphi_1^3\rangle & \cdots & \langle\varphi_{\sigma_1}^1|\varphi_{N_3}^3\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_i}^1|\mathcal{O}|\varphi_1^3\rangle & \cdots & \langle\varphi_{\sigma_i}^1|\mathcal{O}|\varphi_{N_3}^3\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_{N_3}}^1|\varphi_1^3\rangle & \cdots & \langle\varphi_{\sigma_{N_3}}^1|\varphi_{N_3}^3\rangle\end{vmatrix}\times\begin{vmatrix}\langle\varphi_{\sigma_{N_3+1}}^1|\varphi_1^4\rangle & \cdots & \langle\varphi_{\sigma_{N_3+1}}^1|\varphi_{N_4}^4\rangle\\ \vdots & & \vdots\\ \langle\varphi_{N_2}^2|\varphi_1^4\rangle & \cdots & \langle\varphi_{N_2}^2|\varphi_{N_4}^4\rangle\end{vmatrix}$$
$$+\begin{vmatrix}\langle\varphi_{\sigma_1}^1|\varphi_1^3\rangle & \cdots & \langle\varphi_{\sigma_1}^1|\varphi_{N_3}^3\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_{N_3}}^1|\varphi_1^3\rangle & \cdots & \langle\varphi_{\sigma_{N_3}}^1|\varphi_{N_3}^3\rangle\end{vmatrix}$$
$$\times\Bigg\{\sum_{i=N_3+1}^{N_1}\begin{vmatrix}\langle\varphi_{\sigma_{N_3+1}}^1|\varphi_1^4\rangle & \cdots & \langle\varphi_{\sigma_{N_3+1}}^1|\varphi_{N_4}^4\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_i}^1|\mathcal{O}|\varphi_1^4\rangle & \cdots & \langle\varphi_{\sigma_i}^1|\mathcal{O}|\varphi_{N_4}^4\rangle\\ \vdots & & \vdots\\ \langle\varphi_{N_2}^2|\varphi_1^4\rangle & \cdots & \langle\varphi_{N_2}^2|\varphi_{N_4}^4\rangle\end{vmatrix}$$
$$+\sum_{i=1}^{N_2}\begin{vmatrix}\langle\varphi_{\sigma_{N_3+1}}^1|\varphi_1^4\rangle & \cdots & \langle\varphi_{\sigma_{N_3+1}}^1|\varphi_{N_4}^4\rangle\\ \vdots & & \vdots\\ \langle\varphi_i^2|\mathcal{O}|\varphi_1^4\rangle & \cdots & \langle\varphi_i^2|\mathcal{O}|\varphi_{N_4}^4\rangle\\ \vdots & & \vdots\\ \langle\varphi_{N_2}^2|\varphi_1^4\rangle & \cdots & \langle\varphi_{N_2}^2|\varphi_{N_4}^4\rangle\end{vmatrix}\Bigg\}\Bigg]. \qquad (2\cdot2\cdot25)$$

By noting the relation

$$\begin{vmatrix}a_{\sigma_1 1} & \cdots & a_{\sigma_1 n}\\ \vdots & & \vdots\\ b_{\sigma_i 1} & \cdots & b_{\sigma_i n}\\ \vdots & & \vdots\\ a_{\sigma_n 1} & \cdots & a_{\sigma_n n}\end{vmatrix}_{\leftarrow i}=\varepsilon\begin{pmatrix}1\cdots n\\ \sigma_1\cdots\sigma_n\end{pmatrix}\begin{vmatrix}a_{11} & \cdots & a_{1n}\\ \vdots & & \vdots\\ b_{\sigma_i,1} & \cdots & b_{\sigma_i,n}\\ \vdots & & \vdots\\ a_{n1} & \cdots & a_{nn}\end{vmatrix}_{\leftarrow\sigma_i},$$

$$\sum_{i=1}^{n}\begin{vmatrix} a_{\sigma_1 1} & \cdots\cdots & a_{\sigma_1 n} \\ \vdots & & \vdots \\ b_{\sigma_i 1} & \cdots\cdots & b_{\sigma_i n} \\ \vdots & & \vdots \\ a_{\sigma_n 1} & \cdots\cdots & a_{\sigma_n n} \end{vmatrix} = \varepsilon\begin{pmatrix} 1 \cdots n \\ \sigma_1 \cdots \sigma_n \end{pmatrix}\sum_{i=1}^{n}\begin{vmatrix} a_{11} & \cdots\cdots & a_{1n} \\ \vdots & & \vdots \\ b_{i1} & \cdots\cdots & b_{in} \\ \vdots & & \vdots \\ a_{n1} & \cdots\cdots & a_{nn} \end{vmatrix}, \qquad (2\cdot2\cdot26)$$

and again with the aid of Eqs. (2·2·21) and (2·2·23), we get

$$\langle\psi(C_1, \boldsymbol{R}_1)\psi(C_2, \boldsymbol{R}_2)|\sum_{i=1}^{A}\mathcal{O}_i|\psi(C_3, \boldsymbol{R}_3)\psi(C_4, \boldsymbol{R}_4)\rangle$$

$$=\sqrt{\frac{N_2!\,N_3!}{N_1!\,N_4!}}(N_1-N_3)!$$

$$\times\left\{\sum_{i=1}^{N_1}\begin{vmatrix} \langle\varphi_1^1|\varphi_1^3\rangle & \cdots\cdots & \langle\varphi_1^1|\varphi_{N_4}^4\rangle \\ \vdots & & \vdots \\ \langle\varphi_i^1|\mathcal{O}|\varphi_1^3\rangle & \cdots\cdots & \langle\varphi_i^1|\mathcal{O}|\varphi_{N_4}^4\rangle \\ \vdots & & \vdots \\ \langle\varphi_{N_1}^1|\varphi_1^3\rangle & \cdots\cdots & \langle\varphi_{N_1}^1|\varphi_{N_4}^4\rangle \\ & \langle\varphi_1^2|\varphi_1^4\rangle & \cdots\cdots \langle\varphi_1^2|\varphi_{N_4}^4\rangle \\ 0 & \vdots & \vdots \\ & \langle\varphi_{N_2}^2|\varphi_1^4\rangle & \cdots\cdots \langle\varphi_{N_2}^2|\varphi_{N_4}^4\rangle \end{vmatrix}\right.$$

$$\left.+\sum_{i=1}^{N_2}\begin{vmatrix} \langle\varphi_1^1|\varphi_1^3\rangle & \cdots\cdots & \langle\varphi_1^1|\varphi_{N_4}^4\rangle \\ \vdots & & \vdots \\ \langle\varphi_{N_1}^1|\varphi_1^3\rangle & \cdots\cdots & \langle\varphi_{N_1}^1|\varphi_{N_4}^4\rangle \\ & \langle\varphi_1^2|\varphi_1^4\rangle & \cdots\cdots \langle\varphi_1^2|\varphi_{N_4}^4\rangle \\ 0 & \vdots & \vdots \\ & \langle\varphi_i^2|\mathcal{O}|\varphi_1^4\rangle & \cdots\cdots \langle\varphi_i^2|\mathcal{O}|\varphi_{N_4}^4\rangle \\ & \vdots & \vdots \\ & \langle\varphi_{N_2}^2|\varphi_1^4\rangle & \cdots\cdots \langle\varphi_{N_2}^2|\varphi_{N_4}^4\rangle \end{vmatrix}\right\}$$

$$=\sqrt{\frac{N_2!\,N_3!}{N_1!\,N_4!}}(N_1-N_3)!\sum_{i=1}^{A}{}'\sum_{j=1}^{A}{}'\langle\varphi_i|\mathcal{O}|\varphi_j'\rangle(\tilde{B}^{-1})_{ji}, \qquad (2\cdot2\cdot27)$$

where $\{\varphi_i, (i=1\sim A)\}$ is $\{\varphi_{c_1,1}\cdots\varphi_{c_2,1}\cdots\}$ and $\{\varphi_j', (j=1\sim A)\}$ is $\{\varphi_{c_3,1}\cdots\varphi_{c_4,1}\cdots\}$, and $\sum'^{A}_{j=1}$ means that φ_j' runs only on $\varphi_{c_4,j}(j=1\sim N_4)$ when φ_i belongs to $\{\varphi_{c_2,i}\ i=1\sim N_2\}$. Now we consider the direct rearrangement kernel for the two-body operator. Below we show the calculation not for the full operator $\sum_{ij}^{A}\mathcal{O}_{ij}$ but for the case of the operators of the type $\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\mathcal{O}_{ij}$ or $\sum_{i=1}^{N_3}\sum_{j=1}^{N_4}\mathcal{O}_{ij}$ which are of interest for the calculation of the interaction kernels between rearranged channels in the frameworks without full antisymmetrization. Of course the treatment of the two-body operators of the type $\sum_{ij}^{N_1}\mathcal{O}_{ij}$ is similar and is not difficult. Consider first $\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\mathcal{O}_{ij}$. We express this operator as $\sum_{m_1n_1m_2n_2}\langle m_1m_2|\mathcal{O}|n_1n_2\rangle\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\mathcal{O}_{m_1n_1}(i)\mathcal{O}_{m_2n_2}(j)$ and evaluate the matrix element for $\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\mathcal{O}_1(i)\mathcal{O}_2(j)$ $(\mathcal{O}_i=\mathcal{O}_{m_in_i})$ which is summed up as $\sum_{m_1n_1m_2n_2}\langle m_1m_2|\mathcal{O}|n_1n_2\rangle$ to give the final result. The matrix element for such separable operator is

$$\langle\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)|\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\mathcal{O}_1(i)\mathcal{O}_2(j)|\psi(C_3,\boldsymbol{R}_3)\psi(C_4,\boldsymbol{R}_4)\rangle$$

$$=\sqrt{\frac{N_2!}{N_1!\,N_3!\,N_4!}}\sum_{\sigma}\varepsilon\begin{pmatrix}1\cdots N_1\\ \sigma_1\cdots\sigma_{N_1}\end{pmatrix}$$

$$\times\Bigg\{\sum_{i=1}^{N_3}\begin{vmatrix}\langle\varphi_{\sigma_1}^1|\varphi_1^3\rangle & \cdots\cdots\\ \vdots & \\ \langle\varphi_{\sigma_i}^1|\mathcal{O}_1|\varphi_1^3\rangle & \cdots\cdots\\ \vdots & \\ \langle\varphi_{\sigma_{N_3}}^1|\varphi_1^3\rangle & \cdots\cdots\end{vmatrix}\sum_{j=1}^{N_2}\begin{vmatrix}\langle\varphi_{\sigma_{N_3+1}}^1|\varphi_1^4\rangle & \cdots\cdots\\ \vdots & \\ \langle\varphi_j^2|\mathcal{O}_2|\varphi_1^4\rangle & \cdots\cdots\\ \vdots & \\ \langle\varphi_{N_2}^2|\varphi_1^4\rangle & \cdots\cdots\end{vmatrix}$$

$$+\begin{vmatrix}\langle\varphi_{\sigma_1}^1|\varphi_1^3\rangle & \cdots\cdots\\ \vdots & \\ \langle\varphi_{\sigma_{N_3}}^1|\varphi_1^3\rangle & \cdots\cdots\end{vmatrix}\sum_{i=N_3+1}^{N_1}\sum_{j=1}^{N_2}\begin{vmatrix}\langle\varphi_{\sigma_{N_3+1}}^1|\varphi_1^4\rangle & \cdots\cdots\\ \vdots & \\ \langle\varphi_{\sigma_i}^1|\mathcal{O}_1|\varphi_1^4\rangle & \cdots\cdots\\ \vdots & \\ \langle\varphi_j^2|\mathcal{O}_2|\varphi_1^4\rangle & \cdots\cdots\\ \vdots & \\ \langle\varphi_{N_2}^2|\varphi_1^4\rangle & \cdots\cdots\end{vmatrix}\Bigg\}$$

$$=\sqrt{\frac{N_2!\,N_3!}{N_1!\,N_4!}}(N_1-N_3)!\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}$$

$$\times\begin{vmatrix}\langle\varphi_1^1|\varphi_1^3\rangle & \cdots\cdots & & \\ \vdots & & & \\ \langle\varphi_i^1|\mathcal{O}_1|\varphi_1^3\rangle & \cdots\cdots & & \\ \vdots & & & \\ \langle\varphi_{N_1}^1|\varphi_1^3\rangle & \cdots\cdots & & \\ & & \langle\varphi_1^2|\varphi_1^4\rangle & \cdots\cdots\\ & 0 & \vdots & \\ & & \langle\varphi_j^2|\mathcal{O}_2|\varphi_1^4\rangle & \cdots\cdots\\ & & \vdots & \\ & & \langle\varphi_{N_2}^2|\varphi_1^4\rangle & \cdots\cdots\end{vmatrix}$$

$$=\sqrt{\frac{N_2!\,N_3!}{N_1!\,N_4!}}(N_1-N_3)!\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\sum_{k=1}^{A}\sum_{l=1}^{N_4}\langle\varphi_{c_1i}\varphi_{c_2j}|\mathcal{O}_1\mathcal{O}_2|\varphi_k'\varphi_{c_4l}\rangle$$

$$\times\{(\tilde{B}^{-1})_{k,i}(\tilde{B}^{-1})_{N_3+l,N_2+j}-(\tilde{B}^{-1})_{k,N_2+j}(\tilde{B}^{-1})_{N_3+l,i}\},\qquad(2\cdot2\cdot28)$$

which gives the final formula,

$$\langle\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)|\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\mathcal{O}_{ij}|\psi(C_3,\boldsymbol{R}_3)\psi(C_4,\boldsymbol{R}_4)\rangle$$

$$=\sqrt{\frac{N_2!\,N_3!}{N_1!\,N_4!}}(N_1-N_3)!\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\sum_{k=1}^{A}\sum_{l=1}^{N_4}\langle\varphi_{c_1i}\varphi_{c_2j}|\mathcal{O}|\varphi_k'\varphi_{c_4l}\rangle$$

$$\times\{(\tilde{B}^{-1})_{k,i}(\tilde{B}^{-1})_{N_3+l,N_2+j}-(\tilde{B}^{-1})_{k,N_2+j}(\tilde{B}^{-1})_{N_3+l,i}\}.\qquad(2\cdot2\cdot29)$$

The kernel for $\sum_{i=1}^{N_3}\sum_{j=1}^{N_4}\mathcal{O}_{ij}$ is of course obtained by $\langle\psi(C_3,\boldsymbol{R}_3)\psi(C_4,\boldsymbol{R}_4)|\sum_{i=1}^{N_3}\sum_{j=1}^{N_4}\mathcal{O}_{ij}|\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)\rangle^*$.

2.2.b. *On the analytical evaluation*

The analytical evaluation of the GCM kernels is often necessary and especially for the transformation of the GCM kernel to the RGM one it is highly desirable to have analytical form of the GCM kernel. The prescription given in § 2.2.a is straightforward and for lighter systems we can get the analytical form of the GCM kernel in a manual calculation. When we treat heavier systems like as $\alpha+{}^{40}\mathrm{Ca}$, ${}^{16}\mathrm{O}+{}^{16}\mathrm{O}$, however, the manual calculation becomes fairly tedious. So the techniques are developed which give the analytical form of the GCM kernal by the computor evaluation following the prescription of § 2.2.a. The methods of these kinds of the analytical evaluation devised for the computor calculation are discussed in detail in Chap. IV. What we discuss below is about a method which is suitable for a manual evaluation of the analytical form of the GCM kernel.

In the prescription § 2.2.a, the evaluation of the inverse matrix of the matrix B of Eq. (2·2·12) is a main tediousness in the manual treatment. When the system is composed of a heavy cluster and a lighter cluster (or lighter clusters), the form of the B matrix can be made into a simpler form by treating the lighter clusters as the valence clusters around the heavier core cluster.[32]

For the sake of explanation we consider the two-cluster system and investigate some properties of the kernel $\mathcal{O}(\boldsymbol{R}_G, \boldsymbol{R}; \boldsymbol{R}_G', \boldsymbol{R}')$. In the case of the common oscilator parameter we know from Eq. (2·1·13)

$$\mathcal{O}(\boldsymbol{R}_G, \boldsymbol{R}; \boldsymbol{R}_G', \boldsymbol{R}') = \exp\left\{-\frac{1}{2}A\nu(\boldsymbol{R}_G^* - \boldsymbol{R}_G')^2\right\}\mathcal{O}(\boldsymbol{R}, \boldsymbol{R}')$$

$$\text{for } \nu_1 = \nu_2 . \qquad (2\cdot2\cdot30)$$

This means that if we know the GCM kernel $\mathcal{O}(\boldsymbol{R}; \boldsymbol{R}') = \mathcal{O}(\boldsymbol{R}_G=0, \boldsymbol{R}; \boldsymbol{R}_G'=0, \boldsymbol{R}')$ the GCM kernel $\mathcal{O}(\boldsymbol{R}_G, \boldsymbol{R}; \boldsymbol{R}_G', \boldsymbol{R}')$ with four GC is obtained easily. Namely the essential part of the GCM kernel $\mathcal{O}(\boldsymbol{R}_G, \boldsymbol{R}; \boldsymbol{R}_G', \boldsymbol{R}')$ which needs so much computational effort is determined not by the set of full four GC $(\boldsymbol{R}_G, \boldsymbol{R}, \boldsymbol{R}_G', \boldsymbol{R}')$ but by a set of two GC $\boldsymbol{R}$ and $\boldsymbol{R}'$. A set of values of the GC $\boldsymbol{R}_1=0$, $\boldsymbol{R}_2=\boldsymbol{S}$, $\boldsymbol{R}_1'=0$, $\boldsymbol{R}_2'=\boldsymbol{S}'$ which is equivalent to $\boldsymbol{R}_G=(N_2/A)\boldsymbol{S}$, $\boldsymbol{R}=\boldsymbol{S}$, $\boldsymbol{R}_G'=(N_2/A)\boldsymbol{S}'$, $\boldsymbol{R}'=\boldsymbol{S}'$ is important for our later discussion. Using the above Eq. (2·2·30) we know that the GCM kernel $\mathcal{O}$ with arbitrary complex values of four GC $(\boldsymbol{R}_G, \boldsymbol{R}, \boldsymbol{R}_G', \boldsymbol{R}')$ is related to the GCM kernel $\mathcal{O}$ with the above type of set of GC, as follows,

$$\mathcal{O}(\boldsymbol{R}_G, \boldsymbol{R}; \boldsymbol{R}_G', \boldsymbol{R}') = \exp\left[\frac{1}{2}A\nu\left\{\left(\frac{N_2}{A}\right)^2(\boldsymbol{R}^* - \boldsymbol{R}')^2 - (\boldsymbol{R}_G^* - \boldsymbol{R}_G')^2\right\}\right]$$

$$\times\mathcal{O}\left(\frac{N_2}{A}\boldsymbol{R}, \boldsymbol{R}; \frac{N_2}{A}\boldsymbol{R}', \boldsymbol{R}'\right)$$

$$\text{for } \nu_1 = \nu_2 . \qquad (2\cdot2\cdot31)$$

Almost the same results as the above case of $\nu_1=\nu_2$ hold also for the case with unequal oscillator parameters $\nu_1\neq\nu_2$. We first note the following relations,

$$\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)=q\rho(\boldsymbol{X}_G-\boldsymbol{R}_G,\boldsymbol{r}-\boldsymbol{R})\phi\,,$$

$$q\equiv\left(\frac{4N_1N_2\nu_1\nu_2}{\pi^2}\right)^{3/4},\qquad \phi\equiv\phi(C_1)\phi(C_2)\,,$$

$$\rho(\boldsymbol{A},\boldsymbol{B})\equiv\exp\{-\alpha\boldsymbol{A}^2-\beta\boldsymbol{A}\cdot\boldsymbol{B}-\gamma\boldsymbol{B}^2\}\,,$$

$$\rho(\boldsymbol{X}_G-\boldsymbol{R}_G,\boldsymbol{r}-\boldsymbol{R})=\rho(\boldsymbol{R}_G,\boldsymbol{R})\exp\{-\alpha\boldsymbol{X}_G^2-(\beta\boldsymbol{r}-\boldsymbol{E})\cdot\boldsymbol{X}_G\}\times\exp\{-\gamma\boldsymbol{r}^2+\boldsymbol{F}\cdot\boldsymbol{r}\}\,,$$

$$\boldsymbol{E}\equiv2\alpha\boldsymbol{R}_G+\beta\boldsymbol{R}\,,\quad \boldsymbol{F}\equiv\beta\boldsymbol{R}_G+2\gamma\boldsymbol{R}\,. \tag{2·2·32}$$

The GCM kernel (GC are arbitrary complex vectors) is

$$\begin{aligned}&\mathcal{H}(\boldsymbol{R}_G,\boldsymbol{R};\boldsymbol{R}_G',\boldsymbol{R}')\\&\quad=\langle\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)|\mathcal{O}|\mathcal{A}\{\psi(C_1,\boldsymbol{R}_1')\psi(C_2,\boldsymbol{R}_2')\}\rangle\\&\quad=q^2\rho(\boldsymbol{R}_G^*,\boldsymbol{R}^*)\rho(\boldsymbol{R}_G',\boldsymbol{R}')\\&\qquad\times\langle\exp[-\alpha\boldsymbol{X}_G^2-(\beta\boldsymbol{r}-\boldsymbol{E})\cdot\boldsymbol{X}_G]\exp[-\gamma\boldsymbol{r}^2+\boldsymbol{F}\cdot\boldsymbol{r}]\phi|\mathcal{O}\\&\times|\mathcal{A}\{\exp[-\alpha\boldsymbol{X}_G^2-(\beta\boldsymbol{r}-\boldsymbol{E}')\cdot\boldsymbol{X}_G]\exp[-\gamma\boldsymbol{r}^2+\boldsymbol{F}'\cdot\boldsymbol{r}]\phi\}\rangle,\end{aligned}\tag{2·2·33}$$

where $\boldsymbol{E}'=2\alpha\boldsymbol{R}_G'+\beta\boldsymbol{R}'$, $\boldsymbol{F}'=\beta\boldsymbol{R}_G'+2\gamma\boldsymbol{R}'$. Now we express $\mathcal{A}$ as a sum of the permutation operators P_c as $\mathcal{A}=\sum_c\varepsilon_cP_c$ and consider the matrix element $\mathcal{H}_c$ which is obtained by replacing $\mathcal{A}$ by P_c in the above equation. By using the notation $\boldsymbol{r}'=P_c\boldsymbol{r}$, this $\mathcal{H}_c$ is calculated as follows,

$$\begin{aligned}\mathcal{H}_c\propto q^2\langle[&\int d\boldsymbol{X}_G\exp\{-2\alpha\boldsymbol{X}_G^2-(\beta\boldsymbol{r}-\boldsymbol{E}+\beta\boldsymbol{r}'-\boldsymbol{E}'^*)\cdot\boldsymbol{X}_G\}]\\&\times\exp\{-\gamma\boldsymbol{r}^2+\boldsymbol{F}\cdot\boldsymbol{r}\}\phi|\mathcal{O}|P_c[\exp\{-\gamma\boldsymbol{r}^2+\boldsymbol{F}'\cdot\boldsymbol{r}\}\phi]\rangle\\&=q^2\left(\frac{\pi}{2\alpha}\right)^{3/2}\left\langle\exp\left\{\frac{1}{8\alpha}(\beta\boldsymbol{r}-\boldsymbol{E}+\beta\boldsymbol{r}'-\boldsymbol{E}'^*)^2\right\}\right.\\&\left.\times\exp\{-\gamma\boldsymbol{r}^2+\boldsymbol{F}\cdot\boldsymbol{r}\}\phi|\mathcal{O}|P_c[\exp\{-\gamma\boldsymbol{r}^2+\boldsymbol{F}'\cdot\boldsymbol{r}\}\phi]\right\rangle\\&=q^2\left(\frac{\pi}{2\alpha}\right)^{3/2}\exp\left\{\frac{1}{8\alpha}(\boldsymbol{E}^*+\boldsymbol{E}')^2\right\}\left\langle\exp\left\{\frac{\beta^2}{8\alpha}(\boldsymbol{r}+\boldsymbol{r}')^2\right\}\right.\\&\left.\times\exp\{-\gamma\boldsymbol{r}^2+\boldsymbol{G}\cdot\boldsymbol{r}\}\phi|\mathcal{O}|P_c[\exp\{-\gamma\boldsymbol{r}^2+\boldsymbol{G}'\cdot\boldsymbol{r}\}\phi]\right\rangle\\&=q^2\exp\left\{\frac{1}{8\alpha}(\boldsymbol{E}^*+\boldsymbol{E}')^2\right\}\langle\exp(-\alpha\boldsymbol{X}_G^2-\beta\boldsymbol{X}_G\cdot\boldsymbol{r})\exp(-\gamma\boldsymbol{r}^2+\boldsymbol{G}\cdot\boldsymbol{r})\phi|\mathcal{O}\\&\qquad\times|P_c[\exp(-\alpha\boldsymbol{X}_G^2-\beta\boldsymbol{X}_G\cdot\boldsymbol{r})\exp(-\gamma\boldsymbol{r}^2+\boldsymbol{G}'\cdot\boldsymbol{r})\phi]\rangle\end{aligned}$$

$$= \exp\left\{\frac{1}{8\alpha}(\boldsymbol{E}^*+\boldsymbol{E}')^2\right\}\langle \exp(\boldsymbol{G}\cdot\boldsymbol{r})\psi(C_1,0)\psi(C_2,0)\,|\mathcal{O}$$

$$\times |P_c[\exp(\boldsymbol{G}'\cdot\boldsymbol{r})\psi(C_1,0)\psi(C_2,0)]\rangle,$$

$$\boldsymbol{G}\equiv\boldsymbol{F}-\frac{\beta}{4\alpha}(\boldsymbol{E}+\boldsymbol{E}'^*), \qquad \boldsymbol{G}'\equiv\boldsymbol{F}'-\frac{\beta}{4\alpha}(\boldsymbol{E}^*+\boldsymbol{E}'). \tag{2·2·34}$$

Here we assumed that $\mathcal{O}$ does not contain differential operators and so commutes with $\boldsymbol{r}'$. From this equation we get

$$\mathcal{H}(\boldsymbol{R}_G,\boldsymbol{R};\boldsymbol{R}_G',\boldsymbol{R}') = \rho^*(\boldsymbol{R}_G,\boldsymbol{R})\rho(\boldsymbol{R}_G',\boldsymbol{R}')\exp\left\{\frac{1}{8\alpha}(\boldsymbol{E}^*+\boldsymbol{E}')^2\right\}$$

$$\times\langle \exp(\boldsymbol{G}\cdot\boldsymbol{r})\psi(C_1,0)\psi(C_2,0)\,|\mathcal{O}|\mathcal{A}\{\exp(\boldsymbol{G}'\cdot\boldsymbol{r})\psi(C_1,0)\psi(C_2,0)\}\rangle,$$

$$\boldsymbol{E}=2\alpha\boldsymbol{R}_G+\beta\boldsymbol{R}, \qquad \boldsymbol{E}'=2\alpha\boldsymbol{R}_G'+\beta\boldsymbol{R}',$$

$$\boldsymbol{G}=\left(2\gamma-\frac{\beta^2}{4\alpha}\right)\boldsymbol{R}+\frac{\beta}{2}\boldsymbol{R}_G-\frac{\beta^2}{4\alpha}\boldsymbol{R}'^*-\frac{\beta}{2}\boldsymbol{R}_G'^*,$$

$$\boldsymbol{G}'=\left(2\gamma-\frac{\beta^2}{4\alpha}\right)\boldsymbol{R}'+\frac{\beta}{2}\boldsymbol{R}_G'-\frac{\beta^2}{4\alpha}\boldsymbol{R}^*-\frac{\beta}{2}\boldsymbol{R}_G^*. \tag{2·2·35}$$

This equation clearly shows that the essential part of the GCM kernel in the case of the unequal oscillator parameters is also determined by a set of two vectors $\boldsymbol{G}$ and $\boldsymbol{G}'$ not by the original set of full four vectors $\boldsymbol{R}_G$, $\boldsymbol{R}$, $\boldsymbol{R}_G'$, $\boldsymbol{R}'$. The GCM kernels $\mathcal{H}$ with the GC$(\boldsymbol{R}_G,\boldsymbol{R},\boldsymbol{R}_G',\boldsymbol{R}')$ which give the same $\boldsymbol{G}$ and $\boldsymbol{G}'$ vectors are equated to each other by the simple multiplicative factors which are independent of the operator $\mathcal{O}$. Using this Eq. (2·2·35) we obtain a similar relation to Eq. (2·2·31) which expresses the general GCM kernel by the special GCM kernel of the type $\mathcal{H}((N_2/A)\boldsymbol{S},\boldsymbol{S};(N_2/A)\boldsymbol{S}',\boldsymbol{S}')$, as below,

$$\mathcal{H}(\boldsymbol{R}_G,\boldsymbol{R};\boldsymbol{R}_G',\boldsymbol{R}') = \frac{\rho^*(\boldsymbol{R}_G,\boldsymbol{R})\rho(\boldsymbol{R}_G',\boldsymbol{R}')}{\rho^*\left(\frac{N_2}{A}\boldsymbol{S},\boldsymbol{S}\right)\rho\left(\frac{N_2}{A}\boldsymbol{S}',\boldsymbol{S}'\right)}$$

$$\times\frac{\exp\left\{\frac{1}{8\alpha}(\boldsymbol{E}^*+\boldsymbol{E}')^2\right\}}{\exp\left\{\frac{(N_2\nu_2)^2}{2\alpha}(\boldsymbol{S}^*+\boldsymbol{S}')^2\right\}}\mathcal{H}\left(\frac{N_2}{A}\boldsymbol{S},\boldsymbol{S};\frac{N_2}{A}\boldsymbol{S}',\boldsymbol{S}'\right),$$

$$\boldsymbol{S}\equiv\frac{\alpha+A\nu_1}{4N_1N_2\nu_1\nu_2}\boldsymbol{G}+\frac{\nu_2-\nu_1}{4N_1\nu_1\nu_2}\boldsymbol{G}'^*,$$

$$\boldsymbol{S}'\equiv\frac{\alpha+A\nu_1}{4N_1N_2\nu_1\nu_2}\boldsymbol{G}'+\frac{\nu_2-\nu_1}{4N_1\nu_1\nu_2}\boldsymbol{G}^*. \tag{2·2·36}$$

As seen above in Eqs. (2·2·31) and (2·2·36) the GCM kernel can be reduced to the type,

$$\Theta\left(\frac{N_2}{A}\boldsymbol{S}, \boldsymbol{S}; \frac{N_2}{A}\boldsymbol{S}', \boldsymbol{S}'\right)$$
$$=\langle\psi(C_1, 0)\psi(C_2, \boldsymbol{S})|\mathcal{O}|\mathcal{A}\{\psi(C_1, 0)\psi(C_2, \boldsymbol{S}')\}\rangle. \qquad (2\cdot2\cdot37)$$

Since the position of the cluster C_1 in bra and in ket is the same in this matrix element, the sub-matrix of the overlap matrix B which is formed only by the orbitals in C_1 is unity. By choosing C_1 larger than $C_2(N_1\geq N_2)$ the matrix B is thus fairly simplified.

The case when a lighter cluster C_2 is a $0s$-shell cluster (like as n, d, t, α) the kernel $\Theta((N_2/A)\boldsymbol{S}, \boldsymbol{S}; (N_2/A)\boldsymbol{S}', \boldsymbol{S}')$ is calculated as follows.[32] By representing $\psi(C_2, \boldsymbol{S})$ as $(1/\sqrt{N_2!})\det\{\varphi_{0s,1}(\boldsymbol{S})\cdots\varphi_{0s,N_2}(\boldsymbol{S})\}$ we note the following relation,

$$\det\{\varphi_{C_1,1}\cdots\varphi_{C_1N_1}\varphi_{0s,1}(\boldsymbol{S})\cdots\varphi_{0s,N_2}(\boldsymbol{S})\}$$
$$=\det\{\varphi_{C_1,1}\cdots\varphi_{C_1,N_1}\hat{\varphi}_{0s,1}(\boldsymbol{S})\cdots\hat{\varphi}_{0s,N_2}(\boldsymbol{S})\}$$
$$\hat{\varphi}_{0s}(\boldsymbol{S})\equiv\varphi_{0s}(\boldsymbol{S})-\sum_{j=1}^{N_1}|\varphi_{C_1,j}\rangle\langle\varphi_{C_1,j}|\varphi_{0s}(\boldsymbol{S})\rangle, \qquad (2\cdot2\cdot38)$$

which gives us

$$\Theta\left(\frac{N_2}{A}\boldsymbol{S}, \boldsymbol{S}; \frac{N_2}{A}\boldsymbol{S}', \boldsymbol{S}'\right)$$
$$=\langle\varphi_{C_1,1}\cdots\varphi_{C_1,N_1}\hat{\varphi}_{0s,1}(\boldsymbol{S})\cdots\hat{\varphi}_{0s,N_2}(\boldsymbol{S})|\mathcal{O}$$
$$\times|\det\{\varphi_{C_1,1}\cdots\varphi_{C_1,N_1}\hat{\varphi}_{0s,1}(\boldsymbol{S}')\cdots\hat{\varphi}_{0s,N_2}(\boldsymbol{S}')\}\rangle$$
$$=\begin{cases}\text{(I)} & \text{for } \mathcal{O}=\sum_{i=1}^{A}\mathcal{O}_i,\\ \text{(II)} & \text{for } \mathcal{O}=\frac{1}{2}\sum_{i\neq j}^{A}\mathcal{O}_{ij},\end{cases}$$

$$\text{(I)}=\hat{p}^{N_2}\{\sum_{j=1}^{N_1}\langle\varphi_{C_1,j}|\mathcal{O}|\varphi_{C_1,j}\rangle+\hat{p}^{-1}\sum_{j=1}^{N_2}\langle\varphi_{0s,j}(\boldsymbol{S})|\mathcal{O}|\varphi_{0s,j}(\boldsymbol{S}')\rangle\},$$

$$\text{(II)}=\hat{p}^{N_2}\{\tfrac{1}{2}\sum_{i\neq j}^{N_1}\langle\varphi_{C_1,i}\varphi_{C_1,j}|\mathcal{O}|\varphi_{C_1,i}\varphi_{C_1,j}\rangle^a$$
$$+\hat{p}^{-2}\tfrac{1}{2}\sum_{i\neq j}^{N_2}\langle\hat{\varphi}_{0s,i}(\boldsymbol{S})\hat{\varphi}_{0s,j}(\boldsymbol{S})|\mathcal{O}|\hat{\varphi}_{0s,i}(\boldsymbol{S}')\hat{\varphi}_{0s,j}(\boldsymbol{S}')\rangle^a$$
$$+\hat{p}^{-1}\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\langle\varphi_{C_1,i}\hat{\varphi}_{0s,j}(\boldsymbol{S})|\mathcal{O}|\varphi_{C_1,i}\hat{\varphi}_{0s,j}(\boldsymbol{S}')\rangle^a\},$$

$$\hat{p}\equiv\langle\hat{\varphi}_{0s}(\boldsymbol{S})|\hat{\varphi}_{0s}(\boldsymbol{S}')\rangle=\langle\varphi_{0s}(\boldsymbol{S})|\hat{\varphi}_{0s}(\boldsymbol{S}')\rangle=\langle\hat{\varphi}_{0s}(\boldsymbol{S})|\varphi_{0s}(\boldsymbol{S}')\rangle,$$
$$|\varphi_1\varphi_2\rangle^a\equiv|\varphi_1\varphi_2\rangle-|\varphi_2\varphi_1\rangle. \qquad (2\cdot2\cdot39)$$

This is because the B matrix is now diagonal and is given by $B_{ij}=\hat{p}_i\delta_{ij}$ where $\hat{p}_i=1$ if $i\in C_1$ and $\hat{p}_i=\hat{p}=\langle\varphi_{0s}(\boldsymbol{S})|\varphi_{0s}(\boldsymbol{S}')\rangle$ if $i\in C_2$. When $\mathcal{O}$ is a two-nucleon

interaction V, the term in the above equation $\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\langle\varphi_{C_1,i}\varphi_{0s,j}(\boldsymbol{S})|V|\varphi_{C_1,i}\varphi_{0s,j}(\boldsymbol{S}')\rangle^a$ is expressed as $\sum_{j=1}^{N_2}\langle\varphi_{0s,j}(\boldsymbol{S})|U_{\mathrm{HF}}|\varphi_{0s,j}(\boldsymbol{S}')\rangle$ where the Hartree-Fock potential U_{HF} produced by the core (C_1) particles is defined by

$$\langle m|U_{\mathrm{HF}}|n\rangle\equiv\sum_{i=1}^{N_1}\langle m,\varphi_{C_1,i}|V|n,\varphi_{C_1,i}\rangle^a \qquad (2\cdot2\cdot40)$$

for arbitrary single particle states $|m\rangle$ and $|n\rangle$.

It is to be noted that the relations of Eqs. (2·2·31) and (2·2·36) are valid when we treat the direct GCM kernel simply by replacing $\mathcal{H}$ by $\mathcal{H}^D$ as is clear from the derivation of them. It is also easy to show that for $\mathcal{O}=V_r=\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}V_{ij}$ the corresponding kernel $\mathcal{H}^r$ of Eq. (2·1·23) is given by

$$\begin{aligned}&\mathcal{H}^r\left(\frac{N_2}{A}\boldsymbol{S},\boldsymbol{S};\frac{N_2}{A}\boldsymbol{S}',\boldsymbol{S}'\right)\\&=\hat{p}^{N_2-1}\sum_{i=1}^{N_2}\langle\varphi_{0s,i}(\boldsymbol{S})|U_{\mathrm{HF}}|\hat{\varphi}_{0s,i}(\boldsymbol{S}')\rangle\\&\quad-\hat{p}^{N_2-2}\sum_{i,j}^{N_2}\langle\varphi_{0s,i}(\boldsymbol{S})\varphi_{0s,j}(\boldsymbol{S})|V|\hat{\varphi}_{0s,i}(\boldsymbol{S}')\hat{\varphi}_{0s,j}(\boldsymbol{S}')\rangle^a.\end{aligned} \qquad (2\cdot2\cdot41)$$

2.2.c. *Decomposition of kernels according to the number of the nucleons exchanged*

Now we investigate the formulas of Eqs. (2·2·10)$\sim$(2·2·13) by examining the number of exchanged nucleons between clusters. For this, we consider two-cluster system, the wave function of which is given by

$$\begin{aligned}&\frac{1}{\sqrt{A!}}\det\{\varphi_{C_1,1}\cdots\varphi_{C_1,N_1}\varphi_{C_2,1}\cdots\varphi_{C_2,N_2}\}\\&=\frac{1}{\sqrt{\binom{A}{N_1}}}\mathcal{A}\{\psi(C_1,\boldsymbol{R}_1)\psi(C_2,\boldsymbol{R}_2)\}\\&=\frac{1}{\sqrt{\binom{A}{N_1}}}\sum_P\varepsilon(P)P\cdot\frac{1}{\sqrt{N_1!}}\det\{\varphi_{C_1,1}\cdots\varphi_{C_1,N_1}\}\\&\qquad\times\frac{1}{\sqrt{N_2!}}\det\{\varphi_{C_2,1}\cdots\varphi_{C_2,N_2}\},\end{aligned} \qquad (2\cdot2\cdot42)$$

where P denotes the permutation of nucleons between C_1 and C_2 and $\varepsilon(P)$ is the signature of P. Equation (2·2·42) is, of course, just the Laplace expansion of the single Slater determinant into the sum of the products of two Slater determinants. So following Eq. (2·2·2) we can rewrite Eq. (2·2·42) in a more concrete form,

$$\det\{\varphi_{C_1,1}\cdots\varphi_{C_1,N_1}\varphi_{C_2,1}\cdots\varphi_{C_2,N_2}\}$$

$$= \sum_{k_1<k_2<\cdots<k_{N_1}} (-)^{\sum_{i=1}^{N_1}(i+k_i)} \det\{\varphi_{c_1,1}(\boldsymbol{x}_{k_1}-\boldsymbol{R}_1)\cdots\varphi_{c_1,N_1}(\boldsymbol{x}_{k_{N_1}}-\boldsymbol{R}_1)\}$$
$$\times \det\{\varphi_{c_2,1}(\boldsymbol{x}_{p_1}-\boldsymbol{R}_2)\cdots\varphi_{c_2,N_2}(\boldsymbol{x}_{p_{N_2}}-\boldsymbol{R}_2)\}, \qquad (2\cdot2\cdot43)$$

where $(p_1, p_2, \cdots p_{N_2})$ are the numbers which are left after subtracting the set of numbers $(k_1, k_2, \cdots k_{N_1})$ from $(1, 2, \cdots A)$ and satisfy $p_1<p_2<\cdots<p_{N_2}$. By using Eq. (2·2·43) we re-calculate the kernels of Eqs. (2·2·10), (2·2·11) and (2·2·13).

First the overlap is

$$\langle\varphi_1(1)\cdots\varphi_{N_1}(N_1)\varphi_{N_1+1}(N_1+1)\cdots\varphi_A(A)|$$
$$\times\det\{\varphi_1'(1)\cdots\varphi_{N_1}'(N_1)\varphi_{N_1+1}'(N_1+1)\cdots\varphi_A'(A)\}\rangle$$
$$= \sum_{\sigma_1<\sigma_2<\cdots<\sigma_{N_1}} (-)^{\sum_{i=1}^{N_1}(i+\sigma_i)}\langle\varphi_{\sigma_1}(\sigma_1)\cdots\varphi_{\sigma_{N_1}}(\sigma_{N_1})\varphi_{\sigma_{N_1+1}}(\sigma_{N_1+1})\cdots\varphi_{\sigma_A}(\sigma_A)|$$
$$\times\det\{\varphi_1'(\sigma_1)\cdots\varphi_{N_1}'(\sigma_{N_1})\}\det\{\varphi_{N_1+1}'(\sigma_{N_1+1})\cdots\varphi_A'(\sigma_A)\}\rangle$$
$$= \sum_{\sigma_1<\sigma_2<\cdots<\sigma_{N_1}} (-)^{\sum_{i=1}^{N_1}(i+\sigma_i)} \begin{vmatrix} \langle\varphi_{\sigma_1}|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_{\sigma_1}|\varphi_{N_1}'\rangle \\ \vdots & & \vdots \\ \langle\varphi_{\sigma_{N_1}}|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_{\sigma_{N_1}}|\varphi_{N_1}'\rangle \end{vmatrix}$$
$$\times \begin{vmatrix} \langle\varphi_{\sigma_{N_1+1}}|\varphi_{N_1+1}'\rangle & \cdots\cdots & \langle\varphi_{\sigma_{N_1+1}}|\varphi_A'\rangle \\ \vdots & & \vdots \\ \langle\varphi_{\sigma_A}|\varphi_{N_1+1}'\rangle & \cdots\cdots & \langle\varphi_{\sigma_A}|\varphi_A'\rangle \end{vmatrix}, \qquad (2\cdot2\cdot44)$$

where we denoted $\varphi_{c_2,i}$ by φ_{N_1+i}, $\varphi'_{c_2,i}$ as φ'_{N_1+i} and $(k_1, \cdots k_{N_1}, p_1, \cdots p_{N_2})$ as $(\sigma_1, \cdots \sigma_{N_1}, \sigma_{N_1+1}, \cdots \sigma_A)$. This is just the Laplace expansion of the overlap determinant $\det\cdot B$ of Eq. (2·2·12),

$$\det\cdot B = \begin{vmatrix} B^{\mathrm{I}} & B^{\mathrm{I\,II}} \\ B^{\mathrm{II\,I}} & B^{\mathrm{II}} \end{vmatrix}, \quad B^{\mathrm{I}} = \begin{pmatrix} \langle\varphi_1|\varphi_1'\rangle & \cdots & \langle\varphi_1|\varphi_{N_1}'\rangle \\ \vdots & & \vdots \\ \langle\varphi_{N_1}|\varphi_1'\rangle & \cdots & \langle\varphi_{N_1}|\varphi_{N_1}'\rangle \end{pmatrix},$$
$$B^{\mathrm{II}} = \begin{pmatrix} \langle\varphi_{N_1+1}|\varphi_{N_1+1}'\rangle & \cdots & \langle\varphi_{N_1+1}|\varphi_A'\rangle \\ \vdots & & \vdots \\ \langle\varphi_A|\varphi_{N_1+1}'\rangle & \cdots\cdots & \langle\varphi_A|\varphi_A'\rangle \end{pmatrix}, \quad B^{\mathrm{I\,II}} = \begin{pmatrix} \langle\varphi_1|\varphi_{N_1+1}'\rangle & \cdots & \langle\varphi_1|\varphi_A'\rangle \\ \vdots & & \vdots \\ \langle\varphi_{N_1}|\varphi_{N_1+1}'\rangle & \cdots & \langle\varphi_{N_1}|\varphi_A'\rangle \end{pmatrix},$$
$$B^{\mathrm{II\,I}} = \begin{pmatrix} \langle\varphi_{N_1+1}|\varphi_1'\rangle & \cdots & \langle\varphi_{N_1+1}|\varphi_{N_1}'\rangle \\ \vdots & & \vdots \\ \langle\varphi_A|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_A|\varphi_{N_1}'\rangle \end{pmatrix}. \qquad (2\cdot2\cdot45)$$

From the above procedure we can express the full overlap kernel (OV.K.) as the sum of the partial overlap kernel $(\mathrm{OV.K.})_n$ which is coming from the n-particle exchange part of the wave function as follows:

$$(\mathrm{OV.K.}) = \sum_{n=0}(\mathrm{OV.K.})_n,$$
$$(\mathrm{OV.K.})_n = \sum_{(\sigma_1<\sigma_2<\cdots<\sigma_{N_1})}^{(n)} (-)^{\sum_{i=1}^{N_1}(i+\sigma_i)} \begin{vmatrix} \langle\varphi_{\sigma_1}|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_{\sigma_1}|\varphi_{N_1}'\rangle \\ \vdots & & \vdots \\ \langle\varphi_{\sigma_{N_1}}|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_{\sigma_{N_1}}|\varphi_{N_1}'\rangle \end{vmatrix}$$

$$\times\begin{vmatrix}\langle\varphi_{\sigma_{N_1+1}}|\varphi'_{N_1+1}\rangle & \cdots\cdots & \langle\varphi_{\sigma_{N_1+1}}|\varphi_A'\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_A}|\varphi'_{N_1+1}\rangle & \cdots\cdots & \langle\varphi_{\sigma_A}|\varphi_A'\rangle\end{vmatrix}, \qquad (2\cdot2\cdot46)$$

where $\sum^{(n)}$ means to sum over those $(\sigma_1, \cdots, \sigma_{N_1})$ in which the number of σ_i satisfying $\sigma_i > N_1$ is just n. Therefore, it is clear that $(\mathrm{OV.K.})_n$ are obtained from the following relation,[9]

$$\det\cdot B(\lambda) = \sum_{n=0} \lambda^{2n} (\mathrm{OV.K.})_n ,$$

$$B(\lambda) \equiv \begin{pmatrix} B^{\mathrm{I}} & \lambda B^{\mathrm{I\,II}} \\ \lambda B^{\mathrm{II\,I}} & B^{\mathrm{II}} \end{pmatrix}. \qquad (2\cdot2\cdot47)^{*)}$$

The direct overlap kernel is obtained by putting $\lambda=0$ in Eq. (2·2·47) resulting $(\mathrm{OV.K.})_{\mathrm{direct}} = (\mathrm{OV.K.})_{n=0} = \det(B^{\mathrm{I}}) \det(B^{\mathrm{II}})$. Next, for the one-body operator, by using $\sum_i \mathcal{O}_i = \sum_i \mathcal{O}_{\sigma_i}$, we get

$$\begin{aligned}&\langle\varphi_1(1)\cdots\varphi_A(A)\,|\sum_{i=1}^{A}\mathcal{O}_i|\,\det\{\varphi_1(1)\cdots\varphi_A(A)\}\rangle\\ &=\sum_{(\sigma_1<\sigma_2<\cdots<\sigma_{N_1})}(-)^{\sum_{i=1}^{N_1}(i+\sigma_i)}\left\{\sum_{i=1}^{N_1}\begin{vmatrix}\langle\varphi_{\sigma_1}|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_{\sigma_1}|\varphi'_{N_1}\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_i}|\mathcal{O}|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_{\sigma_i}|\mathcal{O}|\varphi'_{N_1}\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_{N_1}}|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_{\sigma_{N_1}}|\varphi'_{N_1}\rangle\end{vmatrix}\right.\\ &\qquad\times\begin{vmatrix}\langle\varphi_{\sigma_{N_1+1}}|\varphi'_{N_1+1}\rangle & \cdots\cdots & \langle\varphi_{\sigma_{N_1+1}}|\varphi_A'\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_A}|\varphi'_{N_1+1}\rangle & \cdots\cdots & \langle\varphi_{\sigma_A}|\varphi_A'\rangle\end{vmatrix}\\ &\left.+\begin{vmatrix}\langle\varphi_{\sigma_1}|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_{\sigma_1}|\varphi'_{N_1}\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_{N_1}}|\varphi_1'\rangle & \cdots\cdots & \langle\varphi_{\sigma_{N_1}}|\varphi'_{N_1}\rangle\end{vmatrix}\cdot\sum_{i=N_1+1}^{A}\begin{vmatrix}\langle\varphi_{\sigma_{N_1+1}}|\varphi'_{N_1+1}\rangle & \cdots\cdots & \langle\varphi_{\sigma_{N_1+1}}|\varphi_A'\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_i}|\mathcal{O}|\varphi'_{N_1+1}\rangle & \cdots\cdots & \langle\varphi_{\sigma_i}|\mathcal{O}|\varphi_A'\rangle\\ \vdots & & \vdots\\ \langle\varphi_{\sigma_A}|\varphi'_{N_1+1}\rangle & \cdots\cdots & \langle\varphi_{\sigma_A}|\varphi_A'\rangle\end{vmatrix}\right\}.\end{aligned} \qquad (2\cdot2\cdot48)$$

Thus by a similar argument to the above we can decompose the one-body operator kernel (OB.K.) as the sum of $(\mathrm{OB.K.})_n$ which are defined in entirely the same manner as $(\mathrm{OV.K.})_n$, as follows:

$$(\mathrm{OB.K.}) = \sum_{n=0} (\mathrm{OB.K.})_n ,$$

$$(\mathrm{OB.K.})(\lambda) = \sum_{n=0} \lambda^{2n} (\mathrm{OB.K.})_n ,$$

$$(\mathrm{OB.K.})(\lambda)$$

*) We note the relations

$$\begin{vmatrix} B^{\mathrm{I}} & \lambda B^{\mathrm{I\,II}} \\ \lambda B^{\mathrm{II\,I}} & B^{\mathrm{II}} \end{vmatrix} = \begin{vmatrix} B^{\mathrm{I}} & B^{\mathrm{I\,II}} \\ \lambda^2 B^{\mathrm{II\,I}} & B^{\mathrm{II}} \end{vmatrix} = \begin{vmatrix} B^{\mathrm{I}} & \lambda^2 B^{\mathrm{I\,II}} \\ B^{\mathrm{II\,I}} & B^{\mathrm{II}} \end{vmatrix}.$$

$$\equiv \sum_{i=1}^{N_1} \begin{vmatrix} \langle\varphi_1|\varphi_1'\rangle & \cdots & \langle\varphi_1|\varphi_{N_1}'\rangle & \lambda\langle\varphi_1|\varphi_{N_1+1}'\rangle & \cdots & \lambda\langle\varphi_1|\varphi_A'\rangle \\ \langle\varphi_i|\mathcal{O}|\varphi_1'\rangle & \cdots & \langle\varphi_i|\mathcal{O}|\varphi_{N_1}'\rangle & \lambda\langle\varphi_i|\mathcal{O}|\varphi_{N_1+1}'\rangle & \cdots & \lambda\langle\varphi_i|\mathcal{O}|\varphi_A'\rangle \\ \langle\varphi_{N_1}|\varphi_1'\rangle & \cdots & \langle\varphi_{N_1}|\varphi_{N_1}'\rangle & \lambda\langle\varphi_{N_1}|\varphi_{N_1+1}'\rangle & \cdots & \lambda\langle\varphi_{N_1}|\varphi_A'\rangle \\ \multicolumn{3}{c}{\lambda B^{\mathrm{II\,I}}} & \multicolumn{3}{c}{B^{\mathrm{II}}} \end{vmatrix}$$

$$+ \sum_{i=N_1+1}^{A} \begin{vmatrix} \multicolumn{3}{c}{B^{\mathrm{I}}} & \multicolumn{3}{c}{\lambda B^{\mathrm{I\,II}}} \\ \lambda\langle\varphi_{N_1+1}|\varphi_1'\rangle & \cdots & \lambda\langle\varphi_{N_1+1}|\varphi_{N_1}'\rangle & \langle\varphi_{N_1+1}|\varphi_{N_1+1}'\rangle & \cdots & \langle\varphi_{N_1+1}|\varphi_A'\rangle \\ \lambda\langle\varphi_i|\mathcal{O}|\varphi_1'\rangle & \cdots & \lambda\langle\varphi_i|\mathcal{O}|\varphi_{N_1}'\rangle & \langle\varphi_i|\mathcal{O}|\varphi_{N_1+1}'\rangle & \cdots & \langle\varphi_i|\mathcal{O}|\varphi_A'\rangle \\ \lambda\langle\varphi_A|\varphi_1'\rangle & \cdots & \lambda\langle\varphi_A|\varphi_{N_1}'\rangle & \langle\varphi_A|\varphi_{N_1+1}'\rangle & \cdots & \langle\varphi_A|\varphi_A'\rangle \end{vmatrix}. \tag{2·2·49}$$

We can calculate (OB.K.) (λ) by the following formula,

$$(\mathrm{OB.K.})\,(\lambda) = \{\det\cdot B(\lambda)\}\sum_{i,j}^{A} \lambda_{ij}\langle\varphi_i|\mathcal{O}|\varphi_j'\rangle (B(\lambda)^{-1})_{ji},$$

$$\lambda_{ij} = \begin{cases} \lambda & \text{for } (1\leq i\leq N_1,\ N_1<j\leq A) \text{ or } (N_1<i\leq A,\ 1\leq j\leq N_1), \\ 1 & \text{for other } (i,j). \end{cases} \tag{2·2·50}$$

Similarly for the two-body operator kernel (TB.K.), we get

$$(\mathrm{TB.K.}) = \sum_{n=0} (\mathrm{TB.K.})_n,$$

$$(\mathrm{TB.K.})\,(\lambda) = \sum_{n=0} \lambda^{2n} (\mathrm{TB.K.})_n,$$

$$(\mathrm{TB.K.})\,(\lambda) = \{\det\cdot B(\lambda)\}\sum_{ijkl} \lambda_{ijkl}\langle\varphi_i\varphi_j|\mathcal{O}|\varphi_k'\varphi_l'\rangle$$

$$\times\{(B(\lambda)^{-1})_{ki}(B(\lambda)^{-1})_{lj} - (B(\lambda)^{-1})_{kj}(B(\lambda)^{-1})_{li}\},$$

$$\lambda_{ijkl} = \begin{cases} \lambda^2 & \text{for } (i,k),\ (j,l)\in N^{\mathrm{I\,II}} \\ \lambda & \text{for } (i,k)\in N^{\mathrm{I\,II}},\ (j,l)\notin N^{\mathrm{I\,II}}, \\ & \text{or} \\ & \text{for } (i,k)\notin N^{\mathrm{I\,II}},\ (j,l)\in N^{\mathrm{I\,II}} \\ 1 & \text{for } (i,k),\ (j,l)\notin N^{\mathrm{I\,II}}, \end{cases} \tag{2·2·51}$$

where $(p,q)\in N^{\mathrm{I\,II}}$ means $(N_1<p\leq A,\ 1\leq q\leq N_1)$ or $(1\leq p\leq N_1,\ N_1<q\leq A)$. Both in Eqs. (2·2·49) and (2·2·51), we obtain the direct kernels calculated in § 2.2.a. by putting $\lambda=0$.

2.2.d. *Range of kernels*

We denote the $0s$ single-particle H.O. wave function around $\boldsymbol{R}_i$ as $\varphi_{i,0s} = (2\nu_i/\pi)^{3/4}\exp\{-\nu_i(x-\boldsymbol{R}_i)^2\}$. $0p$ orbit wave functions are obtained by the differentiation of $\varphi_{i,0s}$ by $\boldsymbol{R}_i$; for example, $\varphi_{i,0p_x} = \nu_i^{-1/2}(\partial/\partial R_{ix})\varphi_{i,0s}$. If we have

the matrix elements by only the $0s$ orbits, the differentiations of them with respect to the GC ($\boldsymbol{R}_i$) give the matrix elements by higher orbitals such as $0p$, $1s$, $0d$ and so on. We give below some formulas of the matrix elements by $0s$ orbitals;[18),33),34)]

$$
\begin{aligned}
&B_{ij}\equiv\langle\varphi_{i,0s}|\varphi_{j,0s}\rangle=\left(\frac{2\sqrt{\nu_i\nu_j}}{\nu_i+\nu_j}\right)^{3/2}\exp\left\{-\frac{\nu_i\nu_j}{\nu_i+\nu_j}(\boldsymbol{R}_i-\boldsymbol{R}_j)^2\right\},\\
&\langle\varphi_{i,0s}|\left(\frac{-\hbar^2}{2m}\nabla^2\right)|\varphi_{j,0s}\rangle=B_{ij}\frac{\hbar^2}{2m}\frac{\nu_i\nu_j}{\nu_i+\nu_j}\left\{3-\frac{2\nu_i\nu_j}{\nu_i+\nu_j}(\boldsymbol{R}_i-\boldsymbol{R}_j)^2\right\},\\
&\langle\varphi_{i,0s}|y_{k\nu}(\boldsymbol{x})|\varphi_{j,0s}\rangle=B_{ij}y_{k\nu}(\boldsymbol{A}_{ij}),\\
&\langle\varphi_{i,0s}\varphi_{j,0s}|e^{-\mu(\boldsymbol{x}_1-\boldsymbol{x}_2)^2}|\varphi_{k,0s}\varphi_{l,0s}\rangle=B_{ik}B_{jl}C^{3/2}e^{-(1-C)\boldsymbol{D}^2},\\
&\langle\varphi_{i,0s}\varphi_{j,0s}|\frac{1}{|\boldsymbol{x}_1-\boldsymbol{x}_2|}|\varphi_{k,0s}\varphi_{l,0s}\rangle=B_{ik}B_{jl}\frac{\mathrm{erf}(|\boldsymbol{D}|)}{\sqrt{2(a_{ik}+a_{jl})}|\boldsymbol{D}|},\\
&a_{ij}\equiv\frac{1}{\nu_i+\nu_j},\qquad \boldsymbol{A}_{ij}\equiv a_{ij}(\nu_i\boldsymbol{R}_i+\nu_j\boldsymbol{R}_j),\\
&C\equiv 1/[1+\mu(a_{ik}+a_{jl})],\qquad \boldsymbol{D}\equiv(\boldsymbol{A}_{ik}-\boldsymbol{A}_{jl})/\sqrt{a_{ik}+a_{jl}},\\
&\mathrm{erf}(x)\equiv(2/\sqrt{\pi})\int_0^x e^{-t^2}dt,\qquad y_{k\nu}(\boldsymbol{x})\equiv x^kY_{k\nu}(\hat{x}).
\end{aligned}
\tag{2·2·52}
$$

For further details, see Refs. 11), 18), 33), 34).

We discuss the range of the GCM kernels below by using Eq. (2·2·52) in the case of the equal oscillator widths $\nu=\nu_1=\nu_2=\cdots$. Usually, the GCM kernels are the sum of terms each of which is the product of the polynomial part of GC's and the Gaussian part of GC's. In the case of the Coulomb interaction kernel there appear the terms which are the product of the error function of GC's and the Gaussian function of GC's. The important factor to determine the range of the GCM kernel is the form of the Gaussian parts of the kernel. What we discuss here is how the Gaussian parts of the GCM kernels are. We will see in the following that the Gaussian parts of the GCM kernels are governed by the number of the exchanged nucleons between clusters.

First we consider the overlap kernel. The Gaussian parts of the matrix elements of overlap matrix B are the same within the same submatrices B^{I}, $B^{\mathrm{I\,II}}$, $B^{\mathrm{II\,I}}$, B^{II} in Eq. (2·2·45). The Gaussian parts of the matrix elements of the submatrix B^{I} are all of the form $\exp\{-(\nu/2)(\boldsymbol{R}_1-\boldsymbol{R}_1')^2\}$, and similarly for $B^{\mathrm{I\,II}}$, $B^{\mathrm{II\,I}}$, B^{II} they are $\exp\{-(\nu/2)(\boldsymbol{R}_1-\boldsymbol{R}_2')^2\}$, $\exp\{-(\nu/2)\times(\boldsymbol{R}_2-\boldsymbol{R}_1')^2\}$, $\exp\{-(\nu/2)(\boldsymbol{R}_2-\boldsymbol{R}_2')^2\}$, respectively, where $\boldsymbol{R}_1=(-N_2/A)\boldsymbol{R}$, $\boldsymbol{R}_2=(N_1/A)\boldsymbol{R}$, $\boldsymbol{R}_1'=(-N_2/A)\boldsymbol{R}'$, $\boldsymbol{R}_2'=(N_1/A)\boldsymbol{R}'$. From the arguments leading to Eq. (2·2·47) it is clear that $(\mathrm{OV.K.})_n$ has a Gaussian part of the form[8)~13)]

$$\left[\exp\left\{-\frac{\nu}{2}(\boldsymbol{R}_1-\boldsymbol{R}_1')^2\right\}\right]^{N_1-n}\left[\exp\left\{-\frac{\nu}{2}(\boldsymbol{R}_2-\boldsymbol{R}_2')^2\right\}\right]^{N_2-n}$$
$$\times\left[\exp\left\{-\frac{\nu}{2}\{(\boldsymbol{R}_1-\boldsymbol{R}_2')^2+(\boldsymbol{R}_2-\boldsymbol{R}_1')^2\}\right\}\right]^n$$
$$=\exp\left[-\frac{\nu}{2}\left\{(N_1-n)\left(\frac{N_1}{A}\right)^2(\boldsymbol{R}-\boldsymbol{R}')^2+(N_2-n)\left(\frac{N_2}{A}\right)^2(\boldsymbol{R}-\boldsymbol{R}')^2\right.\right.$$
$$\left.\left.+\frac{n}{A^2}(N_2\boldsymbol{R}+N_1\boldsymbol{R}')^2+\frac{n}{A^2}(N_1\boldsymbol{R}+N_2\boldsymbol{R}')^2\right\}\right]$$
$$=\exp\left\{-\frac{\nu}{4}\left(\frac{2N_1N_2}{A}-n\right)(\boldsymbol{R}-\boldsymbol{R}')^2-\frac{\nu}{4}n(\boldsymbol{R}+\boldsymbol{R}')^2\right\}$$
$$=\exp\left\{-\frac{N_1N_2}{2A}\nu(\boldsymbol{R}-\boldsymbol{R}')^2-n\nu\boldsymbol{R}\cdot\boldsymbol{R}'\right\}$$
$$=\exp\left\{-\frac{N_1N_2}{2A}\nu(R^2+R'^2)+\left(\frac{N_1N_2}{A}-n\right)\nu\boldsymbol{R}\cdot\boldsymbol{R}'\right\}. \qquad (2\cdot2\cdot53)$$

In the case of the kernels of the one-body operators like as the kinetic energy and the multipole operators, we see from Eq. (2·2·52) and from the arguments leading to Eq. (2·2·50) that the Gaussian part of $(\mathrm{OB.K.})_n$ is the same as that of the overlap kernel given in Eq. (2·2·53). Finally we consider the kernels of the two-body operators. As a representative example we study the kernel of the single-range Gaussian interaction operator $\sum_{i\neq j}\exp\{-\mu(\boldsymbol{x}_i-\boldsymbol{x}_j)^2\}$. From Eq. (2·2·52) we know that, in the present case of the equal oscillator widths, $\langle\varphi_{i,0s}\varphi_{j,0s}|\exp\{-\mu(\boldsymbol{x}_1-\boldsymbol{x}_2)^2\}|\varphi_{k,0s}\varphi_{l,0s}\rangle=B_{ik}B_{jl}\{\nu/(\nu+\mu)\}^{3/2}\exp\{-\nu_\mu(\boldsymbol{R}_i-\boldsymbol{R}_j+\boldsymbol{R}_k-\boldsymbol{R}_l)^2\}$ where $\nu_\mu\equiv\nu\mu/\{4(\nu+\mu)\}$. Then, from the argument leading to Eq. (2·2·51) we see that the Gaussian parts of $(\mathrm{TB.K.})_n$ have five possible forms each of which is the product of the term of Eq. (2·2·53) with one of the following five terms: 1, $\exp\{-\nu_\mu\boldsymbol{R}^2\}$, $\exp\{-\nu_\mu\boldsymbol{R}'^2\}$, $\exp\{-\nu_\mu\cdot(\boldsymbol{R}-\boldsymbol{R}')^2\}$ and $\exp\{-\nu_\mu(\boldsymbol{R}+\boldsymbol{R}')^2\}$.

§ 3. Calculation of RGM kernels

— Transformation from GCM to RGM —

3.1. RGM wave function and kernel

For the sake of notations, we here discuss the form of the wave function and kernel in the RGM framework.[3),36),37)] The wave function in RGM has the following form in the case of the system composed of two spin zero clusters,

$$n_0\mathcal{A}\{\chi(\boldsymbol{r})\phi_0(C_1)\phi_0(C_2)\}=\int d\boldsymbol{a}\chi(\boldsymbol{a})n_0\mathcal{A}\{\delta(\boldsymbol{r}-\boldsymbol{a})\phi_0(C_1)\phi_0(C_2)\},$$
$$n_0\equiv\sqrt{N_1!N_2!/A!}. \qquad (3\cdot1\cdot1)$$

The matrix element of the operator $\mathcal{O}$ with these wave functions is

$$\langle n_0\mathcal{A}\{\chi_1(\boldsymbol{r})\phi_0(C_1)\phi_0(C_2)\}|\mathcal{O}|n_0\mathcal{A}\{\chi_2(\boldsymbol{r})\phi_0(C_1)\phi_0(C_2)\}\rangle$$
$$=\int d\boldsymbol{a}_1 d\boldsymbol{a}_2 \chi_1^*(\boldsymbol{a}_1)\chi_2(\boldsymbol{a}_2)m(\boldsymbol{a}_1,\boldsymbol{a}_2),$$

$$m(\boldsymbol{a}_1,\boldsymbol{a}_2)\equiv\langle\delta(\boldsymbol{r}-\boldsymbol{a}_1)\phi_0(C_1)\phi_0(C_2)|\mathcal{O}|\mathcal{A}\{\delta(\boldsymbol{r}-\boldsymbol{a}_2)\phi_0(C_1)\phi_0(C_2)\}\rangle. \quad (3\cdot1\cdot2)$$

$m(\boldsymbol{a}_1,\boldsymbol{a}_2)$ is called the RGM (integral) kernel of the operator $\mathcal{O}$.

For the multi-cluster system, the RGM wave function has the form $\mathcal{A}\{\chi(\boldsymbol{\xi}_1,\cdots,\boldsymbol{\xi}_{n-1})\prod_{i=1}^{n}\phi_0(C_i)\}$ where $\boldsymbol{\xi}_i$ are the relative coordinates of n clusters (such as Jacobi coordinates), and the RGM kernel of the operator $\mathcal{O}$ is

$$m(\boldsymbol{a}_1,\cdots,\boldsymbol{a}_{n-1};\boldsymbol{b}_1,\cdots,\boldsymbol{b}_{n-1})$$
$$=\langle\prod_{i=1}^{n-1}\delta(\boldsymbol{\xi}_i-\boldsymbol{a}_i)\prod_{i=1}^{n}\phi_0(C_i)|\mathcal{O}|\mathcal{A}\{\prod_{i=1}^{n-1}\delta(\boldsymbol{\xi}_i-\boldsymbol{b}_i)\prod_{i=1}^{n}\phi_0(C_i)\}\rangle. \quad (3\cdot1\cdot3)$$

The RGM wave function of the system including rearrangement channels has the following form,

$$\sum_\alpha\frac{1}{\sqrt{\binom{A}{N_{\alpha1}}}}\mathcal{A}_\alpha\{\chi_\alpha(\boldsymbol{r}_\alpha)\phi(C_{\alpha1})\phi(C_{\alpha2})\}. \quad (3\cdot1\cdot4)$$

The RGM kernels necessary for this system are

$$m_{\alpha,\beta}(\boldsymbol{a}_\alpha,\boldsymbol{a}_\beta)=\frac{1}{\sqrt{\binom{A}{N_{\alpha1}}\binom{A}{N_{\beta1}}}}\langle\mathcal{A}_\alpha\{\delta(\boldsymbol{r}_\alpha-\boldsymbol{a}_\alpha)\phi(C_{\alpha1})\phi(C_{\alpha2})\}$$
$$\times|\mathcal{O}|\mathcal{A}_\beta\{\delta(\boldsymbol{r}_\beta-\boldsymbol{a}_\beta)\phi(C_{\beta1})\phi(C_{\beta2})\}\rangle. \quad (3\cdot1\cdot5)$$

When we treat the relative motion with definite angular momentum, $\chi(\boldsymbol{r})$ is $\chi_L(r)Y_{LM}(\hat{r})$ and the necessary kernel is

$$m_{L_1M_1L_2M_2}(a_1,a_2)=\left\langle\frac{\delta(r-a_1)}{a_1^2}h_{L_1M_1}|\mathcal{O}|\mathcal{A}\left\{\frac{\delta(r-a_2)}{a_2^2}h_{L_2M_2}\right\}\right\rangle,$$

$$h_{LM}\equiv Y_{LM}(\hat{r})\phi_0(C_1)\phi_0(C_2). \quad (3\cdot1\cdot6)$$

Similarly for the multi-cluster system, $\chi(\boldsymbol{\xi}_1,\cdots,\boldsymbol{\xi}_{n-1})$ is $\chi_{L,\alpha}(\xi_1,\cdots,\xi_{n-1})Y_{LM,\alpha}(\hat{\xi}_1,\cdots,\hat{\xi}_{n-1})$ where the definition of $Y_{LM,\alpha}$ is given in Eq. (2·1·15) and the kernel is

$$m^{\alpha_1\alpha_2}_{L_1M_1L_2M_2}(a_1,\cdots,a_{n-1};b_1,\cdots,b_{n-1})$$
$$=\left\langle\prod_{i=1}^{n-1}\frac{\delta(\xi_i-a_i)}{a_i^2}h_{L_1M_1,\alpha_1}|\mathcal{O}|\mathcal{A}\left\{\prod_{i=1}^{n-1}\frac{\delta(\xi_i-b_i)}{b_i^2}h_{L_2M_2,\alpha_2}\right\}\right\rangle, \quad (3\cdot1\cdot7)$$

where the channel wave function $h_{LM,\alpha}$ is defined in Eq. (2·1·15).

The channel coupling systems which involve the excitation of clusters are treated similarly. As an example, the two-cluster system where one cluster

C_1 is allowed to be excited, is described by the wave function

$$\mathcal{A}\{\chi_{J,i}(r)\, h_i^{JM}\},$$
$$h_i^{JM} \equiv [Y_{L_1}(\hat{r})\, \phi_{L_2}(C_1)]_{JM} \phi_0(C_2),$$
$$i \equiv (L_1, L_2). \tag{3·1·8}$$

The RGM kernel for this system is

$$\left\langle \frac{\delta(r-a_1)}{a_1^2} h_i^{J_1 M_1} | \mathcal{O} | \mathcal{A}\left\{ \frac{\delta(r-a_2)}{a_2^2} h_j^{J_2 M_2} \right\} \right\rangle. \tag{3·1·9}$$

The above RGM kernels corresponding to the RGM wave functions with definite angular momentum are calculated by the angular momentum projection of the non-projected kernels m. For example, the kernel of Eq. (3·1·7) is obtained from the kernel of Eq. (3·1·3) as follows:

$$m^{\alpha_1 \alpha_2}_{L_1 M_1 L_2 M_2}(a_1, \cdots; b_1, \cdots)$$
$$= \int (\prod_{i=1}^{n-1} d\hat{a}_i) (\prod_{j=1}^{n-1} d\hat{b}_j) Y^*_{L_1 M_1, \alpha_1}(\hat{a}_1, \cdots) Y_{L_2 M_2, \alpha_2}(\hat{b}_1, \cdots) m(\boldsymbol{a}_1, \cdots; \boldsymbol{b}_1, \cdots). \tag{3·1·10}$$

The RGM wave functions are often expressed by the linear superposition of the suitable basis wave functions like as

$$\chi(\boldsymbol{r}) = \sum_i c_i u_i(\boldsymbol{r}). \tag{3·1·11}$$

Usual choices for $\{u_i(\boldsymbol{r})\}$ are the H.O. functions $\{R_{Nl}(r)\, Y_{lm}(\hat{r})\}$ or the Gaussian wave packets with variable width parameters $\exp\{-\gamma_i r^2\} r^l Y_{lm}(\hat{r})$. The kernels necessary for this kind of wave functions are

$$\hat{m}(i,j) = \langle u_i(\boldsymbol{r})\, \phi_0(C_1)\, \phi_0(C_2) | \mathcal{O} | \mathcal{A}\{u_j(\boldsymbol{r})\, \phi_0(C_1)\, \phi_0(C_2)\} \rangle. \tag{3·1·12}$$

3.2. Transformation of wave function

3.2.a. *Gaussian transformation*

The transformation of the kernels between GCM and RGM is based on that of the wave functions between two methods. We therefore first discuss the relation between GCM and RGM wave functions for the preparation to later investigations. (See also the discussion in Chap. II.) The oscillator widths of all the cluster wave functions in the system are taken to be the same in the arguments of §§ 3.2 and 3.3. The more realistic case of unequal oscillator widths of clusters can be treated in almost similar ways and is discussed in § 3.4.

For the case of the system of two H.O. closed shell clusters, the GCM wave function is written as follows, as is discussed in § 2.1,

$$\Psi \propto \int d\boldsymbol{R} f(\boldsymbol{R}) \mathcal{A}\left\{ \phi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right) \phi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right) \right\}$$

$$= \mathcal{A}\{\chi(\boldsymbol{r})\phi_0(C_1)\phi_0(C_2)\}\omega_0(\boldsymbol{X}_G),$$

$$\chi(\boldsymbol{r}) = \int d\boldsymbol{R} \Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma) f(\boldsymbol{R}), \tag{3·2·1}$$

where

$\phi_0(C_i, \boldsymbol{R})$ = H.O. closed shell wave function centered around $\boldsymbol{R}$

$$= \left(\frac{2N_i\nu}{\pi}\right)^{3/4} e^{-N_i\nu(\boldsymbol{X}_i-\boldsymbol{R})^2}\phi_0(C_i),$$

$$\omega_0(\boldsymbol{X}_G) \equiv \left(\frac{2A\nu}{\pi}\right)^{3/4} e^{-A\nu\boldsymbol{X}_G^2}, \qquad A = N_1+N_2,$$

$$\Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma) \equiv \left(\frac{2\gamma}{\pi}\right)^{3/4} e^{-\gamma(\boldsymbol{r}-\boldsymbol{R})^2}, \qquad \gamma = \frac{N_1N_2}{N_1+N_2}\nu,$$

$\boldsymbol{X}_i, \boldsymbol{X}_G$ = C.M. coordinates of the cluster C_i and the total system, respectively. (3·2·2)

Here the following simple but important relation is utilized,

$$\prod_{i=1}^{2}\left(\frac{2N_i\nu}{\pi}\right)^{3/4} e^{-N_i\nu(\boldsymbol{X}_i-\boldsymbol{R}_i)^2} = \Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma)\omega_0(\boldsymbol{X}_G). \tag{3·2·3}$$

Equation (3·2·1) shows the RGM wave function is related to the GCM one by the Gaussian transformation.[6),7),39)] Similarly, in the multi-cluster system,

$$\Psi \propto \int \prod_{i=1}^{n-1} d\boldsymbol{S}_i \cdot f(\boldsymbol{S}_1, \cdots, \boldsymbol{S}_{n-1})\mathcal{A}\{\prod_{i=1}^{n}\phi_0(C_i, \boldsymbol{R}_i)\}$$

$$= \mathcal{A}\{\chi(\boldsymbol{\xi}_1, \cdots, \boldsymbol{\xi}_{n-1})\prod_{i=1}^{n}\phi_0(C_i)\}\omega_0(\boldsymbol{X}_G),$$

$$\chi(\boldsymbol{\xi}_1, \cdots, \boldsymbol{\xi}_{n-1}) = \int \prod_{i=1}^{n-1} d\boldsymbol{S}_i \Gamma(\boldsymbol{\xi}_i, \boldsymbol{S}_i, \gamma_i) \cdot f(\boldsymbol{S}_1, \cdots, \boldsymbol{S}_{n-1}), \tag{3·2·4}$$

where $\boldsymbol{\xi}_i$ are Jacobi coordinates (or any other suitably defined relative coordinates) obtained by the linear combination of $\boldsymbol{X}_i$, for example, $\boldsymbol{\xi}_1 = \boldsymbol{X}_2 - \boldsymbol{X}_1$, $\boldsymbol{\xi}_2 = \boldsymbol{X}_3 - (N_1\boldsymbol{X}_1 + N_2\boldsymbol{X}_2)/(N_1+N_2)$, $\cdots$, and $\boldsymbol{S}_i$ are the corresponding Jacobi generator coordinates obtained by linearly combining $\boldsymbol{R}_i$ just as in the same manner as the definition of $\boldsymbol{\xi}_i$ by $\boldsymbol{X}_i$, namely $\boldsymbol{S}_1 = \boldsymbol{R}_2 - \boldsymbol{R}_1$, $\boldsymbol{S}_2 = \boldsymbol{R}_3 - (N_1\boldsymbol{R}_1 + N_2\boldsymbol{R}_2)/(N_1+N_2)$, $\cdots$. Here the condition $\boldsymbol{R}_1 + \boldsymbol{R}_2 + \cdots + \boldsymbol{R}_n = 0$ is assumed for $\boldsymbol{R}_i$.

The relative motion with definite angular momentum is treated by the projection procedure applied to the above-mentioned relations. For the two-cluster system with the relative angular momentum L, the GCM wave function is

$$\Psi_L \propto \int_0^\infty dR \cdot R^2 f_L(R) \cdot P_{LM}\mathcal{A}\left\{\phi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right)\right\}$$

$$= \int_0^\infty dR \cdot R^2 f_L(R) \cdot \int d\hat{R} Y_{LM}(\hat{R})\mathcal{A}\left\{\phi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right)\right\}$$

$$= \mathcal{A}\{\chi_L(r) Y_{LM}(\hat{r}) \phi_0(C_1) \phi_0(C_2)\} \omega_0(\boldsymbol{X}_G),$$

$$\chi_L(r) = \int_0^\infty dR \cdot R^2 \Gamma_L(r, R, \gamma) f_L(R), \tag{3·2·5}$$

where

$$P_{LM} \equiv (\text{constant}) \int d\Omega D^{L*}_{M0}(\Omega) R(\Omega),$$

$$\Gamma_L(r, R, \gamma) \equiv \left(\frac{2\gamma}{\pi}\right)^{3/4} 4\pi i_L(2\gamma r R) e^{-\gamma(r^2+R^2)}. \tag{3·2·6}$$

The relation between Γ and Γ_L is

$$\Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma) = \sum_{L=0}^{\infty} \Gamma_L(r, R, \gamma) \sum_M Y^*_{LM}(\hat{R}) Y_{LM}(\hat{r}). \tag{3·2·7}$$

Equation (3·2·5) is just Eq. (3·2·1) with insertion,

$$\chi(\boldsymbol{r}) = \chi_L(r) Y_{LM}(\hat{r}), \quad f(\boldsymbol{R}) = f_L(R) Y_{LM}(\hat{R}). \tag{3·2·8}$$

Similarly for the case of the multi-cluster system,

$$\Psi_L \propto \int \prod_{i=1}^{n-1} dS_i \cdot S_i^2 \cdot f_{L,\alpha}(S_1, \cdots, S_{n-1}) \times \int \prod_{i=1}^{n-1} d\hat{S}_i \cdot Y_{LM,\alpha}(\hat{S}_1, \cdots, \hat{S}_{n-1}) \mathcal{A}\{\prod_{i=1}^{n} \phi_0(C_i, \boldsymbol{R}_i)\}$$

$$= \mathcal{A}\{\chi_{L,\alpha}(\xi_1, \cdots, \xi_{n-1}) Y_{LM,\alpha}(\hat{\xi}_1, \cdots, \hat{\xi}_{n-1}) \prod^{n} \phi_0(C_i)\} \omega_0(\boldsymbol{X}_G),$$

$$\chi_{L,\alpha}(\xi_1, \cdots, \xi_{n-1}) = \int \prod_{i=1}^{n-1} dS_i \cdot S_i^2 \Gamma_{L_i}(\xi_i, S_i, \gamma_i) f_{L,\alpha}(S_1, \cdots, S_{n-1}), \tag{3·2·9}$$

where α stands for the set of quantum numbers $(L_i, L_{12}, L_{123}\cdots)$ as in § 3.1. Equation (3·2·9) is just Eq. (3·2·4) with insertion of $\chi(\boldsymbol{\xi}_1, \cdots, \boldsymbol{\xi}_{n-1}) = \chi_{L,\alpha}(\xi_1, \cdots, \xi_{n-1})[\cdots[Y_{L_1}(\hat{\xi}_1) Y_{L_2}(\hat{\xi}_2)]_{L_{12}}\cdots]_L$ and $f(\boldsymbol{S}_1, \cdots, \boldsymbol{S}_{n-1}) = f_{L,\alpha}(S_1, \cdots, S_{n-1}) \times [\cdots[Y_{L_1}(\hat{S}_1) Y_{L_2}(\hat{S}_2)]_{L_{12}}\cdots]_L$.

The cases when the system involves the non-closed-shell clusters with non-zero spins are also treated similarly. As an example, for the simplest case of the two-cluster system with one non-zero spin cluster C_1, the corresponding transformation formula is

$$\Psi_L \propto \int_0^\infty dR \cdot R^2 f_{L,\alpha}(R) \int d\hat{R} \times \left[Y_{L_1}(\hat{R}) \cdot \mathcal{A}\left\{\phi_{L_2}\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right)\right\}\right]_L$$

$$= \mathcal{A}\{\chi_{L,\alpha}(r)\,[Y_{L_1}(\hat{r})\phi_{L_2}(C_1)]_L \phi_0(C_2)\} \omega_0(\boldsymbol{X}_G),$$

$$\chi_{L,\alpha}(r) = \int_0^\infty dR \cdot R^2 \Gamma_L(r, R, \gamma) f_{L,\alpha}(R), \tag{3·2·10}$$

where $\alpha=(L_1, L_2)$.

3.2.b. *Inverse of Gaussian transformation*

The inverse transformation of the RGM wave function to the GCM one is done by finding the inverse kernel of $\Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma)$ (or $\Gamma_L(r, R, \gamma)$). Since $\Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma)$ is a function of only $(\boldsymbol{r}-\boldsymbol{R})$, the eigen functions of this integral kernel are plane waves;

$$\int d\boldsymbol{R}\Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma)\left(\frac{1}{2\pi}\right)^{3/2}\exp\{i\boldsymbol{k}\boldsymbol{R}\}=\left[\left(\frac{2\pi}{\gamma}\right)^{3/4}\exp\left\{-\frac{k^2}{4\gamma}\right\}\right]\left(\frac{1}{2\pi}\right)^{3/2}\exp\{i\boldsymbol{k}\boldsymbol{r}\}. \tag{3·2·11}$$

The spectral representations of Γ and Γ^{-1} are thus

$$\Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma)=\int d\boldsymbol{k}\left(\frac{1}{2\pi}\right)^{3/2}\exp\{i\boldsymbol{k}\boldsymbol{r}\}\left[\left(\frac{2\pi}{\gamma}\right)^{3/4}\exp\left\{-\frac{k^2}{4\gamma}\right\}\right]\left(\frac{1}{2\pi}\right)^{3/2}\exp\{-i\boldsymbol{k}\boldsymbol{R}\},$$

$$\Gamma^{-1}(\boldsymbol{R}, \boldsymbol{r}, \gamma)=\int d\boldsymbol{k}\left(\frac{1}{2\pi}\right)^{3/2}\exp\{i\boldsymbol{k}\boldsymbol{R}\}\left[\left(\frac{\gamma}{2\pi}\right)^{3/4}\exp\left\{\frac{k^2}{4\gamma}\right\}\right]\left(\frac{1}{2\pi}\right)^{3/2}\exp\{-i\boldsymbol{k}\boldsymbol{r}\}. \tag{3·2·12}$$

Equation (3·2·12) shows Γ^{-1} is a singular kernel[38),40)] which is a well-known fact as a high frequency catastrophe of the real number GCM. This means that for some kind of relative wave functions $\chi(\boldsymbol{r})$ (of Eq. (3·2·1)), there is no corresponding weight function $f(\boldsymbol{R})$ which is non-singular. Denoting the Fourier component of $\chi(\boldsymbol{r})$ as $\chi^F(\boldsymbol{k})$, $f(\boldsymbol{R})$ is expressed by this $\chi^F(\boldsymbol{k})$ as follows,

$$\chi(\boldsymbol{r})=\int d\boldsymbol{k}\left(\frac{1}{2\pi}\right)^{3/2}\exp\{i\boldsymbol{k}\boldsymbol{r}\}\chi^F(\boldsymbol{k}),$$

$$f(\boldsymbol{R})=\int d\boldsymbol{k}\left(\frac{1}{2\pi}\right)^{3/2}\exp\{i\boldsymbol{k}\boldsymbol{R}\}\left[\left(\frac{\gamma}{2\pi}\right)^{3/4}\exp\left\{\frac{k^2}{4\gamma}\right\}\right]\chi^F(\boldsymbol{k}). \tag{3·2·13}$$

In the case when the damping of $\chi^F(\boldsymbol{k})$ at high frequency is overwhelmed by the growth of the factor $\exp(k^2/4\gamma)$, $f(\boldsymbol{R})$ becomes singular. As an example, when the width parameter γ_H of the Gaussian wave packet $\chi(\boldsymbol{r})$ is equal to or larger than γ of Γ, there is no corresponding regular $f(\boldsymbol{R})$, while on the contrary for $\gamma_H<\gamma$ we can find the regular function $f(\boldsymbol{R})$ as below

$$\left(\frac{2\gamma_H}{\pi}\right)^{3/4}\exp\{-\gamma_H r^2\}=\int d\boldsymbol{R}\Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma)\left(\frac{\gamma_H\gamma^3}{\pi^2(\gamma-\gamma_H)^2}\right)^{3/4}\exp\left\{-\frac{\gamma\gamma_H}{\gamma-\gamma_H}R^2\right\}. \tag{3·2·14}$$

When γ_H is near γ this $f(\boldsymbol{R})$ is sharply peaked around the origin and in the limit of $\gamma_H\to\gamma$ it becomes the Dirac delta function $\delta(\boldsymbol{R})$. More generally for $\gamma_H<\gamma$, the H.O. wave function $V_{NLM}(\boldsymbol{r}, \gamma_H)=R_{NL}(\boldsymbol{r}, \gamma_H)Y_{LM}(\hat{r})$ ($N=2n+L$ =number of oscillator quanta) has its corresponding $f(\boldsymbol{R})$ as follows:[11),41)]

$$R_{NL}(r,\gamma_H)Y_{LM}(\hat{r}) = \int d\boldsymbol{R}\Gamma(\boldsymbol{r},\boldsymbol{R},\gamma)B_{NL}(R,\gamma,\gamma_H)Y_{LM}(\hat{R}),$$

$$B_{NL}(R,\gamma,\gamma_H) = \left(\frac{\gamma}{2\pi}\right)^{3/4}\left(\frac{\gamma+\gamma_H}{\gamma-\gamma_H}\right)^{(N+3/2)/2}\cdot\exp\left\{-\frac{\gamma\gamma_H{}^2}{\gamma^2-\gamma_H{}^2}R^2\right\}R_{NL}\left(R,\frac{\gamma^2\gamma_H}{\gamma^2-\gamma_H{}^2}\right),$$

$$R_{NL}(r,\nu) \equiv \left[\frac{(2\nu)^{L+3/2}(\sqrt{2})^{N+L+4}\left(\frac{N-L}{2}\right)!}{\sqrt{\pi}(N+L+1)!!}\right]^{1/2} r^L\exp\{-\nu r^2\}L^{(L+1/2)}_{((N-L)/2)}(2\nu r^2), \tag{3·2·15}$$

where $L_n^{(L+1/2)}(2\nu r^2)$ is the associate Laguerre polynomial and it should be noticed that the number of the H.O. quanta N is used instead of the number of nodes $n(N=2n+L)$. This relation is equivalent to the following relation[42] for the one-dimensional H.O. wave function X_n,

$$X_n(x,\gamma_H) = \int dR_x\left(\frac{2\gamma}{\pi}\right)^{1/4}\exp\{-\gamma(x-R_x)^2\}b_n(R_x,\gamma,\gamma_H),$$

$$b_n(R_x,\gamma,\gamma_H) = \left(\frac{\gamma}{2\pi}\right)^{1/4}\left(\frac{\gamma+\gamma_H}{\gamma-\gamma_H}\right)^{(n+1/2)/2}\cdot\exp\left\{-\frac{\gamma\gamma_H{}^2}{\gamma^2-\gamma_H{}^2}R_x{}^2\right\}X_n\left(R_x,\frac{\gamma^2\gamma_H}{\gamma^2-\gamma_H{}^2}\right),$$

$$X_n(x,\nu) = \left(\frac{2\nu}{\pi}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n(\sqrt{2\nu}\,x)\exp\{-\nu x^2\}, \tag{3·2·16}$$

where H_n is the Hermite polynomial. This transformation equation (3·2·16) is just equivalent to the formula about the Gaussian transformation of the Hermite polynomial,[42]

$$\int dy\cdot\exp\left\{-\frac{1}{p}(z-y)^2\right\}H_n(y) = \sqrt{\pi p}(1-p)^{n/2}H_n\left(\frac{z}{\sqrt{1-p}}\right). \tag{3·2·17}$$

The equivalence of Eq. (3·2·17) to Eq. (3·2·16) is proved by putting $x=\sqrt{(\gamma+\gamma_H)/2\gamma_H(\gamma-\gamma_H)}z$, $R_x=\sqrt{(\gamma^2-\gamma_H{}^2)/2\gamma^2\gamma_H}y$ $p=2\gamma_H/(\gamma+\gamma_H)$ in Eq. (3·2·17). The functional form of $f(R_x)=b_n(R_x,\gamma,\gamma_H)$ of Eq. (3·2·16) was obtained by Griffin and Wheeler[19] by solving directly the GHW equation for the H.O. Hamiltonian in the translated Gaussian basis. (They reported the form of $b_n(R_x,\gamma,\gamma_H)$ for $n=0$, 1 and the recursion relation for higher n instead of the explicit form.) B_{NLM} and b_n are sharply peaked around the origin when γ_H is near γ having the same numbers of the nodal points with the corresponding H.O. functions, and they become singular in the region $\gamma_H \geqq \gamma$. The singular weight functions B_{NLM} and b_n in the case of $\gamma_H \geqq \gamma$ can be expressed in the integral form as was discussed above in Eq. (3·2·13). The Fourier transforms of $R_{NL}(r,\gamma_H)Y_{LM}(\hat{r})$ and $X_n(x,\gamma_H)$ necessary in Eq. (3·2·13) are again the H.O. functions of $\boldsymbol{k}=(k,\hat{k})$ and k_x, namely $R_{NL}(k, 1/4\gamma_H)Y_{LM}(\hat{k})$ and $X_n(k_x, 1/4\gamma_H)$, respectively. These integral forms will be used in later discussion.

The aim of this section 3 is to transform things in GCM space to those in RGM space. As for the wave function, this transformation is done by the Gaussian transformation kernel Γ (or Γ_L) but on the contrary for the integral kernels of operators the transformation is achieved by the inverse Gaussian kernel Γ^{-1}.

For the treatment of the dynamics in the GCM formalism, many works confine the use of the GCM within the interaction region and for dealing with the scattering or reaction problems the connection is done between the inner waves treated by GCM and outer waves whose functional forms are known except the scattering matrix elements, with the use of the R-matrix theory[7),43)~46)] or variational methods.[45)~47)] But there are also many works which treat every thing in the entire GCM space.[48)~53)] In the former we usually need not transform the quantities in RGM to GCM but in the latter the asymptotic boundary condition in the usual space (namely RGM space) must be transformed into that of GCM. Thus in the latter the Coulomb wave functions in the outside region (in RGM) must be transformed into the corresponding weight functions $f_L(R)$ with the use of ${\Gamma_L}^{-1}$. Since we do not discuss this approach later we here only quote the references.

3.2.c. *Expansion of Γ by the H.O. functions*

By using the generating function formula for the Hermite polynomials,

$$e^{-t^2+2tz}=\sum_{n=0}^{\infty}\frac{H_n(z)}{n!}t^n\,, \tag{3·2·18}$$

We can easily derive the expansion formula of the Gaussian transformation kernel Γ by the H.O. functions $X_{\boldsymbol{N}}(\boldsymbol{r},\gamma)$ as follows:[14)]

$$\begin{aligned}
\Gamma(\boldsymbol{r},\boldsymbol{R},\gamma)&=\left(\frac{2\gamma}{\pi}\right)^{3/4}\exp\{-\gamma(\boldsymbol{r}-\boldsymbol{R})^2\}\\
&=\exp\left\{-\frac{\gamma}{2}R^2\right\}\sum_{\boldsymbol{N}}[(\sqrt{\gamma}\boldsymbol{R})^{\boldsymbol{N}}/\sqrt{\boldsymbol{N}!}]X_{\boldsymbol{N}}(\boldsymbol{r},\gamma)\,,\\
X_{\boldsymbol{N}}(\boldsymbol{r},\gamma)&\equiv\prod_{i=1}^{3}\left(\frac{2\gamma}{\pi}\right)^{1/2}\frac{1}{\sqrt{2^{N_i}N_i!}}H_{N_i}(\sqrt{2\gamma}\,r_i)\exp\{-\gamma r_i^2\}\\
&=X_{N_1}(x,\gamma)X_{N_2}(y,\gamma)X_{N_3}(z,\gamma)\,,\\
\boldsymbol{R}^{\boldsymbol{N}}&\equiv\prod_{i=1}^{3}R_i^{N_i},\quad \boldsymbol{N}!\equiv\prod_{i=1}^{3}(N_i!)\,.
\end{aligned} \tag{3·2·19}$$

The angular momentum projection formula for $X_{(0,0,N)}(\boldsymbol{r},\gamma)$,

$$\begin{aligned}
X_{(0,0,N)}(\boldsymbol{r},\gamma)&=\sum_l A_l^N R_{Nl}(r,\gamma)Y_{l0}(\hat{r})\,,\\
A_l^N&\equiv(-)^{(N-l)/2}\sqrt{\frac{(2l+1)\cdot N!}{(N-l)!!(N+l+1)!!}}\,,
\end{aligned} \tag{3·2·20}$$

gives us the expansion formular of Γ as in the following form,*)

$$\Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma) = \exp\left\{-\frac{\gamma}{2}R^2\right\} \sum_{Nlm} \frac{(\gamma R^2)^{N/2}}{\sqrt{N!}} \sqrt{\frac{4\pi}{2l+1}} A_l^N \times Y_{lm}^*(\hat{R})\, R_{Nl}(r, \gamma)\, Y_{lm}(\hat{r}). \tag{3·2·21}$$

3.2.d. *Complex generator coordinates*

The extension of the GC into complex numbers can avoid the difficulties related to the singularity of the inverse Gaussian transformation Γ^{-1} encountered in the real number GCM. And further, as will be seen in later applications, the complex GCM (C-GCM) has many nice properties in the investigation of RGM kernels.

From the form of the C-GCM wave function in § 2.1 the relation of wave functions between C-GCM and RGM is written as follows,

$$\begin{aligned}\Psi &\propto \int d\mu(\boldsymbol{z}) f(\boldsymbol{z})\, e^{(\boldsymbol{z}^*)^2/2} \mathcal{A}\left\{\phi_0\left(C_1, \frac{-N_2\boldsymbol{z}^*}{A\sqrt{\gamma}}\right)\phi_0\left(C_2, \frac{N_1\boldsymbol{z}^*}{A\sqrt{\gamma}}\right)\right\} \\ &= \int d\mu(\boldsymbol{z}) f(\boldsymbol{z})\, \mathcal{A}\{A_\gamma^*(\boldsymbol{r}, \boldsymbol{z})\, \phi_0(C_1)\, \phi_0(C_2)\}\, \omega_0(\boldsymbol{X}_G) \\ &= \mathcal{A}\{\chi(\boldsymbol{r})\, \phi_0(C_1)\, \phi_0(C_2)\}\, \omega_0(\boldsymbol{X}_G), \\ \chi(\boldsymbol{r}) &= \int d\mu(\boldsymbol{z})\, A_\gamma^*(\boldsymbol{r}, \boldsymbol{z}) f(\boldsymbol{z}),\end{aligned} \tag{3·2·22}$$

where $A_\gamma(\boldsymbol{r}, \boldsymbol{z})$ and $d\mu(\boldsymbol{z})$ are defined in Eq. (2·1·29).

The space spanned by the entire analytic functions of $\boldsymbol{z}$ can be made into a Hilbert space (H_B) by defining the inner product by the integral with this measure $d\mu(\boldsymbol{z})$.[29] As an example of the complete orthonormal set of basis vectors of H_B, we can choose the following,

$$U_{\boldsymbol{N}}(\boldsymbol{z}) \equiv \frac{\boldsymbol{z}^{\boldsymbol{N}}}{\sqrt{\boldsymbol{N}!}} = \prod_{i=1}^{3} \frac{z_i^{N_i}}{\sqrt{N_i!}}. \tag{3·2·23}$$

The corresponding complete orthonormal set of basis vectors in the usual configuration space which is transformed by the kernel $A_\gamma^*(\boldsymbol{r}, \boldsymbol{z})$ from $\{U_{\boldsymbol{N}}(\boldsymbol{z})\}$ is just the H.O. wave functions $\{X_{\boldsymbol{N}}(\boldsymbol{r}, \gamma)\}$ of Eq. (3·2·19) as follows,[29]

$$X_{\boldsymbol{N}}(\boldsymbol{r}, \gamma) = \int d\mu(\boldsymbol{z})\, A_\gamma^*(\boldsymbol{r}, \boldsymbol{z})\, U_{\boldsymbol{N}}(\boldsymbol{z}). \tag{3·2·24}$$

Therefore $A_\gamma(\boldsymbol{r}, \boldsymbol{z})$ can be expanded by these two sets $\{U_{\boldsymbol{N}}(\boldsymbol{z})\}$, $\{X_{\boldsymbol{N}}(\boldsymbol{r}, \gamma)\}$, as

$$A_\gamma(\boldsymbol{r}, \boldsymbol{z}) = \sum_{\boldsymbol{N}} X_{\boldsymbol{N}}(\boldsymbol{r}, \gamma)\, U_{\boldsymbol{N}}(\boldsymbol{z}). \tag{3·2·25}$$

*) A way to derive Eq. (3·2·21) is as follows: First we expand $\Gamma(\boldsymbol{r}_z, \boldsymbol{R}, \gamma)$ with $\boldsymbol{r}_z = (0, 0, z)$ by $X_{(0,0,N)}$ using Eq. (3·2·19), and then use $\Gamma(\boldsymbol{r}-\boldsymbol{R}) = \exp(-i\phi J_z)\exp(-i\theta J_y)\Gamma(\boldsymbol{r}_z, \boldsymbol{R}, \gamma)$ with $\hat{r} = (\theta, \phi)$.

This equation is nothing but Eq. (3·2·19) if we replace $\boldsymbol{R}$ by $\boldsymbol{z}/\sqrt{\gamma}$ in Eq. (3·2·19).

From Eq. (3·2·25) we obtain

$$\int d\mu(\boldsymbol{z})\, A_\gamma(\boldsymbol{r}', \boldsymbol{z})\, A_\gamma^*(\boldsymbol{r}, \boldsymbol{z}) = \sum_{\boldsymbol{N}} X_{\boldsymbol{N}}(\boldsymbol{r}', \gamma)\, X_{\boldsymbol{N}}(\boldsymbol{r}, \gamma) = \delta(\boldsymbol{r}' - \boldsymbol{r}),$$

$$\int d\boldsymbol{r} A_\gamma(\boldsymbol{r}, \boldsymbol{z}')\, A_\gamma^*(\boldsymbol{r}, \boldsymbol{z}) = \sum_{\boldsymbol{N}} U_{\boldsymbol{N}}(\boldsymbol{z}')\, U_{\boldsymbol{N}}^*(\boldsymbol{z}) = \exp(\boldsymbol{z}' \cdot \boldsymbol{z}^*). \qquad (3\cdot2\cdot26)$$

As is clear from the relation $\exp(\boldsymbol{z}' \cdot \boldsymbol{z}^*) = \sum_{\boldsymbol{N}} U_{\boldsymbol{N}}(\boldsymbol{z}')\, U_{\boldsymbol{N}}^*(\boldsymbol{z})$, the function $\exp(\boldsymbol{z}' \cdot \boldsymbol{z}^*)$ behaves like the Dirac delta function in H_B,

$$\int d\mu(\boldsymbol{z}) \exp(\boldsymbol{z}' \cdot \boldsymbol{z}^*)\, \omega(\boldsymbol{z}) = \omega(\boldsymbol{z}') \qquad (3\cdot2\cdot27)$$

for an arbitrary element $\omega(\boldsymbol{z})$ of H_B. Therefore, in C-GCM, the inverse of the transformation relation $\chi(\boldsymbol{r}) = \int d\mu(\boldsymbol{z})\, A_\gamma^*(\boldsymbol{r}, \boldsymbol{z}) f(\boldsymbol{z})$ causes no difficultly and can be written as

$$f(\boldsymbol{z}) = \int d\boldsymbol{r} A_\gamma(\boldsymbol{r}, \boldsymbol{z})\, \chi(\boldsymbol{r}). \qquad (3\cdot2\cdot28)$$

As was discussed in § 2.1, the transformation kernel $A_\gamma^*(\boldsymbol{r}, \boldsymbol{z})$ is the so-called coherent state and can be expressed as follows,*)

$$A_\gamma^*(\boldsymbol{r}, \boldsymbol{z}) = e^{\boldsymbol{z}^* \cdot \boldsymbol{a}^\dagger} W_0(\boldsymbol{r}),$$

$$W_0(\boldsymbol{r}) \equiv \left(\frac{2\gamma}{\pi}\right)^{3/4} e^{-\gamma r^2}, \quad \boldsymbol{a}^\dagger \equiv \sqrt{\gamma}\left(\boldsymbol{r} - \frac{1}{2\gamma}\frac{\partial}{\partial \boldsymbol{r}}\right). \qquad (2\cdot1\cdot30)$$

By using Eq. (3·2·27), we get

$$\chi(\boldsymbol{r}) = \int d\mu(\boldsymbol{z}) \cdot \exp(\boldsymbol{z}^* \cdot \boldsymbol{a}^\dagger)\, W_0(\boldsymbol{r})\, f(\boldsymbol{z})$$

$$= f(\boldsymbol{a}^\dagger)\, W_0(\boldsymbol{r}). \qquad (3\cdot2\cdot29)$$

This direct relation between $\chi(\boldsymbol{r})$ and $f(\boldsymbol{z})$ was also noted by Ui and Biedenharn.[24]

3.3. Transformation of kernels

3.3.a. *RGM kernels in coordinate representation*

Throughout § 3.3 we assume that the GCM kernels are already calculated and we discuss how to transform these GCM kernels into RGM kernels. First we consider the RGM kernel of the operator $\mathcal{O}$ in the coordinate representation

*) Equation (2·1·30) is related to Eq. (3·2·25) as follows. By inserting the relation $X_{\boldsymbol{N}}(\boldsymbol{r}, \gamma) = (1/\sqrt{N!})(\boldsymbol{a}^\dagger)^{\boldsymbol{N}} W_0(\boldsymbol{r})$ into Eq. (3·2·25), we obtain

$$A_\gamma(\boldsymbol{r}, \boldsymbol{z}) = \sum_{\boldsymbol{N}} \prod_{i=1}^{3} \frac{1}{N_i!} (z_i a_i^\dagger)^{N_i} W_0(\boldsymbol{r})$$

$$= \exp(\boldsymbol{z} \cdot \boldsymbol{a})^\dagger W_0(\boldsymbol{r}).$$

which in the illustrative case of the system of two closed shell clusters takes the form,

$$m(\boldsymbol{a}_1, \boldsymbol{a}_2) = \langle \delta(\boldsymbol{r}-\boldsymbol{a}_1)\phi_0(C_1)\phi_0(C_2)|\mathcal{O}|\mathcal{A}\{\delta(\boldsymbol{r}-\boldsymbol{a}_2)\phi_0(C_1)\phi_0(C_2)\}\rangle$$
$$= m^D(\boldsymbol{a}_1)\delta(\boldsymbol{a}_1-\boldsymbol{a}_2) - m^E(\boldsymbol{a}_1, \boldsymbol{a}_2). \qquad (3\cdot3\cdot1)$$

Here $m^D(\boldsymbol{a})$ is the direct kernel given by

$$m^D(\boldsymbol{a}) = \langle \phi_0(C_1)\phi_0(C_2)|\delta(\boldsymbol{r}-\boldsymbol{a})\mathcal{O}|\phi_0(C_1)\phi_0(C_2)\rangle, \qquad (3\cdot3\cdot2)$$

and $m^E(\boldsymbol{a}_1, \boldsymbol{a}_2)$ is the exchange kernel given by $m^E(\boldsymbol{a}_1, \boldsymbol{a}_2) = \langle \delta(\boldsymbol{r}-\boldsymbol{a}_1)\phi_0(C_1) \times \phi_0(C_2)|\mathcal{O}|(\mathcal{A}-1)\{\delta(\boldsymbol{r}-\boldsymbol{a}_2)\phi_0(C_1)\phi_0(C_2)\}\rangle$.

Because of $\nu_1=\nu_2$, $\mathcal{H}(\boldsymbol{R}, \boldsymbol{R}') = M_\gamma(\boldsymbol{R}, \boldsymbol{R}')$ and since the GCM kernel M_γ can be written as

$$M_\gamma(\boldsymbol{R}_1, \boldsymbol{R}_2) = \langle \Gamma(\boldsymbol{r}, \boldsymbol{R}_1, \gamma)\phi_0(C_1)\phi_0(C_2)|\mathcal{O}|\mathcal{A}\{\Gamma(\boldsymbol{r}, \boldsymbol{R}_2, \gamma)\phi_0(C_1)\phi_0(C_2)\}\rangle$$
$$= \int d\boldsymbol{a}_1 d\boldsymbol{a}_2 \Gamma(\boldsymbol{a}_1, \boldsymbol{R}_1, \gamma) m(\boldsymbol{a}_1, \boldsymbol{a}_2) \Gamma(\boldsymbol{a}_2, \boldsymbol{R}_2, \gamma)$$
$$= \Gamma m \Gamma, \qquad (3\cdot3\cdot3)$$

the RGM kernel m is obtained by the inverse transformation Γ^{-1} from M_γ as

$$m(\boldsymbol{a}_1, \boldsymbol{a}_2) = \Gamma^{-1} M_\gamma \Gamma^{-1}$$
$$= \int d\boldsymbol{R}_1 d\boldsymbol{R}_2 \Gamma^{-1}(\boldsymbol{R}_1, \boldsymbol{a}_1, \gamma) M_\gamma(\boldsymbol{R}_1, \boldsymbol{R}_2) \Gamma^{-1}(\boldsymbol{R}_2, \boldsymbol{a}_2, \gamma)$$
$$= \left(\frac{1}{2\pi}\right)^6 \left(\frac{\gamma}{2\pi}\right)^{3/2} \int d\boldsymbol{k}_1 d\boldsymbol{k}_2 \exp\{-i\boldsymbol{k}_1\boldsymbol{a}_1 - i\boldsymbol{k}_2\boldsymbol{a}_2\}$$
$$\times \exp\left\{\frac{1}{4\gamma}(k_1^2+k_2^2)\right\} \int d\boldsymbol{R}_1 d\boldsymbol{R}_2 \exp\{i\boldsymbol{k}_1\boldsymbol{R}_1 + i\boldsymbol{k}_2\boldsymbol{R}_2\} M_\gamma(\boldsymbol{R}_1, \boldsymbol{R}_2), \qquad (3\cdot3\cdot4)$$

where we used the integral representation of Γ^{-1} given in Eq. (3·2·12). Equation (3·3·4) shows that the RGM kernel can be obtained from the GCM kernel by two-fold Fourier transformations in bra and ket respectively, first from GC $\boldsymbol{R}$ to linear momentum $\boldsymbol{k}$ and second from the momentum $\boldsymbol{k}$ to the coordinate $\boldsymbol{a}$, as shown in Ref. 7). This procedure is sometimes called "double Fourier transformation."[18]

A more straightforward transformation formula can be obtained by using the Fourier integral representation of the Dirac delta function[54)~57)]

$$\delta(\boldsymbol{r}-\boldsymbol{a}) = \left(\frac{1}{2\pi}\right)^3 \int d\boldsymbol{k} \exp\{i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{a})\}. \qquad (3\cdot3\cdot5)$$

From this equation we get

$$\delta(\boldsymbol{r}-\boldsymbol{a}) = \delta(\boldsymbol{r}-\boldsymbol{a}) \exp\{-\gamma(\boldsymbol{r}-\boldsymbol{a})^2\}$$

$$= \left(\frac{1}{2\pi}\right)^3 \int d\boldsymbol{k} \exp\{i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{a}) - \gamma(\boldsymbol{r}-\boldsymbol{a})^2\}$$

$$= \left(\frac{1}{2\pi}\right)^3 \int d\boldsymbol{k} \exp\left\{-\frac{k^2}{4\gamma}\right\} \exp\left\{-\gamma\left[\boldsymbol{r}-\boldsymbol{a}-\frac{i}{2\gamma}\boldsymbol{k}\right]^2\right\}$$

$$= \left(\frac{1}{2\pi}\right)^3 \left(\frac{\pi}{2\gamma}\right)^{3/4} \int d\boldsymbol{k} \exp\left\{-\frac{k^2}{4\gamma}\right\} \Gamma\left(\boldsymbol{r}, \boldsymbol{a}+\frac{i}{2\gamma}\boldsymbol{k}, \gamma\right), \qquad (3\cdot3\cdot6)^{*)}$$

which when inserted into Eq. (3·3·1) gives us the desired formula,

$$m(\boldsymbol{a}_1, \boldsymbol{a}_2) = \left(\frac{1}{2\pi}\right)^6 \left(\frac{\pi}{2\gamma}\right)^{3/2} \int d\boldsymbol{k}_1 d\boldsymbol{k}_2 \exp\left\{-\frac{1}{4\gamma}(k_1^2+k_2^2)\right\}$$

$$\times M_\gamma\left(\boldsymbol{a}_1+\frac{i}{2\gamma}\boldsymbol{k}_1, \boldsymbol{a}_2+\frac{i}{2\gamma}\boldsymbol{k}_2\right). \qquad (3\cdot3\cdot7)$$

This procedure may be called "single Fourier transformation." Several authors call this "complex generator coordinate technique"[3),56),57)] since we use complex generator coordinates $\boldsymbol{a}_j+(i/2\gamma)\boldsymbol{k}_j$ $(j=1, 2)$ in the GCM kernel M. But this "complex generator coordinate technique" described here is different from our complex GCM (C-GCM) discussed in §§ 2.1 and 3.2 which uses the coherent state (or the Bargmann transformation kernel) $A_\gamma(\boldsymbol{r}, \boldsymbol{z})$ and twice as many integration coordinates $\mathrm{Re}(\boldsymbol{z})$ and $\mathrm{Im}(\boldsymbol{z})$. Thus to avoid the confusion we use the terminology "single Fourier transformation technique" for Eq. (3·3·7).

The framework of C-GCM, of course, provides us the transformation formula from C-GCM kernels to RGM kernels as follows,

$$m(\boldsymbol{a}_1, \boldsymbol{a}_2) = \int d\mu(\boldsymbol{z}_1) d\mu(\boldsymbol{z}_2) A_\gamma^*(\boldsymbol{a}_1, \boldsymbol{z}_1) A_\gamma(\boldsymbol{a}_2, \boldsymbol{z}_2)$$

$$\times \langle A_\gamma^*(\boldsymbol{r}, \boldsymbol{z}_1)\phi_0(C_1)\phi_0(C_2)|\mathcal{O}|\mathcal{A}\{A_\gamma^*(\boldsymbol{r}, \boldsymbol{z}_2)\phi_0(C_1)\phi_0(C_2)\}\rangle$$

$$= \int d\mu(\boldsymbol{z}_1) d\mu(\boldsymbol{z}_2) A_\gamma^*(\boldsymbol{a}_1, \boldsymbol{z}_1) A_\gamma(\boldsymbol{a}_2, \boldsymbol{z}_2)$$

$$\times e^{1/2(\boldsymbol{z}_1^2)+1/2(\boldsymbol{z}_2^2)^*} M_\gamma\left(\frac{\boldsymbol{z}_1^*}{\sqrt{\gamma}}, \frac{\boldsymbol{z}_2^*}{\sqrt{\gamma}}\right), \qquad (3\cdot3\cdot8)$$

where use is made of the relation of Eq. (3·2·27), $\delta(\boldsymbol{r}-\boldsymbol{a}) = \int d\mu(\boldsymbol{z}) A_\gamma(\boldsymbol{a}, \boldsymbol{z})$

*) Equation (3·3·6) can be slightly generalized as follows:

$$\delta(\boldsymbol{r}-\boldsymbol{a}) = \delta(\boldsymbol{r}-\boldsymbol{a}) \exp\{-\gamma(\boldsymbol{r}-\boldsymbol{a})^2 + \boldsymbol{d}(\boldsymbol{r}-\boldsymbol{a})\}$$

$$= \left(\frac{1}{2\pi}\right)^3 \int d\boldsymbol{k} \exp\{(i\boldsymbol{k}+\boldsymbol{d})(\boldsymbol{r}-\boldsymbol{a}) - \gamma(\boldsymbol{r}-\boldsymbol{a})^2\}$$

$$= \left(\frac{1}{2\pi}\right)^3 \left(\frac{\pi}{2\gamma}\right)^{3/4} \int d\boldsymbol{k} \exp\left\{-\frac{(\boldsymbol{k}-i\boldsymbol{d})^2}{4\gamma}\right\} \Gamma\left(\boldsymbol{r}, \boldsymbol{a}+\frac{i\boldsymbol{k}+\boldsymbol{d}}{2\gamma}, \gamma\right).$$

Here $\boldsymbol{d}$ is an arbitrary complex vector.

$\times A_\gamma^*(\boldsymbol{r}, \boldsymbol{z})$.

The above three transformation formulas (double Fourier, single Fourier transformations and C-GCM) are based on the different integral representations of the Dirac delta function $\delta(\boldsymbol{r}-\boldsymbol{a})$ with the use of $I(\boldsymbol{r}, \boldsymbol{R}, \gamma)$, which are summarized as follows:

$$\begin{aligned}\delta(\boldsymbol{r}-\boldsymbol{a}) &= \left(\frac{1}{2\pi}\right)^3\left(\frac{\gamma}{2\pi}\right)^{3/4}\int d\boldsymbol{k}\exp\left\{-i\boldsymbol{k}\boldsymbol{a}+\frac{k^2}{4\gamma}\right\}\int d\boldsymbol{R}\exp\{i\boldsymbol{k}\boldsymbol{R}\} \\ &\quad \times I(\boldsymbol{r}, \boldsymbol{R}, \gamma) \quad \text{(double Fourier)} \\ &= \left(\frac{1}{2\pi}\right)^3\left(\frac{\pi}{2\gamma}\right)^{3/4}\int d\boldsymbol{k}\exp\left\{-\frac{k^2}{4\gamma}\right\} I\left(\boldsymbol{r}, \boldsymbol{a}+\frac{i}{2\gamma}\boldsymbol{k}, \gamma\right) \quad \text{(single Fourier)} \\ &= \int d\mu(\boldsymbol{z})\, A_\gamma(\boldsymbol{a}, \boldsymbol{z})\exp\left\{\frac{1}{2}(\boldsymbol{z}^2)^*\right\} I\left(\boldsymbol{r}, \frac{\boldsymbol{z}}{\sqrt{\gamma}}, \gamma\right) \quad \text{(C-GCM)}.\end{aligned} \tag{3·3·9}$$

The above procedures are all about the calculation of the entire kernel of RGM. These automatically give both direct and exchange kernels $m^D(\boldsymbol{a})$, $m^E(\boldsymbol{a}_1, \boldsymbol{a}_2)$ defined in Eqs. (3·3·1) and (3·3·2). When we want to calculate only the direct kernel $m^D(\boldsymbol{a}_1)\delta(\boldsymbol{a}_1-\boldsymbol{a}_2)$, the calculational procedure of it is simply to replace the GCM full kernels M_γ in Eqs. (3·3·4), (3·3·7) and (3·3·8) by the GCM direct kernel M_γ^D in Eq. (2·1·14),

$$M_\gamma^D(\boldsymbol{R}_1, \boldsymbol{R}_2) \equiv \langle I(\boldsymbol{r}, \boldsymbol{R}_1, \gamma)\phi_0(C_1)\phi_0(C_2)\,|\mathcal{O}|\,I(\boldsymbol{r}, \boldsymbol{R}_2, \gamma)\phi_0(C_1)\phi_0(C_2)\}\rangle\,. \tag{2·1·14}'$$

When the operator $\mathcal{O}$ does not contain the differential operation, the calculation of the direct kernel can be done in the following simplified way. Since the definition of $m^D(\boldsymbol{a})$ of Eq. (3·3·2) contains only one Dirac delta function, we need to express this Dirac delta function by the integral representation which contains two $I(\boldsymbol{r}, \boldsymbol{R}, \gamma)$, in order to relate m^D to M^D. A simple way is to use the relation $\delta(\boldsymbol{r}-\boldsymbol{a}) = (\pi/2\gamma)^{3/4} I(\boldsymbol{r}, \boldsymbol{a}, \gamma)\delta(\boldsymbol{r}-\boldsymbol{a})$ and to insert the integral representations of Eq. (3·3·9) into the right-hand-side $\delta(\boldsymbol{r}-\boldsymbol{a})$ of this relation, yielding

$$\begin{aligned}m^D(\boldsymbol{a}) &= \left(\frac{1}{2\sqrt{2}\pi}\right)^3\int d\boldsymbol{k}\exp\left\{-i\boldsymbol{k}\boldsymbol{a}+\frac{k^2}{4\gamma}\right\}\int d\boldsymbol{R}\exp\{i\boldsymbol{k}\boldsymbol{R}\}\, M_\gamma^D(\boldsymbol{a}, \boldsymbol{R}) \\ &= \left(\frac{1}{2\pi}\right)^3\left(\frac{\pi}{2\gamma}\right)^{3/2}\int d\boldsymbol{k}\exp\left\{-\frac{k^2}{4\gamma}\right\} M_\gamma^D\left(\boldsymbol{a}, \boldsymbol{a}+\frac{i}{2\gamma}\boldsymbol{k}\right) \\ &= \left(\frac{\pi}{2\gamma}\right)^{3/4}\int d\mu(\boldsymbol{z})\, A_\gamma(\boldsymbol{a}, \boldsymbol{z})\exp\left\{\frac{1}{2}(\boldsymbol{z}^2)^*\right\} M_\gamma^D\left(\boldsymbol{a}, \frac{\boldsymbol{z}^*}{\sqrt{\gamma}}\right).\end{aligned} \tag{3·3·10}$$

Here we used the commutability of the operator $\mathcal{O}$ with one I based on the condition that $\mathcal{O}$ does not contain the differential operators. We give here

one more prescription, which utilizes the relation $\Gamma(\boldsymbol{r}, \boldsymbol{R}, 2\gamma) = (\pi/\gamma)^{3/4} \times \Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma)\Gamma(\boldsymbol{r}, \boldsymbol{R}, \gamma)$. First we replace the width parameter γ in Eq. (3·3·9) by 2γ and then insert the above mentioned relation into $\Gamma(\boldsymbol{r}, \boldsymbol{R}, 2\gamma)$. We thus obtain for $m^D(\boldsymbol{a})$ the following formulas,

$$\begin{aligned} m^D(\boldsymbol{a}) &= \left(\frac{1}{2\pi}\right)^3 \int d\boldsymbol{k} \exp\left\{-i\boldsymbol{k}\boldsymbol{a} + \frac{k^2}{8\gamma}\right\} \int d\boldsymbol{R} \exp\{i\boldsymbol{k}\boldsymbol{R}\} M_\gamma{}^D(\boldsymbol{R}, \boldsymbol{R}) \\ &= \left(\frac{1}{2\pi}\right)^3 \left(\frac{\pi}{2\gamma}\right)^{3/2} \int d\boldsymbol{k} \exp\left\{-\frac{k^2}{8\gamma}\right\} M_\gamma{}^D\left(\boldsymbol{a} - \frac{i}{2\gamma}\boldsymbol{k}, \boldsymbol{a} + \frac{i}{2\gamma}\boldsymbol{k}\right) \\ &= \left(\frac{\pi}{\gamma}\right)^{3/4} \int d\mu(\boldsymbol{z}) A_{2\gamma}(\boldsymbol{a}, \boldsymbol{z}) \exp\left\{\frac{1}{2}(\boldsymbol{z}^2)^*\right\} M_\gamma{}^D\left(\frac{\boldsymbol{z}}{\sqrt{2\gamma}}, \frac{\boldsymbol{z}^*}{\sqrt{2\gamma}}\right). \end{aligned} \tag{3·3·11}$$

Here we also used the commutability of the operator $\mathcal{O}$ with one Γ. The double Fourier transformation formula for m^D is especially convenient since it uses only the diagonal elements of GCM direct kernel $M^D(\boldsymbol{R}, \boldsymbol{R})$ which is very easy to compute as is shown below;[11]

$$M_\gamma{}^D(\boldsymbol{R}, \boldsymbol{R}) = \left\langle \psi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right)\psi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right) | \mathcal{O} | \psi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right)\psi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right)\right\rangle$$

$$= \begin{cases} \text{(I)} & \text{for one-body operater } \mathcal{O}, \\ \text{(II)} & \text{for two-body operator } \mathcal{O}, \end{cases}$$

$$\text{(I)} = \left\langle \psi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right) | \sum_{j \in C_1} \mathcal{O}_j | \psi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right)\right\rangle + \left\langle \psi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right) | \sum_{j \in C_2} \mathcal{O}_j | \psi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right)\right\rangle,$$

$$\langle \psi_0(C_i, \boldsymbol{R}_i) | \sum_{j \in C_i} \mathcal{O}_j | \psi_0(C_i, \boldsymbol{R}_i)\rangle = \sum_{j \in C_i} \langle \varphi_j(\boldsymbol{x} - \boldsymbol{R}_i) | \mathcal{O} | \varphi_j(\boldsymbol{x} - \boldsymbol{R}_i)\rangle,$$

$$\text{(II)} = \left\langle \psi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right) \middle| \frac{1}{2}\sum_{j,k \in C_1} \mathcal{O}_{jk} \middle| \psi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right)\right\rangle + \left\langle \psi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right) \middle| \frac{1}{2}\sum_{j,k \in C_2} \mathcal{O}_{jk} \middle| \psi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right)\right\rangle$$

$$+ \left\langle \psi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right)\psi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right) | \sum_{\substack{j \in C_1 \\ k \in C_2}} \mathcal{O}_{jk} | \psi_0\left(C_1, \frac{-N_2}{A}\boldsymbol{R}\right)\psi_0\left(C_2, \frac{N_1}{A}\boldsymbol{R}\right)\right\rangle,$$

$$\left\langle \psi_0(C_i, \boldsymbol{R}_i) \middle| \frac{1}{2}\sum_{j,k \in C_i} \mathcal{O}_{jk} \middle| \psi_0(C_i, \boldsymbol{R}_i)\right\rangle = \left\langle \psi_0(C_i, 0) \middle| \frac{1}{2}\sum_{j,k \in C_i} \mathcal{O}_{jk} \middle| \psi_0(C_i, 0)\right\rangle$$

$$=\frac{1}{2}\sum_{j,k\in C_i}\langle\varphi_j(\boldsymbol{x}_1)\varphi_k(\boldsymbol{x}_2)|\mathcal{O}|\varphi_j(\boldsymbol{x}_1)\varphi_k(\boldsymbol{x}_2)\rangle^a,$$

$$\langle\psi_0(C_1,\boldsymbol{R}_1)\psi_0(C_2,\boldsymbol{R}_2)|\sum_{\substack{j\in C_1\\k\in C_2}}|\mathcal{O}_{jk}|\psi_0(C_1,\boldsymbol{R}_1)\psi_0(C_2,\boldsymbol{R}_2)\rangle$$

$$=\sum_{\substack{j\in C_1\\k\in C_2}}\langle\varphi_j(\boldsymbol{x}_1-\boldsymbol{R}_1)\varphi_k(\boldsymbol{x}_2-\boldsymbol{R}_2)|\mathcal{O}|\varphi_j(\boldsymbol{x}_1-\boldsymbol{R}_1)\varphi_k(\boldsymbol{x}_2-\boldsymbol{R}_2)\rangle,$$

$$|m,n\rangle^a\equiv|mn\rangle-|nm\rangle. \qquad (3\cdot3\cdot12)$$

Our explanation has been limited to the single channel two-cluster system. But it is evident that the methods explained here can be used in other various cases since the essence is how to represent the Dirac delta function by the integral form containing one (or two) $\Gamma(\boldsymbol{r},\boldsymbol{R},\gamma)$.

3.3.b. *RGM kernels in H.O. and other representations*

As discussed in § 3.1, when we express the RGM relative wave function $\chi(\boldsymbol{r})$ by the linear superposition of some basis wave functions $\{u_i(\boldsymbol{r})\}$ as in Eq. (3·1·11), we need to calculate the kernel $\hat{m}(i,j)$ of Eq. (3·1·12). If we know the kernel in coordinate representation $m(\boldsymbol{a}_1,\boldsymbol{a}_2)$, we can, of course, get $\hat{m}(i,j)$ as follows:

$$\hat{m}(i,j)=\int d\boldsymbol{a}_1 d\boldsymbol{a}_2 u_i^*(\boldsymbol{a}_1)\,m(\boldsymbol{a}_1,\boldsymbol{a}_2)\,u_j(\boldsymbol{a}_2). \qquad (3\cdot3\cdot13)$$

What we discuss here are the prescriptions to get $\hat{m}(i,j)$ directly from the GCM kernel $M(\boldsymbol{R}_1,\boldsymbol{R}_2)$ not by the indirect method of Eq. (3·3·13).

A general prescription is to find the functions $W_i=\Gamma^{-1}u_i$ $(u_i(\boldsymbol{r})=\int d\boldsymbol{R}\times\Gamma(\boldsymbol{r},\boldsymbol{R},\gamma)W_i(\boldsymbol{R}))$. Then we get

$$\hat{m}(i,j)=\int d\boldsymbol{R}_1 d\boldsymbol{R}_2 W_i^*(\boldsymbol{R}_1)\,W_j(\boldsymbol{R}_2)$$

$$\times\int d\boldsymbol{a}_1 d\boldsymbol{a}_2\Gamma(\boldsymbol{a}_1,\boldsymbol{R}_1,\gamma)\,m(\boldsymbol{a}_1,\boldsymbol{a}_2)\,\Gamma(\boldsymbol{a}_2,\boldsymbol{R}_2,\gamma)$$

$$=\int d\boldsymbol{R}_1 d\boldsymbol{R}_2 W_i^*(\boldsymbol{R}_1)\,W_j(\boldsymbol{R}_2)\,M_r(\boldsymbol{R}_1,\boldsymbol{R}_2). \qquad (3\cdot3\cdot14)$$

When we adopt for $\{u_i\}$, the H.O. functions $\{R_{Nl}(r,\gamma_H)Y_{lm}(\hat{r})\}$ or the Gaussian wave packets with variable width parameters $\{e^{-\gamma_i r^2}r^l Y_{lm}(\hat{r})\propto R_{N=l,l}(r,\gamma_i)\times Y_{lm}(\hat{r})\}$, we know $W_i(\boldsymbol{R})$ for these $u_i(r)$ as was given in Eq. (3·2·15), under the condition $\gamma_H<\gamma$ or $\gamma_i<\gamma$. This prescription was discussed in detail in Ref. 11).

The complex GC technique provides a similar prescription to the above. We calculate $W_i(\boldsymbol{z})$ such that $u_i(\boldsymbol{r})=\int d\mu(\boldsymbol{z})\,A_r^*(\boldsymbol{r},\boldsymbol{z})\,W_i(\boldsymbol{z})$, and then we get

$$\hat{m}(i,j)=\int d\mu(\boldsymbol{z}_1)\,d\mu(\boldsymbol{z}_2)\,W_i^*(\boldsymbol{z}_1)\,W_j(\boldsymbol{z}_2)$$

$$\times \int d\boldsymbol{a}_1 d\boldsymbol{a}_2 A_\gamma(\boldsymbol{a}_1, \boldsymbol{z}_1)\, m(\boldsymbol{a}_1, \boldsymbol{a}_2)\, A_\gamma{}^*(\boldsymbol{a}_2, \boldsymbol{z}_2)$$

$$= \int d\mu(\boldsymbol{z}_1)\, d\mu(\boldsymbol{z}_2)\, W_i{}^*(\boldsymbol{z}_1)\, W_j(\boldsymbol{z}_2)$$

$$\times \exp\left\{\frac{1}{2}(\boldsymbol{z}_1{}^2) + \frac{1}{2}(\boldsymbol{z}_2{}^2)^*\right\} M_\gamma\left(\frac{\boldsymbol{z}_1{}^*}{\sqrt{\gamma}}, \frac{\boldsymbol{z}_2{}^*}{\sqrt{\gamma}}\right). \qquad (3\cdot3\cdot15)$$

An interesting and important case is when $\{u_i\}$ are H.O. functions $\{X_{\boldsymbol{N}i}(\boldsymbol{r}, \gamma)\}$. Then $W_i(\boldsymbol{z}) = U_{\boldsymbol{N}i}(\boldsymbol{z})$ as was discussed in § 3.2.d. If we define $\widetilde{M}_\gamma$ by

$$\widetilde{M}_\gamma(\boldsymbol{z}_1, \boldsymbol{z}_2{}^*) \equiv \exp\left\{\frac{1}{2}(\boldsymbol{z}_1{}^2) + \frac{1}{2}(\boldsymbol{z}_2{}^2)^*\right\} M_\gamma\left(\frac{\boldsymbol{z}_1{}^*}{\sqrt{\gamma}}, \frac{\boldsymbol{z}_2{}^*}{\sqrt{\gamma}}\right)$$

$$= \langle A_\gamma{}^*(\boldsymbol{r}, \boldsymbol{z}_1)\phi_0(C_1)\phi_0(C_2)\,|\mathcal{O}|\,\mathcal{A}\{A_\gamma{}^*(\boldsymbol{r}, \boldsymbol{z}_2)\phi_0(C_1)\phi_0(C_2)\}\rangle\,, \qquad (3\cdot3\cdot16)$$

$\widehat{m}(i, j)$ are obtained as the expansion coefficients of the power series expansion of $\widetilde{M}_\gamma(\boldsymbol{z}_1, \boldsymbol{z}_2{}^*)$ by $(\boldsymbol{z}_1)^{\boldsymbol{N}_1}$, $(\boldsymbol{z}_2{}^*)^{\boldsymbol{N}_2}$. Let the power series expansion of $\widetilde{M}_\gamma$ be

$$\widetilde{M}_\gamma(\boldsymbol{z}_1, \boldsymbol{z}_2{}^*) = \sum_{\boldsymbol{N}_1\boldsymbol{N}_2} c_{\boldsymbol{N}_1\boldsymbol{N}_2} U_{\boldsymbol{N}_1}(\boldsymbol{z}_1)\, U_{\boldsymbol{N}_2}^*(\boldsymbol{z}_2), \qquad (3\cdot3\cdot17)$$

then from Eq. (3·3·15) and from $W_i(\boldsymbol{z}) = U_{\boldsymbol{N}i}(\boldsymbol{z})$ we obtain

$$\widehat{m}(\boldsymbol{N}_i, \boldsymbol{N}_j) \equiv \langle X_{\boldsymbol{N}i}(\boldsymbol{r}, \gamma)\phi_0(C_1)\phi_0(C_2)\,|\mathcal{O}|\,\mathcal{A}\{X_{\boldsymbol{N}j}(\boldsymbol{r}, \gamma)\phi_0(C_1)\phi_0(C_2)\}\rangle$$

$$= c_{\boldsymbol{N}_i\boldsymbol{N}_j}\,. \qquad (3\cdot3\cdot18)$$

The result Eq. (3·3·18) can be derived in a different way. Consider $M_\gamma(\boldsymbol{R}_1, \boldsymbol{R}_2)$ where $\boldsymbol{R}_i$ need not be complex number vectors. We insert the expansion formula of Γ by H.O. functions which is given in Eq. (3·2·19), into the defining equation Eq. (3·3·16) of $\widetilde{M}_\gamma$, obtaining

$$\widetilde{M}_\gamma(\boldsymbol{R}_1, \boldsymbol{R}_2) = \sum_{\boldsymbol{N}_1\boldsymbol{N}_2} U_{\boldsymbol{N}_1}(\boldsymbol{R}_1)\, U_{\boldsymbol{N}_2}(\boldsymbol{R}_2)$$

$$\times \langle X_{\boldsymbol{N}_1}(\boldsymbol{r}, \gamma)\phi_0(C_1)\phi_0(C_2)\,|\mathcal{O}|\,\mathcal{A}\{X_{\boldsymbol{N}_2}(\boldsymbol{r}, \gamma)\phi_0(C_1)\phi_0(C_2)\}\rangle\,. \qquad (3\cdot3\cdot19)$$

This gives a proof for the relation of Eq. (3·3·18). Therefore we call the above procedure to get $\widehat{m}(\boldsymbol{N}_1, \boldsymbol{N}_2) \equiv \langle X_{\boldsymbol{N}_1}(\boldsymbol{r}, \gamma)\phi_0(C_1)\phi_0(C_2)|\mathcal{O}|\mathcal{A}\{X_{\boldsymbol{N}_2}(\boldsymbol{r}, \gamma)\phi_0(C_1) \times \phi_0(C_2)\}\rangle$, the generating function technique.

If we insert the expansion formula of Γ by H.O. functions with definite angular momenta which is given in Eq. (3·2·21) into Eq. (3·3·16) defining $\widetilde{M}_\gamma$ we obtain[58]

$$\widetilde{M}_\gamma(\boldsymbol{R}_1, \boldsymbol{R}_2) = \sum_{\substack{N_1 l_1 m_1 \\ N_2 l_2 m_2}} (R^{N_1}/\sqrt{N_1!})\,(R^{N_2}/\sqrt{N_2!})\,\frac{4\pi}{\sqrt{(2l_1+1)(2l_2+1)}}$$

$$\times A_{l_1}^{N_1} A_{l_2}^{N_2} Y_{l_1 m_1}(\widehat{R}_1)\, Y_{l_2 m_2}^*(\widehat{R}_2)\, \widehat{m}(N_1 l_1 m_1, N_2 l_2 m_2),$$

$$\widehat{m}(N_1 l_1 m_1, N_2 l_2 m_2) \equiv \langle R_{N_1 l_1}(r, \gamma)\, Y_{l_1 m_1}(\widehat{r})\, \phi_0(C_1)\phi_0(C_2)\,|$$

$$\times \mathcal{O}|\mathcal{A}\{R_{N_2 l_2}(r,\gamma)Y_{l_2 m_2}(\hat{r})\phi_0(C_1)\phi_0(C_2)\}\rangle . \qquad (3\cdot3\cdot20)$$

Eq. (3·3·20) is used to calculate $\hat{m}(N_1 l_1 m_1, N_2 l_2 m_2)$ from $\tilde{M}_\gamma(\boldsymbol{R}_1, \boldsymbol{R}_2)$; namely, we expand $\tilde{M}_\gamma(\boldsymbol{R}_1, \boldsymbol{R}_2)$ by $R_1^{N_1}Y_{l_1 m_1}(\hat{R}_1)R_2^{N_2}Y^*_{l_2 m_2}(\hat{R}_2)$ and then we obtain $\hat{m}(N_1 l_1 m_1, N_2 l_2 m_2)$ as the expansion coefficients of $\tilde{M}_\gamma(\boldsymbol{R}_1, \boldsymbol{R}_2)$.

We finally study the case when the system includes the non-zero spin clusters. The simplest system is that described by the wave function of Eq. (3·1·8) where the SU_3 shell model wave function is adopted for $\phi_L(C_1)$. By using Eq. (2·1·21) we obtain the following relation:[15]

$$\begin{aligned}
&\exp\left\{\frac{1}{2}(R_1^2+R_2^2)\right\}\left\langle\psi^{Q_1}\left(C_1,\frac{-N_2}{A\sqrt{\gamma}}\boldsymbol{R}_1\right)\phi_0\left(C_2,\frac{N_1}{A\sqrt{\gamma}}\boldsymbol{R}_1\right)\right| \\
&\qquad\times\mathcal{O}|\mathcal{A}\left\{\psi^{Q_2}\left(C_1,\frac{-N_2}{A\sqrt{\gamma}}\boldsymbol{R}_2\right)\phi_0\left(C_2,\frac{N_1}{A\sqrt{\gamma}}\boldsymbol{R}_2\right)\right\}\Big\rangle \\
&=\langle A_\gamma(\boldsymbol{r},\boldsymbol{R}_1)\phi^{Q_1}(C_1)\phi_0(C_2)|\mathcal{O}|\mathcal{A}\{A_\gamma(\boldsymbol{r},\boldsymbol{R}_2)\phi^{Q_2}(C_1)\phi_0(C_2)\}\rangle \\
&=\sum_{N_1N_2}R_1^{N_1}R_2^{N_2}/\sqrt{N_1!\,N_2!}\sum_{\substack{ij\\J_1M_1J_2M_2}}\frac{(4\pi)^2A_{l_i}^{N_1}A_{l_j}^{N_2}A_{L_i}^{N}A_{L_j}^{N}}{\sqrt{(2l_i+1)(2l_j+1)(2L_i+1)(2L_j+1)}} \\
&\quad\times[Y_{l_i}(\hat{R}_1)Y_{L_i}(\Omega_1)]_{J_1M_1}[Y_{l_j}(\hat{R}_2)Y_{L_j}(\Omega_2)]_{J_2M_2} \\
&\quad\times\langle R_{N_1 l_i}(r,\gamma)h_i^{J_1M_1}|\mathcal{O}|\mathcal{A}\{R_{N_2 l_j}(r,\gamma)h_j^{J_2M_2}\}\rangle . \qquad (3\cdot3\cdot21)
\end{aligned}$$

3.3.c. *Range of kernels*

Corresponding to § 2.2.d we discuss here the range of the RGM kernels. When the Gaussian form is assumed for the two-nucleon potential, both the norm kernel and the Hamiltonian kernel without Coulomb part in two-cluster system have in general the following form in GCM,

$$\sum_i c_i R^{2l_i}R'^{2m_i}(\boldsymbol{R}\cdot\boldsymbol{R}')^{n_i}\exp\{-E_{1i}R^2-E_{2i}R'^2-E_{3i}\boldsymbol{R}\cdot\boldsymbol{R}'\}, \qquad (3\cdot3\cdot22)$$

where $E_{ki}(k=1\sim3)$ are shown in § 2.2.d to be determined by the number of the exchanged nucleons between clusters. What we discuss is the range of the RGM kernel transformed from GCM one of Eq. (3·3·22). By using the prescriptions of § 3.3.a, the transformed RGM kernel from the GCM one of Eq. (3·3·22) is[13]

$$\begin{aligned}
&\left(\frac{\gamma}{2\pi}\right)^{3/2}\sum_i c_i(-)^{l_i+m_i+n_i}\left(\frac{\partial}{\partial E_{1i}}\right)^{l_i}\left(\frac{\partial}{\partial E_{2i}}\right)^{m_i}\left(\frac{\partial}{\partial E_{3i}}\right)^{n_i}C_0^{-3/2} \\
&\qquad\times\exp\{-E'_{1i}r^2-E'_{2i}r'^2-E'_{3i}\boldsymbol{r}\cdot\boldsymbol{r}'\} \\
&=\sum_i c_i'r^{2l_i'}r'^{2m_i'}(\boldsymbol{r}\cdot\boldsymbol{r}')^{n_i'}\exp\{-E'_{1i}r^2-E'_{2i}r'^2-E'_{3i}\boldsymbol{r}\cdot\boldsymbol{r}'\},
\end{aligned}$$

$$C_0\equiv1-(E_{1i}+E_{2i})/\gamma+F_i/(4\gamma^2),\quad F_i\equiv4E_{1i}E_{2i}-E_{3i}^2,$$

$$E'_{1i}\equiv\{E_{1i}-F_i/(4\gamma)\}/C_0,\quad E'_{2i}\equiv\{E_{2i}-F_i/(4\gamma)\}/C_0,$$

$$E'_{3i} \equiv E_{3i}/C_0 \,. \tag{3·3·23}$$

In the case of the overlap and kinetic energy kernels, $E_{ki}\,(k=1\sim3)$ are, from Eq. (2·2·53),

$$E_{1i}=E_{2i}=\frac{N_1N_2}{2A}\nu=\frac{\gamma}{2}\,,\quad E_{3i}=\left(n-\frac{N_1N_2}{A}\right)\nu=n\nu-\gamma\,, \tag{3·3·24}$$

where n is the number of nucleons exchanged. Then the range parameters $E'_{ki}\,(k=1\sim3)$ of the RGM kernels are calculated by Eq. (3·3·23) to be[8]

$$\begin{aligned} E'_{1i}&=E'_{2i}=\frac{\gamma}{2}\left\{\frac{n\nu}{2\gamma-n\nu}+\frac{2\gamma-n\nu}{n\nu}\right\},\\ E'_{3i}&=\gamma\left\{\frac{n\nu}{2\gamma-n\nu}-\frac{2\gamma-n\nu}{n\nu}\right\}. \end{aligned} \tag{3·3·25}$$

We can similarly evaluate $E'_{ki}\,(k=1\sim3)$ of the RGM kernel of the Gaussian two-nucleon interaction although they are slightly more complicated compared with Eq. (3·3·25).

3.4. System of clusters with unequal oscillator widths

3.4.a. *Transformation formulas*

As was discussed in § 2.1, when the clusters of the system are represented by the H.O. shell model wave functions with unequal oscillator width parameters, the GCM wave functions contain the spurious component of the excitation of the center-of-mass motion. Nevertheless, the GCM kernels constructed with these GCM wave functions containing spurious components can be used[11),54)~57),95)] to evaluate the RGM kernels which have no problem of the spuriousness since RGM wave functions do not contain the center-of-mass variable at all.

First we give a prescription which uses the two-fold Fourier transformation. Using the relation of Eq. (2·1·6), we obtain

$$\begin{aligned} &\int d\boldsymbol{R}\exp\{i\boldsymbol{k}\boldsymbol{R}\}\phi_0\left(C_1,\frac{-N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2,\frac{N_1}{A}\boldsymbol{R}\right)\\ &=\left(\frac{2N_1\nu_1}{\pi}\cdot\frac{2N_2\nu_2}{\pi}\right)^{3/4}\int d\boldsymbol{R}\exp\{i\boldsymbol{k}\boldsymbol{R}\}\\ &\quad\times\exp\{-\alpha\boldsymbol{X}_G{}^2-\beta\boldsymbol{X}_G(\boldsymbol{r}-\boldsymbol{R})-\gamma(\boldsymbol{r}-\boldsymbol{R})^2\}\phi_0(C_1)\phi_0(C_2)\\ &=\left(\frac{4N_1N_2\nu_1\nu_2}{\pi^2}\right)^{3/4}\left(\frac{\pi}{\gamma}\right)^{3/2}\exp\left\{-\frac{k^2}{4\gamma}\right\}\exp\left\{-\left(\alpha-\frac{\beta^2}{4\gamma}\right)\boldsymbol{X}_G{}^2+\frac{i\beta}{2\gamma}\boldsymbol{k}\cdot\boldsymbol{X}_G\right\}\\ &\quad\times\exp\{i\boldsymbol{k}\boldsymbol{r}\}\phi_0(C_1)\phi_0(C_2)\,, \end{aligned}$$

$$\int d\boldsymbol{R}_1d\boldsymbol{R}_2\exp\{i\boldsymbol{k}_1\boldsymbol{R}_1+i\boldsymbol{k}_2\boldsymbol{R}_2\}$$

$$\times\left\langle\psi_0\left(C_1,\frac{-N_2}{A}\boldsymbol{R}_1\right)\psi_0\left(C_2,\frac{N_1}{A}\boldsymbol{R}_1\right)|\mathcal{O}|\mathcal{A}\left\{\psi_0\left(C_1,\frac{-N_2}{A}\boldsymbol{R}_2\right)\psi_0\left(C_2,\frac{N_1}{A}\boldsymbol{R}_2\right)\right\}\right\rangle$$

$$=\left(\frac{4N_1N_2\nu_1\nu_2}{\pi^2}\right)^{3/2}\left(\frac{\pi}{\gamma}\right)^3\exp\left\{-\frac{1}{4\gamma}(k_1^2+k_2^2)\right\}$$

$$\times\left\langle\exp\left\{-\left(\alpha-\frac{\beta^2}{4\gamma}\right)\boldsymbol{X}_G^2-\frac{i\beta}{2\gamma}\boldsymbol{k}_1\boldsymbol{X}_G\right\}\middle|\exp\left\{-\left(\alpha-\frac{\beta^2}{4\gamma}\right)\boldsymbol{X}_G^2+\frac{i\beta}{2\gamma}\boldsymbol{k}_2\boldsymbol{X}_G\right\}\right\rangle$$

$$\times\langle\exp[-i\boldsymbol{k}_1\boldsymbol{r}]\phi_0(C_1)\phi_0(C_2)|\mathcal{O}|\mathcal{A}\{\exp[i\boldsymbol{k}_2\boldsymbol{r}]\phi_0(C_1)\phi_0(C_2)\}\rangle$$

$$=\left(\frac{2\pi}{\gamma}\right)^{3/2}\exp\{-p(k_1^2+k_2^2)-q\boldsymbol{k}_1\boldsymbol{k}_2\}$$

$$\times\langle\exp[-i\boldsymbol{k}_1\boldsymbol{r}]\phi_0(C_1)\phi_0(C_2)|\mathcal{O}|\mathcal{A}\{\exp[i\boldsymbol{k}_2\boldsymbol{r}]\phi_0(C_1)\phi_0(C_2)\}\rangle,$$

$$\alpha\equiv N_1\nu_1+N_2\nu_2,\quad \beta\equiv\frac{2N_1N_2}{N_1+N_2}(\nu_2-\nu_1),\quad \gamma\equiv\frac{N_1N_2}{(N_1+N_2)^2}(N_2\nu_1+N_1\nu_2),$$

$$p\equiv\frac{1}{4\gamma}+\frac{\beta^2}{32\gamma^2\left(\alpha-\frac{\beta^2}{4\gamma}\right)},\quad q\equiv\frac{\beta^2}{16\gamma^2\left(\alpha-\frac{\beta^2}{4\gamma}\right)}. \tag{3·4·1}$$

Thus the desired formula for m is

$$m(\boldsymbol{a}_1,\boldsymbol{a}_2)=\left(\frac{1}{2\pi}\right)^6\left(\frac{\gamma}{2\pi}\right)^{3/2}\int d\boldsymbol{k}_1d\boldsymbol{k}_2\exp\{-i\boldsymbol{k}_1\boldsymbol{a}_1-i\boldsymbol{k}_2\boldsymbol{a}_2\}$$

$$\times\exp\{p(k_1^2+k_2^2)+q\boldsymbol{k}_1\boldsymbol{k}_2\}\int d\boldsymbol{R}_1d\boldsymbol{R}_2$$

$$\times\exp\{i\boldsymbol{k}_1\boldsymbol{R}_1+i\boldsymbol{k}_2\boldsymbol{R}_2\}\Theta(\boldsymbol{R}_1,\boldsymbol{R}_2). \tag{3·4·2}$$

Equation (3·4·2) reduces to Eq. (3·3·4) when $\nu_1=\nu_2(\beta=0)$ and so it may also be called the double Fourier transformation formula.

Secondly we give another formula[54)~57)] which reduces to Eq. (3·3·7) when $\nu_1=\nu_2$. We note the relation,

$$\delta(\boldsymbol{r}-\boldsymbol{a})\exp\{-\alpha\boldsymbol{X}_G^2\}=\delta(\boldsymbol{r}-\boldsymbol{a})\exp\{-\alpha\boldsymbol{X}_G^2-\beta\boldsymbol{X}_G(\boldsymbol{r}-\boldsymbol{a})-\gamma(\boldsymbol{r}-\boldsymbol{a})^2\}$$

$$=\delta(\boldsymbol{r}-\boldsymbol{a})\exp\left\{-N_1\nu_1\left(\boldsymbol{X}_1+\frac{N_2}{A}\boldsymbol{a}\right)^2-N_2\nu_2\left(\boldsymbol{X}_2-\frac{N_1}{A}\boldsymbol{a}\right)^2\right\},$$

$$\delta(\boldsymbol{r}-\boldsymbol{a})=\left(\frac{1}{2\pi}\right)^3\int d\boldsymbol{k}\exp\{i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{a})\}$$

$$=\left(\frac{1}{2\pi}\right)^3\int d\boldsymbol{k}\exp\left[i\boldsymbol{k}\left\{\left(\boldsymbol{X}_2-\frac{N_1}{A}\boldsymbol{a}\right)-\left(\boldsymbol{X}_1+\frac{N_2}{A}\boldsymbol{a}\right)\right\}\right],$$

$$\delta(\boldsymbol{r}-\boldsymbol{a})\exp\{-\alpha\boldsymbol{X}_G^2\}\phi_0(C_1)\phi_0(C_2)$$

$$=\left(\frac{1}{2\pi}\right)^3\int d\boldsymbol{k}\exp\left\{-\left(\frac{1}{N_1\nu_1}+\frac{1}{N_2\nu_2}\right)\frac{k^2}{4}\right\}$$

$$\times\exp\left\{-N_1\nu_1\left(\boldsymbol{X}_1+\frac{N_2}{A}\boldsymbol{a}+\frac{i}{2N_1\nu_1}\boldsymbol{k}\right)^2\right\}$$
$$\times\exp\left\{-N_2\nu_2\left(\boldsymbol{X}_2-\frac{N_1}{A}\boldsymbol{a}-\frac{i}{2N_2\nu_2}\boldsymbol{k}\right)^2\right\}\phi_0(C_1)\,\phi_0(C_2)$$
$$=\left(\frac{1}{2\pi}\right)^3\left(\frac{\pi^2}{4N_1N_2\nu_1\nu_2}\right)^{3/4}\int d\boldsymbol{k}\exp\left\{-\left(\frac{1}{N_1\nu_1}+\frac{1}{N_2\nu_2}\right)\frac{k^2}{4}\right\}$$
$$\times\phi_0\left(C_1,\frac{-N_2}{A}\boldsymbol{a}-\frac{i}{2N_1\nu_1}\boldsymbol{k}\right)\phi_0\left(C_2,\frac{N_1}{A}\boldsymbol{a}+\frac{i}{2N_2\nu_2}\boldsymbol{k}\right). \qquad (3\cdot4\cdot3)^{*)}$$

From this relation we obtain

$$m(\boldsymbol{a}_1,\boldsymbol{a}_2)=\left(\frac{1}{2\pi}\right)^6\left(\frac{\pi}{2\tilde{\gamma}}\right)^{3/2}\int d\boldsymbol{k}_1d\boldsymbol{k}_2\exp\left\{-\frac{1}{4\tilde{\gamma}}(k_1^2+k_2^2)\right\}$$
$$\times\Theta\left(\frac{i(\nu_1-\nu_2)}{2A\nu_1\nu_2}\boldsymbol{k},\boldsymbol{a}_1+\frac{i}{2\tilde{\gamma}}\boldsymbol{k};\frac{i(\nu_1-\nu_2)}{2A\nu_1\nu_2}\boldsymbol{k},\boldsymbol{a}_2+\frac{i}{2\tilde{\gamma}}\boldsymbol{k}\right),$$
$$\tilde{\gamma}\equiv\frac{N_1N_2\nu_1\nu_2}{N_1\nu_1+N_2\nu_2}. \qquad (3\cdot4\cdot4)$$

It is clear that Eq. (3·4·4) reduces to Eq. (3·3·7) when $\nu_1=\nu_2$, and therefore we may call this formula also the single Fourier transformation formula.

The trouble of the system of clusters with unequal oscillator widths lies in the non-separability of the center-of-mass motion. So the trouble vanishes away simply by effacing[11] the dependence of the GCM wave function on the center-of-mass coordinate. We note the following relation,

$$\int d\boldsymbol{R}_G\phi_0\left(C_1,\boldsymbol{R}_G-\frac{N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2,\boldsymbol{R}_G+\frac{N_1}{A}\boldsymbol{R}\right)$$
$$=\left(\frac{4N_1N_2\nu_1\nu_2}{\pi^2}\right)^{3/4}\left[\int d\boldsymbol{R}_G\exp\{-\alpha(\boldsymbol{X}_G-\boldsymbol{R}_G)^2-\beta(\boldsymbol{X}_G-\boldsymbol{R}_G)(\boldsymbol{r}-\boldsymbol{R})\}\right]$$
$$\times\exp\{-\gamma(\boldsymbol{r}-\boldsymbol{R})^2\}\phi_0(C_1)\,\phi_0(C_2)$$
$$=\left(\frac{4N_1N_2\nu_1\nu_2}{\alpha^2}\right)^{3/4}\exp\left\{-\left(\gamma-\frac{\beta^2}{4\alpha}\right)(\boldsymbol{r}-\boldsymbol{R})^2\right\}\phi_0(C_1)\,\phi_0(C_2),$$
$$\int d\boldsymbol{R}_G\left\langle\phi_0\left(C_1,\boldsymbol{R}_G-\frac{N_2}{A}\boldsymbol{R}_1\right)\phi_0\left(C_2,\boldsymbol{R}_G+\frac{N_1}{A}\boldsymbol{R}_1\right)|\mathcal{O}\right.$$
$$\left.\times|\mathcal{A}\left\{\phi_0\left(C_1,\frac{-N_2}{A}\boldsymbol{R}_2\right)\phi_0\left(C_2,\frac{N_1}{A}\boldsymbol{R}_2\right)\right\}\right\rangle$$
$$=\left(\frac{4N_1N_2\nu_1\nu_2}{\pi\alpha}\right)^{3/2}\left\langle\exp\left\{-\left(\gamma-\frac{\beta^2}{4\alpha}\right)(\boldsymbol{r}-\boldsymbol{R}_1)^2\right\}\phi_0(C_1)\,\phi_0(C_2)\,|\mathcal{O}\right.$$
$$\left.\times|\mathcal{A}\{\exp[-\alpha\boldsymbol{X}_G^2-\beta\boldsymbol{X}_G(\boldsymbol{r}-\boldsymbol{R}_2)]\exp[-\gamma(\boldsymbol{r}-\boldsymbol{R}_2)^2]\phi_0(C_1)\,\phi_0(C_2)\}\right\rangle$$

*) Just as in the case of Eq. (3·3·6), Eq. (3·4·3) also can be generalized slightly by introducing an arbitrary complex vector $\boldsymbol{d}$ as $\delta(\boldsymbol{r}-\boldsymbol{a})\exp\{-\alpha X_G^2\}=\delta(\boldsymbol{r}-\boldsymbol{a})\exp\{-\alpha X_G^2-\beta\boldsymbol{X}_G(\boldsymbol{r}-\boldsymbol{a})-\gamma(\boldsymbol{r}-\boldsymbol{a})^2+\boldsymbol{d}(\boldsymbol{r}-\boldsymbol{a})\}$. This results in replacing $\boldsymbol{k}$ in Eq. (3·4·3) by $\boldsymbol{k}-i\boldsymbol{d}$.

$$= \left(\frac{4N_1N_2\nu_1\nu_2}{\alpha^2}\right)^{3/2} \left\langle \exp\left[-\left(\gamma-\frac{\beta^2}{4\alpha}\right)(\boldsymbol{r}-\boldsymbol{R}_1)^2\right]\phi_0(C_1)\phi_0(C_2)\,|\mathcal{O}\right.$$
$$\left.\times|\mathcal{A}\left\{\exp\left[-\left(\gamma-\frac{\beta^2}{4\alpha}\right)(\boldsymbol{r}-\boldsymbol{R}_2)^2\right]\phi_0(C_1)\phi_0(C_2)\right\}\right\rangle . \qquad (3\cdot4\cdot5)$$

This last equality which can be rewritten as

$$M_{\tilde{\gamma}}(\boldsymbol{R}_1, \boldsymbol{R}_2) = \left(\frac{\alpha}{2\pi}\right)^{3/2} \int d\boldsymbol{R}_G \Theta(\boldsymbol{R}_G\boldsymbol{R}_1, \boldsymbol{R}_2)$$
$$= \left(\frac{\alpha}{2\pi}\right)^{3/2} \int d\boldsymbol{R}_G \Theta(\boldsymbol{R}_1, \boldsymbol{R}_G\boldsymbol{R}_2),$$
$$\tilde{\gamma} \equiv \gamma - \frac{\beta^2}{4\alpha} = \frac{N_1N_2\nu_1\nu_2}{N_1\nu_1+N_2\nu_2}, \qquad (3\cdot4\cdot6)$$

gives the desired quantity $M_{\tilde{\gamma}}$ from which we obtain $m(\boldsymbol{a}_1, \boldsymbol{a}_2)$ by using Eq. (3·3·4), Eq. (3·3·7) or Eq. (3·3·8). Of course, we can use this quantity $M_{\tilde{\gamma}}$ for the evaluation of $\hat{m}(i,j)$ following the prescriptions described in § 3.3.b.

The calculation of the direct kernel $m^D(\boldsymbol{a}_1)\delta(\boldsymbol{a}_1-\boldsymbol{a}_2)$ is done simply by replacing Θ by Θ^D in Eqs. (3·4·2) and (3·4·4). When we use Eq. (3·3·2) for $m^D(\boldsymbol{a})$, we can utilize Eq. (3·3·10) or Eq. (3·3·11) by inserting for M_γ^D in these equations the kernel $M_{\tilde{\gamma}}^D$ calculated by $M_{\tilde{\gamma}}^D(\boldsymbol{R}_1, \boldsymbol{R}_2) = (\alpha/2\pi)^{3/2} \times \int d\boldsymbol{R}_G \Theta^D(\boldsymbol{R}_G, \boldsymbol{R}_1; \boldsymbol{R}_2) = (\alpha/2\pi)^{3/2} \int d\boldsymbol{R}_G \Theta^D(\boldsymbol{R}_1; \boldsymbol{R}_G, \boldsymbol{R}_2)$ following the same argument which has lead to Eq. (3·4·6). The calculation of $m^D(\boldsymbol{a})$ of Eq. (3·3·2) without using $M_{\tilde{\gamma}}^D$ is, of course, possible. We only give here some formulas which are analogous to Eqs. (3·3·10) and (3·3·11) and are easy to prove,

$$m^D(\boldsymbol{a}) = \left(\frac{1}{2\pi}\right)^3 \left(\frac{\pi}{2\tilde{\gamma}}\right)^{3/2} \int d\boldsymbol{k} \exp\left\{-\frac{k^2}{4\tilde{\gamma}}\right\} \Theta^D\left(\boldsymbol{a}; \frac{i(\nu_1-\nu_2)}{2A\nu_1\nu_2}\boldsymbol{k}, \boldsymbol{a}+\frac{i}{2\tilde{\gamma}}\boldsymbol{k}\right)$$
$$= \left(\frac{1}{2\pi}\right)^3 \int d\boldsymbol{k} \exp\{-i\boldsymbol{k}\boldsymbol{a}+p'k^2\} \int d\boldsymbol{R} \exp\{i\boldsymbol{k}\boldsymbol{R}\} \Theta^D(\boldsymbol{R}, \boldsymbol{R}),$$
$$p' \equiv \frac{1}{8\gamma} + \frac{\beta^2}{32\gamma^2\left(\alpha-\frac{\beta^2}{4\gamma}\right)}. \qquad (3\cdot4\cdot7)$$

The diagonal elements of the direct GCM kernel $\Theta^D(\boldsymbol{R}; \boldsymbol{R})$ (more generally $\Theta^D(\boldsymbol{R}_G, \boldsymbol{R}; \boldsymbol{R}_G, \boldsymbol{R})$) are very easy to compute just like as $M_\gamma^D(\boldsymbol{R}, \boldsymbol{R})$ for $\nu_1=\nu_2$ and we can calculate them entirely in the same way as in Eq. (3·3·12).

3.4.b. *Some extensions*

When the wave function of the system is expressed by

$$\sum_i \mathcal{A}\{\chi_i(\boldsymbol{r})\phi_0(C_1, \nu_{1i})\phi_0(C_2, \nu_{2i})\}, \qquad (3\cdot4\cdot8)$$

we need to calculate the kernels of the type

$$\langle \delta(\boldsymbol{r}-\boldsymbol{a})\phi_0(C_1,\nu_1)\phi_0(C_2,\nu_2)|\mathcal{O}|\mathcal{A}\{\delta(\boldsymbol{r}-\boldsymbol{b})\phi_0(C_1,\nu_1')\phi_0(C_2,\nu_2')\}\rangle. \quad (3\cdot4\cdot9)$$

Kernels of this type also appear when the internal wave function of the cluster is expressed as

$$\phi_0(C)=\sum_j c_j\phi_0(C,\nu_j). \quad (3\cdot4\cdot10)$$

It is evident that the calculation of the kernel of Eq. (3·4·9) can be done entirely in the same manner as in Eqs. (3·4·1) and (3·4·3).

The size parameters of the clusters may change depending on the inter-cluster distance. One way to treat this effect is to use the wave function of Eq. (3·4·8). As another prescription we may adopt the wave function of the type,

$$\mathcal{A}\{\chi(\boldsymbol{r})\phi_0(C_1,\nu_1(r))\phi_0(C_2,\nu_2(r))\}$$
$$=\int d\boldsymbol{a}\chi(\boldsymbol{a})\mathcal{A}\{\delta(\boldsymbol{r}-\boldsymbol{a})\phi_0(C_1,\nu_1(a))\phi_0(C_2,\nu_2(a))\}, \quad (3\cdot4\cdot11)$$

where we assume $\nu_1(a)$ and $\nu_2(a)$ are the width parameter function depending smoothly on the distance parameter of $a=|\boldsymbol{a}|$. The necessary kernel for this type of wave function is of the type of Eq. (3·4·9) and can be calculated in the same way.

§ 4. RGM norm kernel

4.1. Eigen-value problem

4.1.a. *Orthonormal basis functions of the system*

In general, to solve the eigen-value problem of the norm kernel (or overlap kernel) of the system is equivalent to construct the orthonormal basis functions of the system.

In our case of the systems composed of composite particles, the wave functions have the form,

$$\sum_j \mathcal{A}_j'\{\chi_j(\hat{\xi}_j)\phi_j\},$$

$$\mathcal{A}_j'\equiv\frac{1}{\sqrt{n_j}}\mathcal{A}_j, \quad n_j\equiv A!/(N_{j1}!N_{j2}!\cdots), \quad (4\cdot1\cdot1)$$

where ϕ_j denote the channel wave functions which are product of internal cluster wave functions (and the spherical harmonics of the angle variables of relative coordinates) and $\hat{\xi}_j$ mean the set of relative coordinates in j-channel. Now we choose a suitable complete orthonormal set of function for each channel which is denoted by $\chi_j^{n_j}$ $(n_j=1,2,\cdots)$. The set of functions $\{\mathcal{A}_j'\times\{\chi_j^{n_j}\phi_j\}\}$ covers our functional space of the system. The orthonormal basis

wave functions Φ_α are obtained by constructing the Gram matrix by these functions $\mathcal{A}_j'\{\chi_j^{n_j}\phi_j\}$ and by solving the eigen-value problem of this Gram matrix, as follows:

$$\sum_{jn_j}\langle\mathcal{A}_i'\{\chi_i^{n_i}\phi_i\}|\mathcal{A}_j'\{\chi_j^{n_j}\phi_j\}\rangle C^\alpha_{jn_j}=\mu_\alpha C^\alpha_{in_i},$$

$$\Phi_\alpha=\frac{1}{\sqrt{\mu_\alpha}}\sum_{jn_j}C^\alpha_{jn_j}\mathcal{A}_j'\{\chi_j^{n_j}\phi_j\}. \tag{4·1·2}$$

From this Eq. (4·1·2) we obtain

$$\sum_{jn_j}\langle\mathcal{A}_i'\{\delta(\xi_i-a_i)\phi_i\}|\mathcal{A}_j'\{\chi_j^{n_j}(\xi_j)\phi_j\}\rangle C^\alpha_{jn_j}=\mu_\alpha\sum_{n_i}C^\alpha_{in_i}\chi_i^{n_i}(a_i), \tag{4·1·3}$$

because if we expand the left-hand-side quantity of Eq. (4·1·3) which is a function of a_i by the complete orthonormal set of functions $\chi_i^{n_i}(a_i)$ ($n_i=1, 2, \cdots$) as

$$\sum_{jn_j}\langle\mathcal{A}_i'\{\delta(\xi_i-a_i)\phi_i\}|\mathcal{A}_j'\{\chi_j^{n_j}(\xi_j)\phi_j\}\rangle C^\alpha_{jn_j}=\sum_{n_i}p_{n_i}\chi_i^{n_i}(a_i), \tag{4·1·4}$$

we easily get $p_{n_i}=\mu_\alpha C^\alpha_{in_i}$ due to the orthonormal property of $\{\chi_i^{n_i};\ n_i=1, 2, \cdots\}$ and from Eq. (4·1·2). If we define

$$\chi_i^\alpha(\xi_i)\equiv\sum_{n_i}C^\alpha_{in_i}\chi_i^{n_i}(\xi_i), \tag{4·1·5}$$

we can rewrite Eq. (4·1·3) as follows:

$$\sum_j\int db_j\langle\mathcal{A}_i'\{\delta(\xi_i-a_i)\phi_i\}|\mathcal{A}_j'\{\delta(\xi_j-b_j)\phi_j\}\rangle\chi_j^\alpha(b_j)=\mu_\alpha\chi_i^\alpha(a_i). \tag{4·1·6}$$

This is just the equation of the eigen-value problem of the RGM norm kernel, and we see that the eigen-values μ_α obtained from Eq. (4·1·2) are just the eigen-values of the RGM norm kernel and functions χ_i^α defined by Eq. (4·1·5) with the use of $C^\alpha_{in_i}$ obtained from Eq. (4·1·2) are eigen-functions of the RGM norm kernel. We need to show that there are no other eigen-functions of the RGM norm kernel besides $\chi_i^\alpha=\sum_{n_i}C^\alpha_{in_i}\chi_i^{n_i}$ obtained from Eq. (4·1·2). This is done by inverting our discussion from Eq. (4·1·2) to Eq. (4·1·6). Let us consider any eigen-function χ_i^α belonging to the eigen-value μ_α of the RGM norm kernel which satisfies Eq. (4·1·6). We expand this χ_i^α by the complete orthonormal set of functions $\chi_i^{n_i}$ as in Eq. (4·1·5), by the expansion coefficients $C^\alpha_{in_i}$. By inserting this expanded form of χ_i^α into Eq. (4·1·6), we easily know that μ_α and $C^\alpha_{in_i}$ just satisfy Eq. (4·1·2).

We can, of course, choose as a set of functions which covers our functional space of the system, $\{\mathcal{A}_j'\{\delta(\xi_j-a_j)\phi_j\}\}$ instead of $\{\mathcal{A}_j'\{\chi_j^{n_j}\phi_j\}\}$. In this case the equation of the eigen-value problem of the Gram matrix of these functions $\mathcal{A}_j'\{\delta(\xi_j-a_j)\phi_j\}$ is nothing but Eq. (4·1·6), and so we immediately know that the orthonormal basis wave functons Φ_α of our functional space are given by

$$\Phi_\alpha=\frac{1}{\sqrt{\mu_\alpha}}\sum_j \mathcal{A}_j'\{\chi_j^\alpha(\xi_j)\phi_j\}, \qquad (4\cdot1\cdot7)$$

by the eigen-functions χ_j^α of the RGM norm kernel.

The eigen-value $\mu_\alpha=0$ needs a special attention. Since $\mu_\alpha=\|\sum_j \mathcal{A}_j' \times\{\chi_j^\alpha(\xi_j)\phi_j\}\|^2$, $\mu_\alpha=0$ means $\sum_j\mathcal{A}_j'\{\chi_j^\alpha(\xi_j)\phi_j\}\equiv0$. This is the linear dependence among the functions $\mathcal{A}_j'\{\chi_j^\alpha\phi_j\}$ which is caused by the Pauli principle. Needless to say, the basis functions of the system, Φ_α are defined for $\mu_\alpha\neq0$ by Eq. (4·1·2) or Eq. (4·1·7).

When the wave functions of the constituent clusters are described by the harmonic oscillator (H.O.) shell model wave functions with common oscillator parameters $\nu_1=\nu_2=\cdots=\nu$, the eigen-value problem of the RGM norm kernel can be solved analytically. The eigen-functions χ_i^α are the linear combinations of the finite number of H.O. functions. We prove this below following the argument from Eq. (4·1·2) to Eq. (4·1·6). We adopt as $\chi_j^{n_j}(\xi_j)$ the H.O. functions. Then $\mathcal{A}_j'\{\chi_j^{n_j}(\xi_j)\phi_j\}$ are the eigen functions of the operator of the total H.O. quanta, $N^{op}=\sum_{i=1}^{A}\boldsymbol{a}_i^\dagger\cdot\boldsymbol{a}_i-\boldsymbol{a}^\dagger(\boldsymbol{x}_G)\cdot\boldsymbol{a}(\boldsymbol{x}_G)$, where $\boldsymbol{a}_i^\dagger(\boldsymbol{a}_i)$ are the creation (destruction) operator of the H.O. quanta of i-th nucleon and $\boldsymbol{a}^\dagger(\boldsymbol{x}_G)$ $(\boldsymbol{a}(\boldsymbol{x}_G))$ that of center-of-mass coordinate. The Gram matrix by these functions clearly decomposes into submatrices which are constructed by the functions $\mathcal{A}_j'\{\chi_j^{n_j}\phi_j\}$ having the same number of the total H.O. quanta. Thus the eigen-value equation of Eq. (4·1·2) is reduced to the infinite sets of the eigen-value problems of the submatrices which are of finite dimension. The diagonalization of the matrix of finite dimension is treated easily by numerical evaluation but as we see below in many cases this diagonalization can be done analytically (or algebraically). In this subsection we therefore investigate the eigen-value problem of the RGM norm kernel in the case of the equal oscillator widths. The problem in the case of the unequal oscillator widths is discussed in § 4.3.

4.1.b. *System of two SU_3 scalar clusters*

The eigen-value problem of the two-cluster system is especially simple when the internal wave functions $\phi(C_i)$ are both described by the SU_3 shell model wave functions belonging to the scalar (namely $(\sigma,\tau)=(0,0)$) representations. So the systems composed of the clusters such as nucleon, deuteron, triton or ^{3}He, $\alpha(^4\mathrm{He})$, ^{16}O and ^{40}Ca are the subjects under consideration.

The eigen-value equation is

$$\langle\phi_0(C_1)\phi_0(C_2)|\mathcal{A}\{\chi^\alpha(\boldsymbol{r})\phi_0(C_1)\phi_0(C_2)\}\rangle=\mu_\alpha\chi^\alpha(\boldsymbol{r}), \qquad (4\cdot1\cdot8)$$

and the eigen functions $\chi^\alpha(\boldsymbol{r})$ are the H.O. functions $V_{Nlm}(\boldsymbol{r},\gamma)\equiv R_{Nl}(r,\gamma)\times Y_{lm}(\hat{r})$, $\gamma=(N_1N_2/(N_1+N_2))\nu$, as is shown in § 4.1.a. The eigen-values μ_α are therefore

$$\mu_{Nlm}=\langle V_{Nlm}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)|\mathcal{A}\{V_{Nlm}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)\}\rangle. \qquad (4\cdot1\cdot9)$$

(When C_1 and C_2 are identical, it is usual to define the half of the value of Eq. (4·1·9) as the eigen-value.) First we show that μ_{Nlm} depends only on $N(=2n+l)$ and not on l and m. This fact is due to the SU_3 scalar property of the antisymmetrization operator $\mathcal{A}$ that $\mathcal{A}$ commutes with all the SU_3 generators which are totally symmetric with respect to the permutations of nucleons. Equation (4·1·9) shows that μ_{Nlm} is just the diagonal matrix element of $\mathcal{A}$ by $V_{Nlm}\phi_0(C_1)\phi_0(C_2)$ which has the SU_3 symmetry $(\lambda, \mu)=(N, 0)$ since both $\phi_0(C_1)$ and $\phi_0(C_2)$ are SU_3 scalar. Due to the Wigner-Eckert theorem the matrix element of the SU_3 scalar operator depends only on the label of the irreducible representation (λ, μ) of the wave function and so in our case μ_{Nlm} depends only on N.[14] We therefore denote μ_{Nlm} simply by μ_N. The above argument also means that μ_N can be expressed as $\mu_N=\langle V_{(N,0)i}(\boldsymbol{r})\phi_0(C_1)\times\phi_0(C_2)|\mathcal{A}\{V_{(N,0)i}(\boldsymbol{r})\phi_0(C_1)\phi_0(C_2)\}\rangle$ where $V_{(N,0)i}(\boldsymbol{r})$ is an arbitrary H.O. function of $\boldsymbol{r}$ belonging to $(N, 0)$ representation. We thus obtain

$$\begin{aligned}&\mu_N=\langle X_N(\boldsymbol{r},\gamma)\phi_0|\mathcal{A}\{X_N(\boldsymbol{r},\gamma)\phi_0\}\rangle,\\&X_N(\boldsymbol{r},\gamma)\equiv X_{(0,0,N)}(\boldsymbol{r},\gamma),\ \phi_0\equiv\phi_0(C_1)\phi_0(C_2),\end{aligned}\qquad(4\cdot1\cdot10)$$

where $X_{\boldsymbol{N}}=X_{(N_1,N_2,N_3)}$ denotes the H.O. function with N_1, N_2 and N_3 oscillator quanta in x, y and z directions, respectively as was defined in § 3. Now we use the generating function technique explained in § 3.3.b. which gives the calculational procedure of the RGM kernel in the H.O. representation. From Eqs. (3·3·16) and (3·3·19), we obtain[14]

$$\begin{aligned}\hat{N}(R)&\equiv\langle A_\gamma(\boldsymbol{r},\boldsymbol{R}_z)\phi_0|\mathcal{A}\{A_\gamma(\boldsymbol{r},\boldsymbol{R}_z)\phi_0\}\rangle\\&=e^{R^2}\left\langle\Gamma\left(\boldsymbol{r},\frac{\boldsymbol{R}_z}{\sqrt{\gamma}},\gamma\right)\phi_0|\mathcal{A}\left\{\Gamma\left(\boldsymbol{r},\frac{\boldsymbol{R}_z}{\sqrt{\gamma}},\gamma\right)\phi_0\right\}\right\rangle\\&=\sum_{\boldsymbol{N}_1\boldsymbol{N}_2}U_{\boldsymbol{N}_1}(\boldsymbol{R}_z)U_{\boldsymbol{N}_2}(\boldsymbol{R}_z)\langle X_{\boldsymbol{N}_1}(\boldsymbol{r},\gamma)\phi_0|\mathcal{A}\{X_{\boldsymbol{N}_2}(\boldsymbol{r},\gamma)\phi_0\}\rangle\\&=\sum_N\{U_{(0,0,N)}(\boldsymbol{R}_z)\}^2\langle X_N(\boldsymbol{r},\gamma)\phi_0|\mathcal{A}\{X_N(\boldsymbol{r},\gamma)\phi_0\}\rangle\\&=\sum_{N=0}^{\infty}\frac{R^{2N}}{N!}\mu_N,\\&\boldsymbol{R}_z\equiv(0,0,R),\end{aligned}\qquad(4\cdot1\cdot11)$$

where we used $U_{(N_1,N_2,N_3)}(\boldsymbol{R}_z)=\delta_{N_1,0}\delta_{N_2,0}U_{(0,0,N_3)}(\boldsymbol{R}_z)=\delta_{N_1,0}\delta_{N_2,0}R^{N_3}/\sqrt{N_3!}$ and the fact that $\langle X_{\boldsymbol{N}_1}(\boldsymbol{r},\gamma)\phi_0|\mathcal{A}\{X_{\boldsymbol{N}_2}(\boldsymbol{r},\gamma)\phi_0\}\rangle=\delta_{\boldsymbol{N}_1,\boldsymbol{N}_2}\langle X_{\boldsymbol{N}_1}\phi_0|\mathcal{A}\{X_{\boldsymbol{N}_1}\phi_0\}\rangle$ due to the conservation of the number of the oscillator quanta in each direction. Thus the function $\hat{N}(R)$ which is essentially the GCM norm kernel is the generating function of the eigen values μ_N of the RGM norm kernel.

We here show some examples.[14] Let x be any $0s$-shell cluster like as p, n, d, t, ^{3}He and α(^{4}He) and N_x be the mass number of the cluster x. Then the generating function $\hat{N}(R)$ and the eigen-values μ_N for $\alpha+x$ system

are

$$\hat{N}(R)=\exp\{R^2\}\left(1-\exp\left\{-\frac{4+N_x}{4N_x}R^2\right\}\right)^{N_x},$$

$$\mu_N=\frac{1}{1+\delta_{N_x,4}}\sum_{k=0}^{N_x}\binom{N_x}{k}(-)^k\left(1-\frac{4+N_x}{4N_x}k\right)^N, \qquad (4\cdot1\cdot12)$$

where the factor $1/(1+\delta_{N_x,4})$ is inserted for μ_N because when $N_x=4$ we have the identical two-cluster system of $\alpha+\alpha$ and usual definition of μ_N is just the half of $\langle X_N\phi_0|\mathcal{A}\{X_N\phi_0\}\rangle$. Equation (4·1·12) for μ_N for $\alpha+\alpha$ can be rewritten in a usual form,[59),60)] namely $\mu_N=0$ for $N=$odd and $\mu_N=1-2^{2-N}+3\delta_{N,0}$ for $N=$even. Similarly for $^{16}\mathrm{O}+x$ system,

$$\hat{N}(R)=e^{R^2}\{1-(1+q_xR^2)e^{-q_xR^2}\}^{N_x},$$

$$\mu_N\equiv\sum_{k=0}^{N_x}\binom{N_x}{k}(-)^k\sum_{r=0}^{k}\binom{k}{r}{q_x}^r\theta(N-r)\frac{N!}{(N-r)!}(1-q_xk)^{N-r},$$

$$q_x\equiv\frac{16+N_x}{16N_x}, \qquad (4\cdot1\cdot13)$$

where $\theta(x)$ is defined by $\theta(x)=1$ for $x\geqq0$ and $\theta(x)=0$ for $x<0$. For $^{40}\mathrm{Ca}+x$,

$$\hat{N}(R)=e^{R^2}\left[1-\left\{1+q_xR^2+\frac{1}{2}(q_xR^2)^2\right\}e^{-q_xR^2}\right]^{N_x},$$

$$\mu_N=\sum_{k=0}^{N_x}\binom{N_x}{k}(-)^k\sum_{r=0}^{k}\binom{k}{r}\left(\frac{{q_x}^2}{2}\right)^{(k-r)}\sum_{p=0}^{r}\binom{r}{p}{q_x}^p$$

$$\times\theta(N-p-2k+2r)\frac{N!}{(N-p-2k+2r)!}(1-q_xk)^{(N-p-2k+2r)},$$

$$q_x\equiv\frac{40+N_x}{40N_x}. \qquad (4\cdot1\cdot14)$$

For $^{16}\mathrm{O}+^{16}\mathrm{O}$,

$$\hat{N}(R)=\left\{\left(2\sinh\frac{R^2}{16}\right)^2-\left(\frac{R^2}{4}\sinh\frac{R^2}{16}\right)^4\right\}^4,$$

$$\mu_N\equiv\frac{1}{2}\langle X_N\phi_0|\mathcal{A}\{X_N\phi_0\}\rangle$$

$$=\begin{cases}\displaystyle\sum_{k=0}^{4}\left(\frac{-1}{64}\right)^k\binom{4}{k}\frac{N!}{(N-2k)!}\sum_{r=0}^{7-k}(-)^r\binom{16-2k}{r}\left(1-\frac{k+r}{8}\right)^{N-2k} \\ \qquad\text{for}\quad N\geqq24, \\ 0\qquad\text{for}\quad N\leqq22. \end{cases} \qquad (4\cdot1\cdot15)$$

Values of μ_N for $\alpha+\alpha$, $\alpha+^{16}\mathrm{O}$, $\alpha+^{40}\mathrm{Ca}$ and $^{16}\mathrm{O}+^{16}\mathrm{O}$ systems are given in

Table I $(\alpha+\alpha, {}^{16}O+{}^{16}O)$ and in Table IV $(\alpha+{}^{16}O, \alpha+{}^{40}Ca)$.

Table I. Eigen-values μ_N of the norm kernel for (a) $\alpha+\alpha$ and (b) $^{16}O+^{16}O$ systems. Superfices denote minus power of 10, for example, $3.168^{3}=3.168\times10^{-3}$.

(a) $\alpha+\alpha$

N	4	6	8	10	12	.....
μ_N	0.7500	0.9375	0.9844	0.9961	0.9990	.....

(b) $^{16}O+^{16}O$

N	24	26	28	30	32	34
μ_N	3.168^{3}	1.502^{2}	4.039^{2}	8.141^{2}	0.1371	0.2045
N	36	38	40	42	44	46
μ_N	0.2792	0.3571	0.4345	0.5085	0.5774	0.6399
N	48	50	52	54	56	58
μ_N	0.6955	0.7443	0.7865	0.8227	0.8533	0.8792
N	60	70	80	90	100	110
μ_N	0.9008	0.9644	0.9878	0.9960	0.9987	0.9996

4.1.c. *Two-cluster system including SU_3 non-scalar cluster*

In order to understand the structure of the norm kernel of the system which includes clusters described by the shell model wave functions belonging to the SU_3 non-scalar representations $(\sigma,\tau)\neq(0,0)$, it is instructive to investigate the norm kernel of the enlarged system where all the excited states with the same (σ,τ) are included.

Let C_1 be an SU_3 non-scalar cluster belonging to $(\sigma,\tau)\neq(0,0)$ and C_2 be an SU_3 scalar cluster. The channel coupling wave function of this illustrative two-cluster system where all the excited states of C_1 within (σ,τ) are included is (cf. Eq. (3·1·8))

$$\sum_j \mathcal{A}\{\chi_j(r)\,[Y_{l_j}(\hat{r})\,\phi_{\rho_j L_j}(C_1)]_J\phi_0(C_2)\}, \tag{4·1·16}$$

where j stands for the set of channel quantum numbers (l_j, ρ_j, L_j) and $\phi_{\rho L}$ is the abbreviated notation for $\phi_{(\sigma,\tau)\rho L}$. The eigen-value equation of the norm kernel is

$$\sum_j \langle h_i^J|\mathcal{A}\{\chi_j^{\alpha}(r)\,h_j^J\}\rangle=\mu_\alpha\chi_i^{\alpha}(r),$$

$$h_i^J\equiv[Y_{l_i}(\hat{r})\,\phi_{\rho_i L_i}(C_1)]_J\phi_0(C_2). \tag{4·1·17}$$

To solve this, we follow the procedure from Eq. (4·1·2) to Eq. (4·1·6). We choose as the set of functions which cover our system space, the following one,

$$\mathcal{A}\{[V_{(N,0)}(\boldsymbol{r},\gamma)\,\phi_{(\sigma,\tau)}(C_1)]_{(\lambda,\mu)\kappa J}\phi_0(C_2)\}, \tag{4·1·18}$$

where

$$[V_{(N,0)}(\boldsymbol{r},\gamma)\phi_{(\sigma,\tau)}(C_1)]_{(\lambda,\mu)\kappa J}$$
$$=\sum_j \langle (N,0)l_i,\ (\sigma,\tau)\rho_j L_j \| (\lambda,\mu)\kappa J\rangle [V_{Nl_j}(\boldsymbol{r},\gamma)\phi_{\rho_j L_j}(C_1)]_J,$$
$$[V_{Nl_j}(\boldsymbol{r},\gamma)\phi_{\rho_j L_j}(C_1)]_J = R_{Nl_j}(r,\gamma)h_j^J. \qquad (4\cdot1\cdot19)$$

Here $\langle (N,0)l,\ (\sigma,\tau)\rho L\|(\lambda,\mu)\kappa J\rangle$ is the reduced Clebsch-Gordan (or Wigner) coefficient (abbreviated as C-G coefficient) of SU_3 group for the coupling $(N,0)\times(\sigma,\tau)\to(\lambda,\mu)$. Due to the SU_3 scalar property of $\mathcal{A}$, these antisymmetrized functions of Eq. (4·1·18) have the SU_3 quantum numbers (λ,μ), κ, J. Thus the Gram matrix constructed by these functions is already diagonal. The answer of Eq. (4·1·17) is therefore[15]

$$\chi_i^{\alpha}(r) = \langle (N,0)l_i,\ (\sigma,\tau)\rho_i L_i\|(\lambda,\mu)\kappa J\rangle R_{Nl_i}(r,\gamma),$$
$$\mu_\alpha = \langle g^N_{(\lambda,\mu)\kappa J}|\mathcal{A}\{g^N_{(\lambda,\mu)\kappa J}\}\rangle,$$
$$g^N_{(\lambda,\mu)\kappa J} \equiv [V_{(N,0)}(\boldsymbol{r},\gamma)\phi_{(\sigma,\tau)}(C_1)]_{(\lambda,\mu)\kappa J}\phi_0(C_2),$$
$$\alpha = \{N,\ (\lambda,\mu),\ \kappa,\ J\}. \qquad (4\cdot1\cdot20)$$

From the SU_3 scalar property of $\mathcal{A}$, we know that μ_α depends only on N and (λ,μ) and it is independent of κ and J.[15] We therefore denote μ_α by $\mu^N_{(\lambda,\mu)}$.

The practical calculational procedure of the eigen-values $\mu^N_{(\lambda,\mu)}$ is to evaluate the matrix elements $\langle R_{Nl_i}h_i^J|\mathcal{A}\{R_{Nl_j}h_j^J\}\rangle$ by the methods given in § 3.3.b and then to diagonalize the matrix. This procedure gives us not only $\mu^N_{(\lambda,\mu)}$ but also the C-G coefficients; namely the solution of

$$\sum_j \langle R_{Nl_i}(r,\gamma)h_i^J|\mathcal{A}\{R_{Nl_j}(r,\gamma)h_j^J\}\rangle C_j^{\alpha} = \mu_\alpha C_i^{\alpha}, \qquad (4\cdot1\cdot21)$$

gives us

$$\mu_\alpha = \mu^N_{(\lambda,\mu)},$$
$$C_i^{\alpha} = \langle (N,0)l_i,\ (\sigma,\tau)\rho_i L_i\|(\lambda,\mu)\kappa J\rangle. \qquad (4\cdot1\cdot22)$$

There is a method of calculating the eigen-values $\mu^N_{(\lambda,\mu)}$ which avoids the numerical diagonalization procedure of Eq. (4·1·21). In order to interpret this method,[15] we consider a simple case of $(\sigma,\tau)=(\sigma,0)$. Then, (λ,μ) resulting from $(N,0)\times(\sigma,0)$ are $(N+\sigma-2k,k)$ with $k=0,1,\cdots\min(N,\sigma)$. Here we are reminded of Elliott's rule for obtaining the representation of R_3 (rotation group) contained in a representation of SU_3. For a given (λ,μ), the possible J values (angular momenta) are

$$J=K,K+1,\cdots,K+\lambda \qquad \text{for } K\neq0,$$
$$=\lambda,\lambda-2,\cdots,1 \text{ or } 0 \qquad \text{for } K=0 \qquad (4\cdot1\cdot23)$$

with the integer K taking the values

$$K=\mu, \mu-2, \cdots, 1 \text{ or } 0. \tag{4·1·24}$$

From this rule, we find that $J=N+\sigma$ is contained only in $(\lambda, \mu)=(N+\sigma, 0)$ with multiplicity one. So with the use of the notation

$$a(J, i) \equiv \langle R_{Nl_i}(r, \gamma) h_i^J | \mathcal{A}\{R_{Nl_i}(r, \gamma) h_i^J\} \rangle, \tag{4·1·25}$$

we get

$$\mu^N_{(N+\sigma, 0)} = a(J=N+\sigma, i), \tag{4·1·26}$$

where, of course, possible i is unique, namely $i=(l_i=N, L_i=\sigma)$. Similarly $J=N+\sigma-1$ is contained only in $(\lambda, \mu)=(N+\sigma-2, 1)$ with multiplicity one. Thus we get

$$\mu^N_{(N+\sigma-2, 1)} = a(J=N+\sigma-1, i), \tag{4·1·27}$$

where the unique channel number i is also $i=(l_i=N, L_i=\sigma)$. For $J=N+\sigma-2$, there are three (λ, μ) which contain this J value. They are $(\lambda, \mu)=(N+\sigma, 0)$, $(N+\sigma-2, 1)$ and $(N+\sigma-4, 2)$ each of which contains $J=N+\sigma-2$ with multiplicity one. Three channel numbers which yield this $J=N+\sigma-2$ are $i=(l_i=N, L_i=\sigma)$, $(l_i=N, L_i=\sigma-2)$ and $(l_i=N-2, L_i=\sigma)$. The essence of our method lies in the use of the invariance of the trace in the diagonalization procedure of Eq. (4·1·21). From this invariance of the trace we get

$$\sum_i a(J=N+\sigma-2, i) = \mu^N_{(N+\sigma, 0)} + \mu^N_{(N+\sigma-2, 1)} + \mu^N_{(N+\sigma-4, 2)}. \tag{4·1·28}$$

Since we already know values of $\mu^N_{(N+\sigma, 0)}$ and $\mu^N_{(N+\sigma-2, 1)}$ by Eqs. (4·1·26) and (4·1·27), we can calculate $\mu^N_{(N+\sigma-4, 2)}$ from the known quantities as

$$\mu^N_{(N+\sigma-4, 2)} = \sum_i a(J=N+\sigma-2, i) - \mu^N_{(N+\sigma, 0)} - \mu^N_{(N+\sigma-2, 1)}. \tag{4·1·29}$$

In this way similarly, we can calculate all the eigen-values $\mu^N_{(\lambda, \mu)}$. Since the matrix elements $a(J, i)$ are obtained analytically by the method in § 3.3.b, this calculational method of $\mu^N_{(\lambda, \mu)}$ gives us the analytical expressions for $\mu^N_{(\lambda, \mu)}$.

Equation (4·1·20) shows that the structure of the norm kernel is governed by the relatively small number of quantities $\mu^N_{(\lambda, \mu)}$ which are independent of κ and J. (The eigen-functions are determined automatically with the use of the known quantities, the SU_3 C-G coefficients.)

We express below by using $\mu^N_{(\lambda, \mu)}$ the quantities in the norm kernel problem of the narrower system where the excitation of the cluster C_1 is restricted. Let us consider the case where only one state of C_1 with the wave function $\phi_{\rho L}(C_1)$ is involved. The wave function of this system is

$$\sum_i \mathcal{A}\{\chi_l(r)[Y_l(\hat{r})\phi_{\rho L}(C_1)]_J \phi_0(C_2)\}, \tag{4·1·30}$$

and the eigen-value equation of the norm kernel is

$$\sum_{l'}\langle h_l^J|\mathcal{A}\{\chi_{l'}^{\alpha}(r)\,h_{l'}^J\}\rangle=\mu_\alpha\chi_l{}^{\alpha}(r),$$

$$h_l{}^J\equiv[Y_l(\hat{r})\,\phi_{\rho L}(C_1)]_J\phi_0(C_2). \tag{4·1·31}$$

The answer to this equation is obtained by solving the following equation,

$$\sum_{l'}\langle R_{Nl}(r,\gamma)\,h_l{}^J|\mathcal{A}\{R_{Nl'}(r,\gamma)\,h_{l'}^J\}\rangle C_{l'}^{\alpha}=\mu_\alpha C_l{}^{\alpha}, \tag{4·1·32}$$

which gives us μ_α and $\chi_l{}^{\alpha}$

$$\chi_l{}^{\alpha}=C_l{}^{\alpha}R_{Nl}(r,\gamma). \tag{4·1·33}$$

The matrix elements in Eq. (4·1·32) are expressed by

$$\langle R_{Nl}h_l{}^J|\mathcal{A}\{R_{Nl'}h_{l'}^J\}\rangle=\sum_{(\lambda,\mu)\kappa}\langle(N,0)\,l,\ (\sigma,\tau)\rho L\|(\lambda,\mu)\kappa J\rangle$$
$$\times\langle(N,0)\,l',\ (\sigma,\tau)\rho L\|(\lambda,\mu)\kappa J\rangle\mu^N_{(\lambda,\mu)}, \tag{4·1·34}$$

which is due to the relation

$$R_{Nl}(r,\gamma)\,h_l{}^J=[V_{Nl}(\boldsymbol{r},\gamma)\,\phi_{\rho L}(C_1)]_J\phi_0(C_2)$$
$$=\sum_{(\lambda,\mu)\kappa}\langle(N,0)\,l,\ (\sigma,\tau)\rho L\|(\lambda,\mu)\kappa J\rangle g^N_{(\lambda,\mu)\kappa J}. \tag{4·1·35}$$

It is easy to show that the answer to Eq. (4·1·32) is also obtained by solving the following equation,

$$\sum_{(\lambda,\mu)\kappa}W[(\lambda',\mu')\kappa'|(\lambda,\mu)\kappa]\,d^{\alpha}_{(\lambda,\mu)\kappa}=\mu_\alpha d^{\alpha}_{(\lambda',\mu')\kappa'},$$

$$W[(\lambda',\mu')\kappa'|(\lambda,\mu)\kappa]\equiv\sqrt{\mu^N_{(\lambda',\mu')}\mu^N_{(\lambda,\mu)}}$$
$$\times\sum_l\langle(N,0)\,l,\ (\sigma,\tau)\rho L\|(\lambda',\mu')\kappa' J\rangle\langle(N,0)\,l,\ (\sigma,\tau)\rho L\|(\lambda,\mu)\kappa J\rangle, \tag{4·1·36}$$

which gives us μ_α and $C_l{}^{\alpha}$;

$$C_l{}^{\alpha}=\frac{1}{\sqrt{\mu_\alpha}}\sum_{(\lambda,\mu)\kappa}d^{\alpha}_{(\lambda,\mu)\kappa}\langle(N,0)\,l,\ (\sigma,\tau)\rho L\|(\lambda,\mu)\kappa J\rangle$$
$$\text{for}\quad \mu_\alpha\neq 0, \tag{4·1·37}$$

while $C_l{}^{\alpha}$ for $\mu_\alpha=0$ are obtained as the vectors which are orthogonal to $C_l{}^{\alpha}$ with $\mu_\alpha\neq 0$.

As an example, let us consider $^{12}\mathrm{C}+\alpha$ system,[15] where $^{12}\mathrm{C}$ is described by the SU_3 shell model wave function $(0s)^4(0p)^8[4]$ which has $(\sigma,\tau)=(0,4)$. $\mu^N_{(\lambda,\mu)}$ with $(\lambda,\mu)=(N,0)\times(0,4)=\sum_{k=0}^{4}(N-k,4-k)$ are obtained by

$$\mu^N_{(N,4)}=a\,(J=N+4,i),$$

$$\mu^N_{(N-1,3)}=\sum_i a\,(J=N+2,i)-2\mu^N_{(N,4)},$$

$$\mu^N_{(N-2,2)}=\sum_i a\,(J=N,i)-3\mu^N_{(N,4)}-2\mu^N_{(N-1,3)},$$

$$\mu^N_{(N-3,1)}=\sum_i a(J=N-2,i)-3\mu^N_{(N,4)}-2\mu^N_{(N-1,3)}-2\mu^N_{(N-2,2)}\,,$$

$$\mu^N_{(N-4,0)}=\sum_i a(J=N-4,i)-3\mu^N_{(N,4)}-2\mu^N_{(N-1,3)}-2\mu^N_{(N-2,2)}-\mu^N_{(N-3,1)}\,. \tag{4·1·38}$$

The matrix elements $a(J,i)$ are obtained by using the generating function technique of § 3.3.b. The generating function for the general overlap matrix elements $\langle R_{Nl_i}h_i^J|\mathcal{A}\{R_{Nl_j}h_j^J\}\rangle$ is

$$\begin{aligned}&F(R,\hat{R},\hat{R}',\Omega,\Omega')\\&\equiv e^{R^2}\left\langle\phi^{\Omega}\left({}^{12}\mathrm{C},\frac{-\boldsymbol{R}}{4\sqrt{\gamma}}\right)\phi_0\left(\alpha,\frac{3\boldsymbol{R}}{4\sqrt{\gamma}}\right)|\mathcal{A}\left\{\phi^{\Omega'}\left({}^{12}\mathrm{C},\frac{-\boldsymbol{R}'}{4\sqrt{\gamma}}\right)\phi_0\left(\alpha,\frac{3\boldsymbol{R}'}{4\sqrt{\gamma}}\right)\right\}\right\rangle\\&=\sum_{N=0}^{\infty}\frac{R^{2N}}{N!}\sum_{\substack{i,j\\J,M}}\frac{(4\pi)^2A^N_{l_i}A^N_{l_j}A^4_{L_i}A^4_{L_j}}{\sqrt{(2l_i+1)(2l_j+1)(2L_i+1)(2L_j+1)}}[Y_{l_i}(\hat{R})Y_{L_i}(\Omega)]_{JM}\\&\quad\times[Y_{l_j}(\hat{R}')Y_{L_j}(\Omega')]^*_{JM}\langle R_{Nl_i}(r,\gamma)h_i^J|\mathcal{A}\{R_{Nl_j}(r,\gamma)h_j^J\}\rangle\,,\end{aligned} \tag{4·1·39}$$

where $\boldsymbol{R}$ and $\boldsymbol{R}'$ have the common length R. The calculated results for the generating function F and the matrix elements $\langle R_{Nl_i}h_i^J|\mathcal{A}\{R_{Nl_j}h_j^J\}\rangle$ are[15),61)]

$$\begin{aligned}&F(R,\hat{R},\hat{R}',\Omega,\Omega')\\&=\exp\left\{-\frac{1}{3}\boldsymbol{R}\cdot\boldsymbol{R}'\right\}\left[\boldsymbol{u}\cdot\boldsymbol{u}'\left\{\exp\left(\frac{1}{3}\boldsymbol{R}\cdot\boldsymbol{R}'\right)-1-\frac{1}{3}\boldsymbol{R}\cdot\boldsymbol{R}'\right\}\right.\\&\quad\left.+\frac{1}{3}(\boldsymbol{R}\cdot\boldsymbol{u})(\boldsymbol{R}'\cdot\boldsymbol{u}')\right]^4,\end{aligned}$$

$$\begin{aligned}&\langle R_{Nl_i}(r,\gamma)h_i^J|\mathcal{A}\{R_{Nl_j}(r,\gamma)h_j^J\}\rangle\\&=\frac{\sqrt{(2l_i+1)(2l_j+1)(2L_i+1)(2L_j+1)}}{A^N_{l_i}A^N_{l_j}A^4_{L_i}A^4_{L_j}}\frac{N!}{3^N}\sum_{k=0}^{4}\sum_{r=0}^{k}\sum_{s=0}^{r}\theta(N+k-4-s)\\&\quad\times\binom{4}{k}(-)^r\binom{k}{r}\binom{r}{s}\frac{(k-r-1)^{N+k-4-s}}{(N+k-4-s)!}\sum_{q=0}^{[(4-k)/2]}\sum_{q'=0}^{[(4-k)/2]}\sum_{p=0}^{[k/2]}\sum_{p'=0}^{[(N+k-4)/2]}\\&\quad\times[A^{4-k}_{4-k-2q}A^{4-k}_{4-k-2q'}A^{k}_{k-2p}A^{N+k-4}_{N+k-4-2p'}]^2\\&\quad\times W(N+k-4-2p',k-2p,l_i,L_i,J,4-k-2q)\\&\quad\times W(N+k-4-2p',k-2p,l_j,L_j,J,4-k-2q')\\&\quad\times C(4-k-2q,N+k-4-2p',l_i)C(4-k-2q',N+k-4-2p',l_j)\\&\quad\times C(4-k-2q,k-2p,L_i)C(4-k-2q',k-2p,L_j)\,,\end{aligned} \tag{4·1·40}$$

where $\boldsymbol{u}$ and $\boldsymbol{u}'$ are unit vectors whose polar angles are Ω and Ω', respectively, $[x]$ denotes the integer I which satisfies $I+1>x\geqq I$, W is the R_3 Racah

coefficient, and $C(s,t,v)$ is the R_3 Clebsch-Gordan coefficient $(s,0,t,0|v,0)$.

The calculated values of $\mu^{N}_{(\lambda,\mu)}$ for the above $^{12}C+\alpha$ system are given in Ref. 15). For reference we give here the generating function of $\mu^{N}_{(\lambda,\mu)}$ for the $^{20}Ne+\alpha$ system where for ^{20}Ne the SU_3 shell model wave function $(sd)^4[4]$ $(\lambda,\mu)=(8,0)$ is adopted;

$$
\begin{aligned}
&F(R,\hat{R},\hat{R}',\Omega,\Omega')\\
&\equiv\exp\{R^2\}\left\langle\psi^{\Omega}\left(^{20}\mathrm{Ne},\frac{-\boldsymbol{R}}{6\sqrt{\gamma}}\right)\phi_0\left(\alpha,\frac{5\boldsymbol{R}}{6\sqrt{\gamma}}\right)\right|\\
&\qquad\times\mathcal{A}\left\{\psi^{\Omega'}\left(^{20}\mathrm{Ne},\frac{-\boldsymbol{R}'}{6\sqrt{\gamma}}\right)\phi_0\left(\alpha,\frac{5\boldsymbol{R}'}{6\sqrt{\gamma}}\right)\right\}\Big\rangle\\
&=\exp\left(-\frac{1}{5}\boldsymbol{R}\cdot\boldsymbol{R}'\right)\left[(\boldsymbol{u}\cdot\boldsymbol{u}')^2\left\{\exp\left(\frac{3}{10}\boldsymbol{R}\cdot\boldsymbol{R}'\right)-1-\frac{3}{10}\boldsymbol{R}\cdot\boldsymbol{R}'\right\}\right.\\
&\qquad\left.-\frac{1}{2}\left\{\frac{3}{10}(\boldsymbol{R}\cdot\boldsymbol{u}')(\boldsymbol{R}'\cdot\boldsymbol{u})\right\}^2\right]^4, \qquad (4\cdot1\cdot41)
\end{aligned}
$$

where also $R=|\boldsymbol{R}|=|\boldsymbol{R}'|$ and $\boldsymbol{u}$ and $\boldsymbol{u}'$ are unit vectors in the directions Ω and Ω', respectively. The overlap matrix elements $\langle R_{Nl_i}h_i^J|\mathcal{A}\{R_{Nl_j}h_j^J\}\rangle$ are extracted from this $F(R,\hat{R},\hat{R}',\Omega,\Omega')$ by the same expansion formula as Eq. (4·1·39) except the replacement of $A^4_{L_i}A^4_{L_j}$ by $A^8_{L_i}A^8_{L_j}$.

When we treat more complex systems where both clusters C_1 and C_2 are SU_3 non-scalar, we generally have an SU_3 representation (λ,μ) more than once. For the (λ,μ) with the multiplicity more than one, we need to diagonalize the antisymmetrizer $\mathcal{A}$ by the states with the same quantum numbers N, (λ,μ), κ, J. Thus the SU_3 classification is necessary but not sufficient for the complete determination of the eigen-functions of the norm kernel for the general complex two-cluster systems.

4.1.d. *Multi-cluster system*

For the sake of the explanation, we consider the system of three SU_3 scalar clusters. The eigen-value equation of the norm kernel is

$$
\langle\phi_0|\mathcal{A}\{\chi^{\alpha}(\xi_1,\xi_2)\phi_0\}\rangle=\mu_{\alpha}\chi^{\alpha}(\xi_1,\xi_2),\quad \phi_0\equiv\prod_{i=1}^{3}\phi_0(C_i). \qquad (4\cdot1\cdot42)
$$

The eigen-functions χ^{α} are classified by the number of the H.O. quanta N and the SU_3 labels (λ,μ), κ, J, and so we denote χ^{α} by $\chi_{N(\lambda,\mu)\kappa J,p}$, where p is the quantum number to distinguish the states with the same N, (λ,μ), κ, J. The eigen-functions are obtained by the following diagonalization:

$$
\sum_{N_1'+N_2'=N}\langle V^{(\lambda,\mu)\kappa J}_{N_1N_2}\phi_0|\mathcal{A}\{V^{(\lambda,\mu)\kappa J}_{N_1'N_2'}\phi_0\}\rangle A^{N(\lambda,\mu)}_{p,N_2'}=\mu^{N}_{(\lambda,\mu),p}A^{N(\lambda,\mu)}_{p,N_2},
$$

$$
\begin{aligned}
V^{N(\lambda,\mu)\kappa J}_{N_1N_2}(\xi_1,\xi_2)&\equiv[V_{(N_1,0)}(\xi_1,\gamma_1)V_{(N_2,0)}(\xi_2,\gamma_2)]_{(\lambda,\mu)\kappa J}\\
&=\sum_{l_1l_2}\langle(N_1,0)l_1,\ (N_2,0)l_2\|(\lambda,\mu)\kappa J\rangle V^{N_1l_1N_2l_2}_{J}(\xi_1,\xi_2),
\end{aligned}
$$

$$V^{N_1 N_2}_{l_1 l_2 J}(\xi_1, \xi_2) \equiv [V_{N_1 l_1}(\xi_1, \gamma_1)\, V_{N_2 l_2}(\xi_2, \gamma_2)]_J \tag{4·1·43}$$

which gives

$$\chi_{N(\lambda,\mu)\kappa J, p}(\xi_1, \xi_2) = \sum_{N_1+N_2=N} A^{N(\lambda,\mu)}_{p, N_2}\, V^{N(\lambda,\mu)\kappa J}_{N_1 N_2}(\xi_1, \xi_2). \tag{4·1·44}$$

Here we shold note that the matrix elements $\langle V^{N(\lambda,\mu)\kappa J}_{N_1 N_2}\phi_0 | \mathcal{A}\{V^{N(\lambda,\mu)\kappa J}_{N_1' N_2'}\phi_0\}\rangle$ do not depend on κ and J due to the SU_3 scalar property of $\mathcal{A}$ and this fact means that the coefficients $A^{N(\lambda,\mu)}_{p,N_2}$ which are eigen-vectors of this overlap matrix also do not depend on κ and J. The eigen-values $\mu^N_{(\lambda,\mu),p}$ are of course independent of κ and J just like as in §§ 4.1.b and 4.1.c. We show in Table II the SU_3-classification of the functional space spanned by $V_{N_1 l_1 m_1}(\xi_1, \gamma_1)\, V_{N_2 l_2 m_2}(\xi_2, \gamma_2)$ with fixed $N = N_1 + N_2$, by using the rule $(N_1, 0)\times(N_2, 0) = \sum_{k=0}^{N_{\min}} (N_1 + N_2 - 2k, k)$ with $N_{\min} = \min(N_1, N_2)$.

Table II. SU_3 classification of the three-body relative H. O. wave functions with the total number of H. O. quanta N. $S_\pm$ denote the quasi-spin operators defined by Eq. (5.2.14).

N_1	N_2	$(\lambda, \mu) = (N-2k, k)$					
N	0	$(N, 0)$					
N-1	1	$(N, 0)$	$(N-2, 1)$				$\uparrow S_+$
N-2	2	$(N, 0)$	$(N-2, 1)$	$(N-4, 2)$			
⋮	⋮	⋮	⋮	⋮	⋮	⋰	
1	N-1	$(N, 0)$	$(N-2, 1)$				$\downarrow S_-$
0	N	$(N, 0)$					

In order to solve Eq. (4·1·43) we need to calculate the matrix elements $\langle V^{N_1 N_2}_{l_1 l_2 J}(\xi_1, \xi_2)\phi_0 | \mathcal{A}\{V^{N_3 N_4}_{l_3 l_4 J}(\xi_1, \xi_2)\phi_0\}\rangle$, which is done by the generating function technique of § 3.3.b as follows:

$$\begin{aligned}
\hat{N}(\boldsymbol{S}_1, \boldsymbol{S}_2; \boldsymbol{S}_3, \boldsymbol{S}_4) &\equiv \langle A_{\gamma_1}(\xi_1, \boldsymbol{S}_1)\, A_{\gamma_2}(\xi_2, \boldsymbol{S}_2)\phi_0 | \mathcal{A}\{A_{\gamma_1}(\xi_1, \boldsymbol{S}_3)\, A_{\gamma_2}(\xi_2, \boldsymbol{S}_4)\phi_0\}\rangle \\
&= \exp\left\{\frac{1}{2}\sum_i^4 S_i^2\right\} \left\langle \Gamma\left(\xi_1, \frac{\boldsymbol{S}_1}{\sqrt{\gamma_1}}, \gamma_1\right)\Gamma\left(\xi_2, \frac{\boldsymbol{S}_2}{\sqrt{\gamma_2}}, \gamma_2\right)\phi_0 \right| \\
&\qquad \times \mathcal{A}\left\{\Gamma\left(\xi_1, \frac{\boldsymbol{S}_3}{\sqrt{\gamma_1}}, \gamma_1\right)\Gamma\left(\xi_2, \frac{\boldsymbol{S}_4}{\sqrt{\gamma_2}}, \gamma_2\right)\phi_0\right\}\right\rangle \\
&= \sum_{\substack{N_i l_i \\ JM}} \left(\prod_{i=1}^4 \frac{S_i^{N_i}}{\sqrt{N_i!}}\sqrt{\frac{4\pi}{2l_i+1}}A^{N_i}_{l_i}\right)[Y_{l_1}(\hat{S}_1)Y_{l_2}(\hat{S}_2)]_{JM}[Y_{l_3}(\hat{S}_3)Y_{l_4}(\hat{S}_4)]^*_{JM} \\
&\qquad \times \langle V^{N_1 N_2}_{l_1 l_2 J}(\xi_1, \xi_2)\phi_0 | \mathcal{A}\{V^{N_3 N_4}_{l_3 l_4 J}(\xi_1, \xi_2)\phi_0\}\rangle.
\end{aligned} \tag{4·1·45}$$

Kato and Bando[62] have proposed an interesting and powerful method to solve the eigen-value problem of the multi-cluster system. Their method is especially suited for the systems composed of α-nuclei (self-conjugate $4n$ nuclei or clusters with $[44\cdots]$ orbital symmetry). For such systems the generating

function of Eq. (4·1·45) has generally the form,[18]

$$\hat{N}(\boldsymbol{S}_1, \boldsymbol{S}_2; \boldsymbol{S}_3, \boldsymbol{S}_4) = \{\hat{n}(\boldsymbol{S}_1, \boldsymbol{S}_2; \boldsymbol{S}_3, \boldsymbol{S}_4)\}^4 . \tag{4·1·46}$$

Here for the sake of interpretation, we consider the case when clusters are all SU_3 scalar (like as α, ^{16}O or ^{40}Ca). To investigate the properties of $\hat{n}$, we write $\hat{N}$ as follows,

$$\begin{aligned}
\hat{N}(\boldsymbol{S}_1, \boldsymbol{S}_2; \boldsymbol{S}_3, \boldsymbol{S}_4) &= \exp\left\{\frac{1}{2}\sum_i^4 S_i^2\right\} \langle \prod_{i=1}^3 \psi(C_i, \boldsymbol{R}_i) | \mathcal{A}\{\prod_{i=1}^3 \psi(C_i, \boldsymbol{R}_i')\}\rangle \\
&= \exp\left\{\frac{1}{2}\sum_i^4 S_i^2\right\} \langle \varphi_{\sigma_1 1}^4 \cdots \varphi_{\sigma_2 1}^4 \cdots \varphi_{\sigma_3 1}^4 \cdots | \det\{\varphi_{\sigma_1' 1}^4 \cdots \varphi_{\sigma_2' 1}^4 \cdots \varphi_{\sigma_3' 1}^4 \cdots\}\rangle \\
&= \exp\left\{\frac{1}{2}\sum_i^4 S_i^2\right\} [\langle \varphi_{\sigma_1 1} \cdots \varphi_{\sigma_2 1} \cdots \varphi_{\sigma_3 1} \cdots | \det\{\varphi_{\sigma_1' 1} \cdots \varphi_{\sigma_2' 1} \cdots \varphi_{\sigma_3' 1} \cdots\}\rangle]^4 \\
&= \exp\left\{\frac{1}{2}\sum_i^4 S_i^2\right\} [\langle \prod_{i=1}^3 \hat{\psi}(C_i, \boldsymbol{R}_i) | \hat{\mathcal{A}}\{\prod_{i=1}^3 \hat{\psi}(C_i, \boldsymbol{R}_i')\}\rangle]^4 ,
\end{aligned} \tag{4·1·47}$$

where

$$\begin{aligned}
&\psi(C_i, \boldsymbol{R}_i) = \frac{1}{\sqrt{N_i!}} \det\{\varphi_{\sigma_i 1}^4 \cdots\}, \quad \sum_{i=1}^3 N_i \boldsymbol{R}_i = 0 , \\
&\boldsymbol{R}_2 - \boldsymbol{R}_1 = \boldsymbol{S}_1/\sqrt{\gamma_1} , \quad \boldsymbol{R}_3 - (N_1\boldsymbol{R}_1 + N_2\boldsymbol{R}_2)/(N_1+N_2) = \boldsymbol{S}_2/\sqrt{\gamma_2} , \\
&\hat{\psi}(C_i, \boldsymbol{R}_i) \equiv \frac{1}{\sqrt{(N_i/4)!}} \det\{\varphi_{\sigma_i 1} \cdots\},
\end{aligned} \tag{4·1·48}$$

and $\hat{\mathcal{A}}$ is an antisymmetrizer of $A/4$ particles which have no spin-isospin coordinates. Just like as the relation of Eq. (2·1·4) we can express $\hat{\psi}(C_i, \boldsymbol{R}_i)$ as

$$\begin{aligned}
&\hat{\psi}(C_i, \boldsymbol{R}_i) = \left(\frac{N_i\nu}{2\pi}\right)^{3/4} \exp\left\{-\frac{N_i}{4}\nu(\boldsymbol{y}_i - \boldsymbol{R}_i)^2\right\} \hat{\phi}_0(C_i), \\
&\boldsymbol{y}_i \equiv \frac{1}{(N_i/4)} \boldsymbol{x}_j ,
\end{aligned} \tag{4·1·49}$$

where $\hat{\phi}_0(C_i)$ are functions of only the relative coordinates $\boldsymbol{x}_j - \boldsymbol{x}_k$ and are SU_3 scalar since $\phi_0(C_i)$ are assumed to be SU_3 scalar. $\hat{n}(\boldsymbol{S}_1, \cdots)$ of Eq. (4·1·46) is now written as

$$\begin{aligned}
\hat{n}(\boldsymbol{S}_1, \boldsymbol{S}_2; \boldsymbol{S}_3, \boldsymbol{S}_4) &= \exp\left\{\frac{1}{2}\sum_i^4 S_i^2\right\} \langle \prod_{i=1}^3 \hat{\psi}_0(C_i, \boldsymbol{R}_i) | \mathcal{A}\{\prod_{i=1}^3 \hat{\psi}_0(C_i, \boldsymbol{R}_i')\}\rangle \\
&= \exp\left\{\frac{1}{8}\sum_i^4 S_i^2\right\} \left\langle \Gamma\left(\eta_1, \frac{\boldsymbol{S}_1}{\sqrt{\gamma_1}}, \frac{\gamma_1}{4}\right) \Gamma\left(\eta_2, \frac{\boldsymbol{S}_2}{\sqrt{\gamma_2}}, \frac{\gamma_2}{4}\right) \hat{\phi}_0 | \right. \\
&\quad \left. \times \hat{\mathcal{A}}\left\{\Gamma\left(\eta_1, \frac{\boldsymbol{S}_3}{\sqrt{\gamma_1}}, \frac{\gamma_1}{4}\right) \Gamma\left(\eta_2, \frac{\boldsymbol{S}_4}{\sqrt{\gamma_2}}, \frac{\gamma_2}{4}\right) \hat{\phi}_0\right\}\right\rangle
\end{aligned}$$

$$= \left\langle A_{\gamma_1/4}\left(\eta_1, \frac{S_1}{2}\right) A_{\gamma_2/4}\left(\eta_2, \frac{S_2}{2}\right)\hat{\phi}_0 \right|$$

$$\times \hat{\mathcal{A}}\left\{A_{\gamma_1/4}\left(\eta_1, \frac{S_3}{2}\right) A_{\gamma_2/4}\left(\eta_2, \frac{S_4}{2}\right)\hat{\phi}_0\right\}\Big\rangle,$$

$$\eta_1 \equiv y_2 - y_1, \quad \eta_2 \equiv y_3 - (N_1 y_1 + N_2 y_2)/(N_1+N_2),$$

$$\hat{\phi}_0 \equiv \prod_{i=1}^{3} \hat{\phi}_0(C_i). \tag{4·1·50}$$

We expand $\hat{n}$ in power series of S_i by using Eq. (3·2·19) or Eq. (3·2·25) as follows,

$$\hat{n}(S_1, S_2; S_3, S_4) = \sum_{M_i} \tau(M_1, M_2; M_3, M_4) \prod_{i=1}^{4} U_{M_i}(S_i),$$

$$\tau(M_1, M_2; M_3, M_4) \equiv \left(\frac{1}{2}\right)^{M_0} \left\langle X_{M_1}\left(\eta_1, \frac{\gamma_1}{4}\right) X_{M_2}\left(\eta_2, \frac{\gamma_2}{4}\right)\hat{\phi}_0 \right|$$

$$\times \hat{\mathcal{A}}\left\{X_{M_3}\left(\eta_1, \frac{\gamma_1}{4}\right) X_{M_4}\left(\eta_2, \frac{\gamma_2}{4}\right)\hat{\phi}_0\right\}\Big\rangle,$$

$$M_0 \equiv \sum_{i=1}^{4}\sum_{x=1}^{3} M_{ix}. \tag{4·1·51}$$

Here we should note that $\tau(M_1, \cdots)$ has a property

$$\tau(M_1, M_2; M_3, M_4) = 0, \quad \text{if} \quad M_1 + M_2 \neq M_3 + M_4, \tag{4·1·52}$$

which means that the matrix $\tau(M_1, M_2; M_3, M_4)$ with row indices (M_1, M_2) and column indices (M_3, M_4) has a decomposed form into submatrices with finite dimension. By diagonalizing these submatrices of τ as follows,

$$\sum_{M_3+M_4=M} \tau(M_1, M_2; M_3, M_4)\, e_\lambda(M_3, M_4) = \sigma_\lambda e_\lambda(M_1, M_2), \tag{4·1·53}$$

we obtain

$$\hat{n}(S_1, S_2; S_3, S_4) = \sum_{\lambda} \sigma_\lambda p_\lambda(S_1, S_2) p_\lambda(S_3, S_4),$$

$$p_\lambda(S_i, S_j) \equiv \sum_{M_i+M_j=M} e_\lambda(M_i, M_j) U_{M_i}(S_i) U_{M_j}(S_j). \tag{4·1·54}$$

By inserting this expression into Eq. (4·1·46), we get

$$\hat{N}(S_1, S_2; S_3, S_4) = \sum_{\lambda_1 \sim \lambda_4} \left(\prod_{i=1}^{4} \sigma_{\lambda_i}\right) \left(\prod_{i=1}^{4} p_{\lambda_i}(S_1, S_2)\right) \left(\prod_{i=1}^{4} p_{\lambda_i}(S_3, S_4)\right). \tag{4·1·55}$$

On the other hand, by inserting the power series expansion of A_γ or Γ given by Eq. (3·2·19) or Eq. (3·2·25) into Eq. (4·1·45) we have

$$\hat{N}(S_1, S_2; S_3, S_4) = \sum_{N_i} \langle X_{N_1}(\xi_1, \gamma_1) X_{N_2}(\xi_2, \gamma_2)\phi_0 | \mathcal{A}$$

$$\times\{X_{\boldsymbol{N}_3}(\boldsymbol{\xi}_1,\gamma_1)X_{\boldsymbol{N}_4}(\boldsymbol{\xi}_2,\gamma_2)\phi_0\}\rangle\prod_{i=1}^{4}U_{\boldsymbol{N}_i}(\boldsymbol{S}_i). \qquad (4\cdot1\cdot56)$$

Comparing Eq. (4·1·56) with Eq. (4·1·57) we obtain

$$\langle X_{\boldsymbol{N}_1}(\boldsymbol{\xi}_1,\gamma_1)X_{\boldsymbol{N}_2}(\boldsymbol{\xi}_2,\gamma_2)\phi_0|\mathcal{A}\{X_{\boldsymbol{N}_3}(\boldsymbol{\xi}_1,\gamma_1)X_{\boldsymbol{N}_4}(\boldsymbol{\xi}_2,\gamma_2)\phi_0\}\rangle$$
$$=(\prod_{i=1}^{4}\boldsymbol{N}_i!)^{1/2}\sum_{\lambda_1\sim\lambda_4}\sum_{\boldsymbol{M}_1{}^1\sim\boldsymbol{M}_1{}^4}\sum_{\boldsymbol{M}_2{}^1\sim\boldsymbol{M}_2{}^4}\sum_{\boldsymbol{M}_3{}^1\sim\boldsymbol{M}_3{}^4}\sum_{\boldsymbol{M}_4{}^1\sim\boldsymbol{M}_4{}^4}$$
$$\times\prod_{i=1}^{4}\sigma_{\lambda_i}e_{\lambda_i}(\boldsymbol{M}_1{}^i,\boldsymbol{M}_2{}^i)\,e_{\lambda_i}(\boldsymbol{M}_3{}^i,\boldsymbol{M}_4{}^i)\,(\prod_{k=1}^{4}\boldsymbol{M}_k{}^i!)^{-1/2},$$

$$\sum_{\boldsymbol{M}_k{}^1\sim\boldsymbol{M}_k{}^4}=\text{summation over }\boldsymbol{M}_k{}^1\sim\boldsymbol{M}_k{}^4\text{ under the condition }\sum_{i=1}^{4}\boldsymbol{M}_k{}^i=\boldsymbol{N}_k, \qquad (4\cdot1\cdot57)$$

which is the formula of the Kato-Bando method to calculate the matrix elements of the norm kernel in the Cartesian H.O. function representation.

The diagonalization process of Eq. (4·1·53) is equivalent to solving the following equation:

$$\langle\hat{\phi}_0|\hat{\mathcal{A}}\{\hat{\chi}^\lambda(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2)\hat{\phi}_0\}\rangle=\sigma_\lambda\hat{\chi}^\lambda(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2), \qquad (4\cdot1\cdot58)$$

the eigen-functions $\hat{\chi}^\lambda$ of which are given by

$$\hat{\chi}^\lambda(\boldsymbol{\eta}_1,\boldsymbol{\eta}_2)=\sum_{\boldsymbol{M}_1+\boldsymbol{M}_2=\boldsymbol{M}}e_\lambda(\boldsymbol{M}_1,\boldsymbol{M}_2)X_{\boldsymbol{M}_1}(\boldsymbol{\eta}_1,\gamma_1/4)X_{\boldsymbol{M}_2}(\boldsymbol{\eta}_2,\gamma_2/4). \qquad (4\cdot1\cdot59)$$

Since $\hat{\mathcal{A}}$ and $\hat{\phi}_0$ are both SU_3 scalar, it is evident that $\hat{\chi}^\lambda$ are classified by the SU_3 scheme, the labels of which are the Cartesian ones M, (λ,ε), ε, Λ, ν,

$$M\equiv M_x+M_y+M_z,\quad \varepsilon\equiv 2M_z-M_x-M_y,\quad \nu\equiv\tfrac{1}{2}(M_x-M_y), \qquad (4\cdot1\cdot60)$$

where we used the notation $\boldsymbol{M}=(M_x,M_y,M_z)$.

Our explanation of the Kato-Bando method given above is in the Cartesian coordinates. It goes without saying that everything can be restated in the spherical (or angular momentum) coordinates.

The powerful points of the Kato-Bando method are as follows. The small-generating-function $\hat{n}(\boldsymbol{S}_1,\cdots)$ is simpler than $\hat{N}(\boldsymbol{S}_1,\cdots)$ and the dimensions of the matrices to be diagonalized are smaller than the case of treating $\hat{N}(\boldsymbol{S}_1,\cdots)$. Moreover what is important is that for low H.O. quanta $M=\sum_x^3 M_x$, most eigen-values σ_λ of Eq. (4·1·53) are zero usually which is due to the Pauli principle expressed by the operator $\hat{\mathcal{A}}$. Therefore when we need the solutions of the eigen-value problem of Eq. (4·1·42) with low H.O. quanta, this method is especially convenient.

The Kato-Bando method acquires the mathematical transparency when it is formulated in framework of complex-GCM.[16] The eigen-value equation of the RGM norm kernel which is expressed in Eq. (4·1·42) is equivalent to the following eigen-value equation of the C-GCM norm kernel,

$$\int d\mu(\boldsymbol{S}_3)\, d\mu(\boldsymbol{S}_4)\, \hat{N}(\boldsymbol{S}_1,\boldsymbol{S}_2;\boldsymbol{S}_3^*,\boldsymbol{S}_4^*) f^\alpha(\boldsymbol{S}_3,\boldsymbol{S}_4) = \mu_\alpha f^\alpha(\boldsymbol{S}_1,\boldsymbol{S}_2), \qquad (4\cdot1\cdot61)$$

where C-GCM norm kernel $\hat{N}$ has entirely the same form as the generating function $\hat{N}$ of Eq. (4·1·45) except that now the generator coordinates are all complex number vectors;

$$\hat{N}(\boldsymbol{S}_1,\boldsymbol{S}_2;\boldsymbol{S}_3^*,\boldsymbol{S}_4^*) = \langle A_{\gamma_1}^*(\boldsymbol{\xi}_1,\boldsymbol{S}_1) A_{\gamma_2}^*(\boldsymbol{\xi}_2,\boldsymbol{S}_2)\phi_0 | \mathcal{A}\{A_{\gamma_1}^*(\boldsymbol{\xi}_1,\boldsymbol{S}_3) A_{\gamma_2}^*(\boldsymbol{\xi}_2,\boldsymbol{S}_4)\phi_0\}\rangle. \qquad (4\cdot1\cdot62)$$

The relation between χ^α and f^α is

$$\chi^\alpha(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2) = \int d\mu(\boldsymbol{S}_1)\, d\mu(\boldsymbol{S}_2)\, A_{\gamma_1}^*(\boldsymbol{\xi}_1,\boldsymbol{S}_1) A_{\gamma_2}^*(\boldsymbol{\xi}_2,\boldsymbol{S}_2) f^\alpha(\boldsymbol{S}_1,\boldsymbol{S}_2). \qquad (4\cdot1\cdot63)$$

The eigen-value equation of the small-norm-kernel of C-GCM $\hat{n}(\boldsymbol{S}_1,\boldsymbol{S}_2;\boldsymbol{S}_3^*,\boldsymbol{S}_4^*)$ defined by Eq. (4·1·46) is

$$\int d\mu(\boldsymbol{S}_3)\, d\mu(\boldsymbol{S}_4)\, \hat{n}(\boldsymbol{S}_1,\boldsymbol{S}_2;\boldsymbol{S}_3^*,\boldsymbol{S}_4^*) p_\lambda(\boldsymbol{S}_3,\boldsymbol{S}_4) = \sigma_\lambda p_\lambda(\boldsymbol{S}_1,\boldsymbol{S}_2), \qquad (4\cdot1\cdot64)$$

which is equivalent to Eq. (4·1·58). It is easy to see that σ_λ and p_λ are given by Eqs. (4·1·53) and (4·1·54). By using the form of $\hat{N}$ given in Eq. (4·1·55), we obtain the solution of Eq. (4·1·61) as follows:

$$f^\alpha(\boldsymbol{S}_1,\boldsymbol{S}_2) = \frac{1}{\sqrt{\mu_\alpha}} \sum_{\lambda_1\sim\lambda_4} C^\alpha_{\lambda_1\cdots\lambda_4} \sqrt{\prod_{i=1}^4 \sigma_{\lambda_i}} \prod_{i=1}^4 p_{\lambda_i}(\boldsymbol{S}_1,\boldsymbol{S}_2), \qquad (4\cdot1\cdot65)$$

where $C^\alpha_{\lambda_1,\cdots,\lambda_4}$ and μ_α are obtained by solving the secular equation,

$$\sum_{\nu_1\sim\nu_4} \sqrt{\prod_{i=1}^4 \sigma_{\lambda_i}} \langle \prod_{i=1}^4 p_{\lambda_i}(\boldsymbol{S}_1,\boldsymbol{S}_2) | \prod_{j=1}^4 p_{\nu_j}(\boldsymbol{S}_1,\boldsymbol{S}_2)\rangle \sqrt{\prod_{j=1}^4 \sigma_{\nu_j}} C^\alpha_{\nu_1\cdots\nu_4} = \mu_\alpha C^\alpha_{\lambda_1\cdots\lambda_4}, \qquad (4\cdot1\cdot66)$$

where $\langle \prod p_{\lambda_i} | \prod p_{\nu_j}\rangle$ denotes the inner product with the use of the measure $d\mu(\boldsymbol{S}_1)\, d\mu(\boldsymbol{S}_2)$. For $\mu_\alpha = 0$, the corresponding f^α are obtained as the functions which are orthogonal to f^α with $\mu_\alpha \neq 0$.

As an example, we consider an application to many-alpha system. $\hat{N}$ and $\hat{n}$ are given by

$$\hat{N}(\boldsymbol{S}_1',\cdots\boldsymbol{S}_{A-1}';\boldsymbol{S}_1^*,\cdots\boldsymbol{S}_{A-1}^*) = \langle \prod_{i=1}^{A-1} A_\gamma^*(\boldsymbol{\xi}_i,\boldsymbol{S}_i')\phi_0 | \mathcal{A}\{\prod_{i=1}^{A-1} A_\gamma^*(\boldsymbol{\xi}_i,\boldsymbol{S}_i)\phi_0\}\rangle,$$

$$\hat{n}(\boldsymbol{S}_1',\cdots\boldsymbol{S}_{A-1}';\boldsymbol{S}_1^*,\cdots\boldsymbol{S}_{A-1}^*) = \left\langle \prod_{i=1}^{A} A_\nu^*\left(\boldsymbol{x}_i,\frac{\boldsymbol{R}_i'}{2}\right) \middle| \det\left\{\prod_{i=1}^{A} A_\nu^*\left(\boldsymbol{x}_i,\frac{\boldsymbol{R}_i}{2}\right)\right\} \right\rangle$$

$$= \begin{vmatrix} \exp\{\boldsymbol{R}_1'\cdot\boldsymbol{R}_1^*/4\} & \cdots & \exp\{\boldsymbol{R}_1'\cdot\boldsymbol{R}_A^*/4\} \\ \vdots & & \vdots \\ \exp\{\boldsymbol{R}_A'\cdot\boldsymbol{R}_1^*/4\} & \cdots & \exp\{\boldsymbol{R}_A'\cdot\boldsymbol{R}_A^*/4\} \end{vmatrix}$$

$$= \sum_P^{A!} \varepsilon(P) \exp\left\{\frac{1}{4}\sum_{i=1}^{A} \boldsymbol{R}_i' P \boldsymbol{R}_i^*\right\}$$

$$=\sum_{P}^{A!}\varepsilon(P)\exp\left\{\frac{1}{4}\sum_{i=1}^{A-1}\boldsymbol{S}_i'P\boldsymbol{S}_i^*\right\}, \qquad (4\cdot1\cdot67)$$

where $\gamma=4\nu$, $\phi_0\equiv\sum_{i=1}^{A}\phi_0(C_i)$ and P are permutation operators of $\boldsymbol{R}_1\sim\boldsymbol{R}_A$. The definition of the Jacobi coordinates $\boldsymbol{\xi}_i$ is slightly changed from that of Eq. (2·1·6) with respect to their lengths and it is

$$\boldsymbol{\xi}_i\equiv\sqrt{\frac{i}{i+1}}\left(\boldsymbol{X}_{i+1}-\frac{1}{i}\sum_{j=1}^{i}\boldsymbol{X}_j\right),\ 1\leq i\leq A-1,$$

$$\boldsymbol{\xi}_A\equiv\frac{1}{\sqrt{A}}\sum_{j=1}^{A}\boldsymbol{X}_j. \qquad (4\cdot1\cdot68)$$

The relation between $(\boldsymbol{S}_i, i=1\sim A)$ and $(\boldsymbol{R}_i, i=1\sim A)$ is entirely the same as that between $(\boldsymbol{\xi}_i, i=1\sim A)$ and $(\boldsymbol{X}_i, i=1\sim A)$ and the restriction $\sum_{j=1}^{A}\boldsymbol{R}_j=\sqrt{A}\boldsymbol{S}_A=0$ is imposed. By using the delta function property of $\exp(\boldsymbol{z}\cdot\boldsymbol{z}^*)$ given by Eq. (3·2·27), we can write the eigen-value equation of $\hat{n}$ as

$$\sum_{P}^{A!}\varepsilon(P)p_\lambda(\tfrac{1}{4}P\boldsymbol{S}_1,\cdots,\tfrac{1}{4}P\boldsymbol{S}_{A-1})=\sigma_\lambda p_\lambda(\boldsymbol{S}_1,\cdots,\boldsymbol{S}_{A-1}). \qquad (4\cdot1\cdot69)$$

As is seen in Eq. (4·1·54) p_λ is a homogeneous polynomial of $\boldsymbol{S}_1, \cdots, \boldsymbol{S}_{A-1}$, and so we obtain

$$\left(\frac{1}{A!}\sum_{P}^{A!}\varepsilon(P)P\right)p_\lambda(\boldsymbol{S}_1,\cdots,\boldsymbol{S}_{A-1})=\frac{4^{I_\lambda}\sigma_\lambda}{A!}p_\lambda(\boldsymbol{S}_1,\cdots,\boldsymbol{S}_{A-1}), \qquad (4\cdot1\cdot70)$$

where I_λ is the degree of the homogeneous polynomial p_λ. From Eq. (4·1·70), $\sigma_\lambda=A!/4^{I_\lambda}$ and p_λ is an arbitrary totally antisymmetric function (with respect to the permutations of $\boldsymbol{R}_1\sim\boldsymbol{R}_A$) of the polynomial degree I_λ. Further and detailed discussion of the 3α and 4α systems is given in Ref. 16).

4.1.e. *SU_4 symmetry*

In previous subsections §§ 4.1.b∼4.1.d, we have seen that the (Elliott) SU_3 group plays a vital role in solving the eigen-value problem of the RGM norm kernel. This originates from the use of the H.O. shell model wave functions in representing the internal states $\phi(C)$ of the constituent clusters. The SU_3 classification is valid and necessary for any kind of systems (including the rearrangement channels which are not treated explicitly in previous subsections), but, needless to say, this group does not give the complete classification of the eigen-functions for complicated systems.

Since the H.O. functions are used to describe the radial (or spatial) parts of the nucleon orbitals, the SU_3 group is concerned with the symmetry of the radial or spatial part of the cluster wave function. As for the spin-isospin degrees of freedom of nucleons, the SU_4 supermultiplet symmetry*) is valid

*) The author is indebted to Professor A. Arima for his remark on this symmetry.

and necessary[63] as is shown below.

As an illustrative example, we consider the systems of $3N+N$, namely $^3\mathrm{He}+n$ and $t+p$ configurations which are coupled to good total spin S and isospin T.[93] The eigen-value problem of the norm kernel of $3N+N$ system with definite S and T is

$$\langle Y_l(\hat{r})\, h_{TS} | \mathcal{A}\{R_{Nl}(r,\gamma)\, Y_l(\hat{r})\, h_{TS}\}\rangle = \mu^N_{TS} R_{Nl}(r,\gamma),$$
$$\boldsymbol{r} \equiv \boldsymbol{X}_N - \boldsymbol{X}_{3N},\ \gamma = \tfrac{3}{4}\nu,$$
$$h_{TS} \equiv [\phi(3N)\eta(N)]_{TS} = \sum_{m_t m_s m_t' m_s'} (\tfrac{1}{2} m_t \tfrac{1}{2} m_t' | T M_T)\ (\tfrac{1}{2} m_s \tfrac{1}{2} m_s' | S M_S) \times \phi_{m_t m_s}(3N)\, \eta_{m_t' m_s'}(N), \qquad (4\cdot1\cdot71)$$

where $\eta_{m_t m_s}(N)$ is the isospin-spin function of a single nucleon (neutron ($m_t = 1/2$), proton ($m_t = -1/2$)), and $\phi_{m_t m_s}(3N)$ is the internal wave function of $3N$(t ($m_t = 1/2$), $^3\mathrm{He}$ ($m_t = -1/2$)). In Eq. (4·1·71), the eigenvalue μ^N_{TS} does not depend on the orbital angular momentum l due to the SU_3 symmetry discussed in § 4.1.b. By expressing μ^N_{TS} as

$$\mu^N_{TS} = \langle R_{Nl}(r,\gamma)\, Y_l(\hat{r})\, h_{TS} | \mathcal{A} | R_{Nl}(r,\gamma)\, Y_l(\hat{r})\, h_{TS}\rangle, \qquad (4\cdot1\cdot72)$$

and by noting the SU_4 scalar property of $\mathcal{A}$ (which means $\mathcal{A}$ commutes with all the SU_4 generators), we know that the dependence of μ^N_{TS} on T and S is unified to the dependence on the label $[\tilde{f}]$ of the irreducible representation of SU_4 group to which h_{TS} belongs. This can be said to be due to the Wigner-Eckart theorem of the SU_4 group. Since the spatial permutation symmetry $[f]$ of $\mathcal{A}\{R_{Nl}(r,\gamma)\, Y_l(\hat{r})\, h_{TS}\}$ is conjugate to the above label $[\tilde{f}]$ of the SU_4 symmetry, we use $[f]$ instead of $[\tilde{f}]$. Thus we can say that within the same $[f]$, μ^N_{TS} does not depend on T and S.[63] In this sense we can use more appropriate notation $\mu^N_{[f]}$. With the use of the generating function technique of § 4.1.b we get

$$\hat{N}(R) = \langle A_\gamma(\boldsymbol{r}, \boldsymbol{R}_z)\, h_{TS} | \mathcal{A}\{A_\gamma(\boldsymbol{r}, \boldsymbol{R}_z)\, h_{TS}\}\rangle = \sum_{N=0}^{\infty} \frac{R^{2N}}{N!} \mu^N_{TS},$$
$$\boldsymbol{R}_z \equiv (0, 0, R). \qquad (4\cdot1\cdot73)$$

The calculated result of $\hat{N}(R)$ is

$$\hat{N}(R) = e^{R^2}\{1 + (4\delta_{T,0}\delta_{S,0} - 1)\, e^{-(4/3)R^2}\}, \qquad (4\cdot1\cdot74)$$

from which we obtain

$$\mu^N_{T=0,S=0} = \mu^N_{[4]} = 1 - \left(\frac{-1}{3}\right)^{N-1},$$
$$\mu^N_{T,S} = \mu^N_{[3,1]} = 1 - \left(\frac{-1}{3}\right)^{N}, \quad \text{where} \quad (T,S) \neq (0,0). \qquad (4\cdot1\cdot75)$$

4.2. Calculation of kernels or physical quantities related to norm kernel

What we here add about the calculation of the kernels or physical quantities is the use of the knowledge of the norm kernel by which we obtain simpler or more convenient procedure of calculation than the general calculational procedures given in §§ 2 and 3. In this subsection we assume all the oscillator parameters of clusters are the same.

4.2.a. *Kinetic energy and Hamiltonian*

We divide the kinetic energy operator into the intrinsic and relative kinetic energies as follows:

$$T=\sum_{i=1}^{A} T_i - T_G = T_{C_1}+T_{C_2}+T_r\,,\quad T_{C_1}\equiv\sum_{i\in C_1} T_i - T_{G_1}\,,$$

$$T_{C_2}\equiv\sum_{i\in C_2} T_i - T_{G_2}\,,\quad T_G\equiv\frac{-\hbar^2}{2Am}\left(\frac{\partial}{\partial \boldsymbol{X}_G}\right)^2,\quad T_r\equiv\frac{-\hbar^2}{2(N_1N_2/A)m}\left(\frac{\partial}{\partial \boldsymbol{r}}\right)^2,$$

$$T_{G_1}\equiv\frac{-\hbar^2}{2N_1m}\left(\frac{\partial}{\partial \boldsymbol{X}_1}\right)^2,\quad T_{G_2}\equiv\frac{-\hbar^2}{2N_2m}\left(\frac{\partial}{\partial \boldsymbol{X}_2}\right)^2. \qquad (4\cdot2\cdot1)$$

The matrix elements of T in the H.O. representation can be calculated in the following way; we assume $N\leq N'$. First we get

$$\begin{aligned}T(N,N',l)\equiv&\langle V_{Nl}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)|T|\mathcal{A}\{V_{N'l}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)\}\rangle\\ =&\langle V_{Nl}\phi_0(C_1)\phi_0(C_2)|\mathcal{A}\{(T_rV_{N'l})\phi_0(C_1)\phi_0(C_2)\}\rangle\\ &+\langle V_{Nl}\phi_0(C_1)\phi_0(C_2)|\mathcal{A}\{V_{N'l}(T_{C_1}\phi_0(C_1))\phi_0(C_2)\}\rangle\\ &+\langle V_{Nl}\phi_0(C_1)\phi_0(C_2)|\mathcal{A}\{V_{N'l}\phi_0(C_1)\,(T_{C_2}\phi_0(C_2))\}\rangle. \qquad (4\cdot2\cdot2)\end{aligned}$$

Next we insert the following expansions into Eq. (4·2·2),

$$\begin{aligned}T_rV_{N'l}=&\langle V_{N'l}|T_r|V_{N'l}\rangle V_{N'l}+\langle V_{N'+2,l}|T_r|V_{N'l}\rangle V_{N'+2,l}\\ &+\langle V_{N'-2,l}|T_r|V_{N',l}\rangle V_{N'-2,l}\,,\\ T_{C_1}\phi_0(C_1)=&\langle\phi_0(C_1)|T_{C_1}|\phi_0(C_1)\rangle\cdot\phi_0(C_1)\\ &+(\text{higher H.O. quantum states of } C_1),\\ T_{C_2}\phi_0(C_2)=&\langle\phi_0(C_2)|T_{C_2}|\phi_0(C_2)\rangle\cdot\phi_0(C_2)\\ &+(\text{higher H.O. quantum states of } C_2). \qquad (4\cdot2\cdot3)\end{aligned}$$

By considering the conservation of the number of the H.O. quanta between bras and kets, we get

$$\begin{aligned}T(N,N',l)=&\delta_{N,N'}\{\langle V_{Nl}|T_r|V_{Nl}\rangle+\langle\phi_0(C_1)|T_{C_1}|\phi_0(C_1)\rangle\\ &+\langle\phi_0(C_2)|T_{C_2}|\phi_0(C_2)\rangle\}\mu_N+\delta_{N+2,N'}\langle V_{Nl}|T_r|V_{N'l}\rangle\mu_N\,, \qquad (4\cdot2\cdot4)\end{aligned}$$

where $\mu_N\equiv\langle V_{Nl}\phi_0(C_1)\phi_0(C_2)|\mathcal{A}\{V_{Nl}\phi_0(C_1)\phi_0(C_2)\}\rangle$ according to Eq. (4·1·9).

When $N>N'$, we get a similar expression by operating T in this time to the ket state $V_{Nl}\phi_0(C_1)\phi_0(C_2)$. The final result valid for arbitrary N and N' is,

$$\begin{aligned}&\langle V_{Nl}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)|T|\mathcal{A}\{V_{N'l}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)\}\rangle\\&=\delta_{N,N'}\cdot\mu_N\cdot\tfrac{1}{2}\hbar\omega(N(C_1)+N(C_2)+N+3/2)\\&\quad+\delta_{N+2,N'}\cdot\mu_N\cdot\tfrac{1}{4}\hbar\omega\sqrt{(N-l+2)(N+l+3)}\\&\quad+\delta_{N,N'+2}\cdot\mu_{N'}\cdot\tfrac{1}{4}\hbar\omega\sqrt{(N'-l+2)(N'+l+3)},\end{aligned}\tag{4·2·5}$$

where use is made of the following relations and definitions:

$$\begin{aligned}&\langle V_{Nl}|T_r|V_{Nl}\rangle=\tfrac{1}{2}\hbar\omega(N+\tfrac{3}{2}),\\&\langle V_{N-2,l}|T_r|V_{N,l}\rangle=\tfrac{1}{4}\hbar\omega\sqrt{(N-l)(N+l+1)},\\&N(C_i)=\text{number of the total H.O. quanta of }\phi_0(C_i).\end{aligned}\tag{4·2·6}$$

Similarly for the case of the total Hamiltonian, by dividing it into the internal and relative parts,

$$\begin{aligned}&H=\sum_{i=1}^{A}T_i-T_G+\tfrac{1}{2}\sum_{i\neq j}^{A}V_{ij}=H_{C_1}+H_{C_2}+T_r+V_r,\\&H_{C_i}=T_{C_i}+\tfrac{1}{2}\sum_{i,j\in C_i}V_{ij},\quad V_r=\sum_{i\in C_1}\sum_{j\in C_2}V_{ij}\quad\text{(Eq. (2·1·25))},\end{aligned}\tag{4·2·7}$$

we get, by entirely the same procedure,

$$\begin{aligned}&\langle V_{Nl}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)|H|\mathcal{A}\{V_{N'l}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)\}\rangle\\&=\delta_{N,N'}\cdot\mu_N\{E(C_1)+E(C_2)+\tfrac{1}{2}\hbar\omega(N+\tfrac{3}{2})\}\\&\quad+\delta_{N+2,N'}\cdot\mu_N\cdot\tfrac{1}{4}\hbar\omega\sqrt{(N-l+2)(N+l+3)}\\&\quad+\delta_{N,N'+2}\cdot\mu_{N'}\cdot\tfrac{1}{4}\hbar\omega\sqrt{(N'-l+2)(N'+l+3)}\\&\quad+\langle V_{Nl}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)|W|V_{N'l}(\boldsymbol{r},\gamma)\phi_0(C_1)\phi_0(C_2)\rangle,\\&E(C_i)\equiv\langle\phi_0(C_i)|H_{C_i}|\phi_0(C_i)\rangle,\\&W=\begin{cases}V_r\mathcal{A} & \text{for}\quad N\geq N',\\ \mathcal{A}V_r & \text{for}\quad N\leq N'.\end{cases}\end{aligned}\tag{4·2·8}$$

This expression is useful when we measure the energies from the two-body threshold energy $E(C_1)+E(C_2)$.

4.2.b. *Multipole operators*

Essentially the same technique as in § 4.2.a is applicable to the case of the multipole operators. What is necessary for us is to divide the multipole operators into the internal and relative parts and their coupling part.

What we consider here is the multipole operator

$$T_{\lambda 0}\equiv\sum_{i=1}^{A}y_{\lambda 0}(\boldsymbol{x}_i-\boldsymbol{X}_G),\quad y_{\lambda\mu}(\boldsymbol{a})\equiv a^{\lambda}Y_{\lambda\mu}(\hat{a}).\tag{4·2·9}$$

In order to treat this operator, we introduce the operator

$$T_{\lambda 0}(k) \equiv \sum_{i=1}^{A} j_\lambda(k|\boldsymbol{x}_i - \boldsymbol{X}_G|)\, Y_{\lambda 0}(\widehat{\boldsymbol{x}_i - \boldsymbol{X}_G}). \tag{4·2·10}$$

With slight modification we can use the results for these operators to the cases of the electric multipole transition operators in gamma decay and electron scattering. The relation of $T_{\lambda 0}$ with $T_{\lambda 0}(k)$ is

$$T_{\lambda 0} = (2\lambda+1)!! \lim_{k\to 0} k^{-\lambda} T_{\lambda 0}(k). \tag{4·2·11}$$

We first express $T_{\lambda 0}(k)$ as follows,

$$T_{\lambda 0}(k) = \frac{i^{-\lambda}}{4\pi} \int d\hat{k}\, Y_{\lambda 0}(\hat{k}) \sum_{i=1}^{A} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}_i - \boldsymbol{X}_G)}. \tag{4·2·12}$$

We introduce the function $k(i)$ which tells us that i-th nucleon is included in $k(i)$-th cluster $C_{k(i)}$. By using this function $k(i)$ we get

$$\boldsymbol{x}_i - \boldsymbol{X}_G = (\boldsymbol{x}_i - \boldsymbol{X}_{k(i)}) + (\boldsymbol{X}_{k(i)} - \boldsymbol{X}_G). \tag{4·2·13}$$

Since $\boldsymbol{X}_{k(i)} - \boldsymbol{X}_G$ is expressed by the Jacobi coordinates $\boldsymbol{\xi}_j$ as

$$\boldsymbol{X}_{k(i)} - \boldsymbol{X}_G = \sum_{j=1}^{n-1} \alpha_{k(i)}^{j} \boldsymbol{\xi}_j, \tag{4·2·14}$$

we get

$$\begin{aligned}
\sum_{i=1}^{A} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}_i - \boldsymbol{X}_G)} &= \sum_{i=1}^{A} \prod_{j=1}^{n-1} \exp\{i\alpha_{k(i)}^{j} \boldsymbol{k}\cdot\boldsymbol{\xi}_j\} \cdot \exp\{i\boldsymbol{k}\cdot(\boldsymbol{x}_i - \boldsymbol{X}_{k(i)})\} \\
&= \sum_{i=1}^{A} (4\pi)^n \sum_{\substack{\lambda_1\sim\lambda_n \\ \mu_1\sim\mu_n}} i^{(\sum_{j=1}^{n}\lambda_j)} \prod_{j=1}^{n-1} j_{\lambda_j}(\alpha_{k(i)}^{j} k\xi_j) \cdot j_{\lambda_n}(k|\boldsymbol{x}_i - \boldsymbol{X}_{k(i)}|) \\
&\quad \times \prod_{j=1}^{n-1} Y^*_{\lambda_j\mu_j}(\hat{k})\, Y_{\lambda_j\mu_j}(\hat{\xi}_j) \cdot Y^*_{\lambda_n\mu_n}(\hat{k})\, Y_{\lambda_n\mu_n}(\widehat{\boldsymbol{x}_i - \boldsymbol{X}_{k(i)}}).
\end{aligned} \tag{4·2·15}$$

For simplicity, we consider the three-cluster system. Then we have

$$\begin{aligned}
T_{\lambda 0}(k) &= (4\pi)^2 \sum_{\lambda_1\sim\lambda_3} i^{\lambda_1+\lambda_2+\lambda_3-\lambda} \sum_{J} e(\lambda_1\lambda_2 J)\, e(J\lambda_3\lambda) \\
&\quad \times \sum_{i=1}^{A} \prod_{j=1}^{2} j_{\lambda_j}(\alpha_{k(i)}^{j} k\xi_j)\, j_{\lambda_3}(k|\boldsymbol{x}_i - \boldsymbol{X}_{k(i)}|) \\
&\quad \times [[Y_{\lambda_1}(\hat{\xi}_1)\, Y_{\lambda_2}(\hat{\xi}_2)]_J\, Y_{\lambda_3}(\widehat{\boldsymbol{x}_i - \boldsymbol{X}_{k(i)}})]_{\lambda 0}, \\
e(j_1 j_2 j_3) &\equiv (j_1 0\, j_2 0 | j_3 0) \sqrt{\frac{(2j_1+1)(2j_2+1)}{4\pi(2j_3+1)}}.
\end{aligned} \tag{4·2·16}$$

By using Eq. (4·2·11) we obtain

$$T_{\lambda 0} = (4\pi)^2 \sum_{\lambda_1+\lambda_2+\lambda_3=\lambda} [(2\lambda+1)!!/\textstyle\sum_{i=1}^{3} \Rightarrow \prod_{i=1}^{3} (2\lambda_i+1)!!]\, e(\lambda_1, \lambda_2, \lambda_1+\lambda_2)$$

$$\times e(\lambda_1+\lambda_2, \lambda_3, \lambda) \sum_{i=1}^{A} (\alpha^1_{k(i)})^{\lambda_1} (\alpha^2_{k(i)})^{\lambda_2}$$
$$\times [[y_{\lambda_1}(\xi_1) y_{\lambda_2}(\xi_2)]_{\lambda_1+\lambda_2} y_{\lambda_3}(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})]_{\lambda 0}. \qquad (4\cdot2\cdot17)$$

(The form of $T_{\lambda 0}(k)$ by Eq. (4·2·16) is useful for the OCM calculation of electron scattering form factor.)

We reduce the form of $T_{\lambda 0}$ of Eq. (4·2·17) into more convenient form by using the following relations,

$$\sum_{i\in C_k} y_{\lambda=1}(\boldsymbol{x}_i-\boldsymbol{X}_k)=0,$$
$$\alpha_1{}^1=\frac{-N_2}{N_1+N_2},\ \alpha_1{}^2=\frac{-N_3}{A},\ \alpha_2{}^1=\frac{N_1}{N_1+N_2},\ \alpha_2{}^2=\frac{N_3}{A},$$
$$\alpha_3{}^1=0,\ \alpha_3{}^2=\frac{N_1+N_2}{A}. \qquad (4\cdot2\cdot18)$$

For $\lambda=2$ we obtain

$$T_{20}=p_1 y_{20}(\xi_1)+p_2 y_{20}(\xi_2)+p_3 \sum_{i=1}^{A} y_{20}(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)}), \qquad (4\cdot2\cdot19)$$

where p_i are constants. Equation (4·2·19) is, of course, directly obtainable from the invariance of the unit quadratic form against the essentially orthogonal transformation $\{\boldsymbol{x}_i-\boldsymbol{X}_G\}\to\{\xi_j, \boldsymbol{x}_i-\boldsymbol{X}_{k(i)}\}$. For $\lambda=3$,

$$T_{30}=q_1 y_{30}(\xi_1)+q_2 y_{30}(\xi_2)+q_3 \sum_{i=1}^{A} y_{30}(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})$$
$$+q_4[y_2(\xi_1) y_1(\xi_2)]_{30}+q_5[y_1(\xi_1) y_2(\xi_2)]_{30}$$
$$+q_6 \sum_{i=1}^{A}[y_1(\xi_1) y_2(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})]_{30}+q_7 \sum_{i=1}^{A}[y_1(\xi_2) y_2(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})]_{30}, \qquad (4\cdot2\cdot20)$$

where q_i are constants. Let all C_i be closed shell clusters and the matrix element I_λ of $T_{\lambda 0}$ is

$$I_\lambda \equiv \langle V^{N_1 N_2}_{l_1 l_2 J_1}\phi_0 | T_{\lambda 0} | \mathcal{A}\{V^{N_3 N_4}_{l_3 l_4 J_2}\phi_0\}\rangle,$$
$$V^{N_1 N_2}_{l_1 l_2 J}(\xi_1, \xi_2) \equiv [V_{N_1 l_1}(\xi_1, \gamma_1) V_{N_2 l_2}(\xi_2, \gamma_2)]_J, \quad \text{(Eq. (4·1·43))}$$
$$\phi_0 \equiv \prod_{i=1}^{3} \phi_0(C_i). \qquad (4\cdot2\cdot21)$$

By assuming $N_1+N_2 \leqq N_3+N_4$ without loss of generality, and by using

$$\sum_{i=1}^{A} y_{20}(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})\phi_0 = \langle\phi_0|\sum_{i=1}^{A} y_{20}(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})|\phi_0\rangle\cdot\phi_0$$
$$+\sum (2\hbar\omega \text{ excited states of } \phi_0),$$
$$\langle\phi_0|\sum_{i=1}^{A} y_{20}(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})|\phi_0\rangle = 0, \qquad (4\cdot2\cdot22)$$

we obtain for $\lambda=2$

$$I_2=\sum_{\substack{l_5,l_6\\ N_5+N_6=N_1+N_2}}\langle V^{N_5N_6}_{l_5l_6J_1}|\{p_1y_{20}(\boldsymbol{\xi}_1)+p_2y_{20}(\boldsymbol{\xi}_2)\}|V^{N_3N_4}_{l_3l_4J_2}\rangle \times\langle V^{N_1N_2}_{l_1l_2J_1}\phi_0|\mathcal{A}\{V^{N_5N_6}_{l_5l_6J_1}\phi_0\}\rangle . \tag{4·2·23}$$

For $\lambda=3$, again by assuming $N_1+N_2\leqq N_3+N_4$ and by using

$$\sum_{i=1}^{A}y_{30}(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})\phi_0=\sum\ (1\text{ or }3\ \hbar\omega\text{ excited states of }\phi_0),$$

$$\sum_{i=1}^{A}[y_1(\boldsymbol{\xi}_j)\,y_2(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})]_{30}V^{N_3N_4}_{l_3l_4J}\phi_0=\sum\ (\text{higher H.O. quantum states than } V^{N_3N_4}_{l_3l_4J}\phi_0 \text{ by at least } 1\hbar\omega), \tag{4·2·24}$$

we obtain

$$I_3=\sum_{\substack{l_5l_6\\ N_5+N_6=N_1+N_2}}\langle V^{N_5N_6}_{l_5l_6J_1}|\{q_1y_{30}(\boldsymbol{\xi}_1)+q_2y_{30}(\boldsymbol{\xi}_2)+q_4[y_2(\boldsymbol{\xi}_1)\,y_1(\boldsymbol{\xi}_2)]_{30} +q_5[y_1(\boldsymbol{\xi}_1)\,y_2(\boldsymbol{\xi}_2)]_{30}\}|V^{N_3N_4}_{l_3l_4J_2}\rangle \times\langle V^{N_1N_2}_{l_1l_2J_1}\phi_0|\mathcal{A}\{V^{N_5N_6}_{l_5l_6J_1}\phi_0\}\rangle . \tag{4·2·25}$$

The case of the system which includes open shell clusters is treated similarly. As an example, we consider a two-cluster system composed of an SU_3-non-scalar cluster C_1 with (σ,τ) symmetry and SU_3 scalar cluster C_2.[61] The forms of $T_{\lambda0}$ are

$$T_{20}=p_1'y_{20}(\boldsymbol{r})+p_2'\sum_{i=1}^{A}y_{20}(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)}),$$

$$T_{30}=q_1'y_{30}(\boldsymbol{r})+q_2'\sum_{i=1}^{A}y_{30}(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)}) +q_3'\sum_{i=1}^{A}[y_1(\boldsymbol{r})\,y_2(\boldsymbol{x}_i-\boldsymbol{X}_{k(i)})]_{30}. \tag{4·2·26}$$

The matrix element I_λ of $T_{\lambda0}$,

$$I_\lambda\equiv\langle[V_{Nl_i}(\boldsymbol{r},\gamma)\phi_{L_i}(C_1)]_{J_1}\phi_0(C_2)|T_{\lambda0}|\mathcal{A}\{[V_{N'l_j}(\boldsymbol{r},\gamma)\phi_{L_j}(C_1)]_{J_2}\phi_0(C_2)\}\rangle \tag{4·2·27}$$

is calculated as follows by assuming $N\leqq N'$ without loss of generality. (When $N>N'$ we operate $T_{\lambda0}$ to the bra state $[V_{Nl_1}\phi_{L_1}(C_1)]_{J_1}\phi_0(C_2)$.) For $\lambda=2$

$$I_2=\sum_k\langle[V_{Nl_k}\phi_{L_k}(C_1)]_{J_1}|\{p_1'y_{20}(\boldsymbol{r})+p_2'\sum_{i\in C_1}y_{20}(\boldsymbol{x}_i-\boldsymbol{X}_1)\}|[V_{N'l_j}\phi_{L_j}(C_1)]_{J_2}\rangle \times\langle[V_{Nl_i}\phi_{L_i}(C_1)]_{J_1}\phi_0(C_2)|\mathcal{A}\{[V_{Nl_k}\phi_{L_k}(C_1)]_{J_1}\phi_0(C_2)\}\rangle, \tag{4·2·28}$$

where we used the fact that the operation of $\sum_{i\in C_1}y_{20}(\boldsymbol{x}_i-\boldsymbol{X}_1)$ to $\phi_{(\sigma,\tau)\rho L}(C_1)$ can change the state within the same irreducible representation (σ,τ) in the $0\hbar\omega$-

jump states, namely

$$\sum_{i\in C_1} y_{20}(\boldsymbol{x}_i-\boldsymbol{X}_1)\phi_{(\sigma,\tau)\rho L}(C_1)=\sum_{\rho' L'}\langle\phi_{(\sigma,\tau)\rho' L'}(C_1)|\sum_{i\in C_1} y_{20}(\boldsymbol{x}_i-\boldsymbol{X}_1)|\phi_{(\sigma,\tau)\rho L}(C_1)\rangle \times\phi_{(\sigma,\tau)\rho' L'}(C_1)+\sum(2\hbar\omega \text{ excited configurations}). \quad (4\cdot2\cdot29)$$

For $\lambda=3$, similarly

$$I_3=\sum_k\langle[V_{Nl_k}\phi_{L_k}(C_1)]_{J_1}|\{q_1' y_{30}(\boldsymbol{r})+q_3'\sum_{i\in C_1}[y_1(\boldsymbol{r})y_2(\boldsymbol{x}_i-\boldsymbol{X}_1)]_{30}\} |[V_{N'l_j}\phi_{L_j}(C_1)]_{J_2}\rangle\langle[V_{Nl_i}\phi_{L_i}(C_1)]_{J_1}\phi_0(C_2)|\mathcal{A}\{[V_{Nl_k}\phi_{L_k}(C_1)]_{J_1}\phi_0(C_2)\}\rangle. \quad (4\cdot2\cdot30)$$

4.2.c. *Reduced width amplitude of cluster decay or transfer*

The calculation of the reduced width amplitude (R.W.A.) of cluster decay or transfer has been discussed for a long time by many authors. What we discuss here is limited to the application of the delta function technique of § 3 and that of the knowledge of the norm kernel. About the other approaches, see Refs. 64)~71).

The R.W.A. of the model wave function Ψ_L with the angular momentum L is

$$y_L(a)\equiv\frac{1}{\sqrt{1+\delta_{C_1C_2}}}\sqrt{\binom{A}{N_1}}\left\langle\frac{\delta(r-a)}{r^2}Y_{L0}(\hat{r})\phi_0(C_1)\phi_0(C_2)\middle|\Phi_L\right\rangle, \quad (4\cdot2\cdot31)$$

where we assume that the model wave function Ψ_L is non-spurious about the C.M. motion and its dependence on $\boldsymbol{X}_G$ is separated from the internal wave function Φ_L as follows:

$$\Psi_L=\omega_0(\boldsymbol{X}_G)\cdot\Phi_L, \quad \omega_0(\boldsymbol{X}_G)\equiv\left(\frac{2A\nu}{\pi}\right)^{3/4}e^{-A\nu\boldsymbol{X}_G^2}. \quad (4\cdot2\cdot32)$$

For simplicity, the channel is considered above where the spins of clusters are zero. We can utilize the delta function technique of § 3.4 for the evaluation of Eq. (4·2·31) with Eq. (4·2·32). From the prescription of Eq. (3·4·1)

$$\int d\boldsymbol{R}\,e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\left\langle\phi_0\left(C_1,\frac{-N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2,\frac{N_1}{A}\boldsymbol{R}\right)\middle|\Psi_L\right\rangle$$
$$=\left(\frac{4N_1N_2\nu_1\nu_2}{\gamma^2}\cdot\frac{2A\nu}{\pi}\right)^{3/4}\exp\left(-\frac{k^2}{4\gamma}\right)$$
$$\times\left\langle\exp\left\{-\left(\alpha-\frac{\beta^2}{4\gamma}\right)X_G^2-\frac{i\beta}{2\gamma}\boldsymbol{k}\cdot\boldsymbol{X}_G\right\}\middle|e^{-A\nu X_G^2}\right\rangle$$
$$\times\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\phi_0(C_1)\phi_0(C_2)|\Phi_L\rangle,$$
$$\langle\delta(\boldsymbol{r}-\boldsymbol{a})\phi_0(C_1)\phi_0(C_2)|\Phi_L\rangle=b_1\int d\boldsymbol{k}\,e^{-i\boldsymbol{k}\cdot\boldsymbol{a}}\cdot e^{b_2k^2}\int d\boldsymbol{R}\,e^{i\boldsymbol{k}\cdot\boldsymbol{R}}$$

$$\times\left\langle\phi_0\left(C_1,\frac{-N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2,\frac{N_1}{A}\boldsymbol{R}\right)\middle|\Psi_L\right\rangle,$$

$$\left\langle\frac{\delta(r-a)}{r^2}Y_{L0}(\hat{r})\phi_0(C_1)\phi_0(C_2)\middle|\Phi_L\right\rangle$$

$$=\begin{cases}\dfrac{1}{Y_{L0}(\hat{a})}\langle\delta(\boldsymbol{r}-\boldsymbol{a})\phi_0(C_1)\phi_0(C_2)|\Phi_L\rangle\\ b_1(4\pi)^2\displaystyle\int_0^\infty dk\cdot k^2 j_L(ka)e^{b_2k^2}\int d\boldsymbol{R}\, j_L(kR)Y_{L0}(\hat{R})\\ \qquad\times\left\langle\phi_0\left(C_1,\dfrac{-N_2}{A}\boldsymbol{R}\right)\phi_0\left(C_2,\dfrac{N_1}{A}\boldsymbol{R}\right)\middle|\Psi_L\right\rangle,\end{cases}\qquad(4\cdot2\cdot33)$$

where b_1, b_2 are constants involving ν, ν_1 and ν_2. From Eq. (3·4·3) we get another formula[54]

$$\langle\delta(\boldsymbol{r}-\boldsymbol{a})\phi_0(C_1)\phi_0(C_2)|\Phi_L\rangle=b_3\int d\boldsymbol{k}\,\exp\left\{-\left(\frac{1}{N_1\nu_1}+\frac{1}{N_2\nu_2}\right)\frac{k^2}{4}\right\}$$

$$\times\left\langle\phi_0\left(C_1,\frac{-N_2}{A}\boldsymbol{a}-\frac{i}{2N_1\nu_1}\boldsymbol{k}\right)\phi_0\left(C_2,\frac{N_1}{A}\boldsymbol{a}+\frac{i}{2N_2\nu_2}\boldsymbol{k}\right)\middle|\Psi_L\right\rangle,\quad(4\cdot2\cdot34)$$

where b_3 is also a constant involving ν, ν_1 and ν_2.

When Φ_L has a definite number of the total oscillator quanta $N(\Phi_L)$ with respect to the oscillator parameter ν, $y_L(a)$ of Eq. (4·2·31) can be expressed by the linear combination of the finite number of the H.O. functions $R_{NL}(a,\gamma_\nu)$ where $\gamma_\nu\equiv N_1N_2\nu/A$;

$$y_L(a)=\sum_{N=0}^{N_F}C_NR_{NL}(a,\gamma_\nu).\qquad(4\cdot2\cdot35)$$

To prove this we expand $\phi_0(C_i,\nu_i)$ by the shell model wave functions with oscillator parameter ν as follows:

$$\phi_0(C_i,\nu_i)=\langle\phi_0(C_i,\nu)|\phi_0(C_i,\nu_i)\rangle\cdot\phi_0(C_i,\nu)$$
$$+\sum\ (\text{higher oscillator quantum states than }\phi_0(C_i,\nu)).\quad(4\cdot2\cdot36)$$

By inserting this expansion into

$$y_L(a)=\frac{1}{\sqrt{1+\delta_{C_1,C_2}}}\sqrt{\binom{A}{N_1}}\sum_N R_{NL}(a,\gamma_\nu)$$
$$\times\langle V_{NL0}(\boldsymbol{r},\gamma_\nu)\phi_0(C_1,\nu_1)\phi_0(C_2,\nu_2)|\Phi_L\rangle,\qquad(4\cdot2\cdot37)$$

and by considering the conservation of the total number of the H.O. quanta between bra and ket, we obtain

$$N_F=N(\Phi_L)-N(C_1)-N(C_2),\qquad(4\cdot2\cdot38)$$

where $N(C_i)$ are the numbers of the H.O. quanta of the states $\phi(C_i,\nu)$.

When Φ_L are of the type of the RGM (or GCM) wave function, we can calculate[14),15),61),68),94] $y_L(a)$ by the knowledge of the norm kernel obtained in § 4.1. Below we assume that all the oscillator constants are the same. For the case

$$\Phi_L=\frac{1}{\sqrt{q_{12}}}\mathcal{A}\{\chi_L(r)Y_{L0}(\hat{r})\phi_0(C_1)\phi_0(C_2)\},\quad q_{12}\equiv\binom{A}{N_1}(1+\delta_{c_1c_2}), \tag{4·2·39}$$

we get

$$y_L(a)=\sum_N e_N\mu_N R_{NL}(a,\gamma), \tag{4·2·40}$$

where e_N are obtained from*)

$$\chi_L(a)=\sum_N e_N R_{NL}(a,\gamma). \tag{4·2·41}$$

In Eq. (4·2·40) we used the usual definition of μ_N that when $C_1\equiv C_2$, μ_N is half of the value of Eq. (4·1·9).

Similarly we can calculate the R.W.A. of Φ_L which are channel-coupling or multi-cluster RGM (or GCM) wave functions. As an example for the case of Eq. (4·1·16),

$$\Phi_J=\frac{1}{\sqrt{\binom{A}{N_1}}}\sum_j\mathcal{A}\{\chi_j(r)[Y_{l_j}(\hat{r})\phi_{(\sigma,\tau)\rho_jL_j}(C_1)]_J\phi_0(C_2)\}, \tag{4·2·42}$$

we get

$$\begin{aligned}y_{iJ}(a)&\equiv\sqrt{\binom{A}{N_1}}\left\langle\frac{\delta(r-a)}{r^2}[Y_{l_i}(\hat{r})\phi(\sigma,\tau)\rho_iL_i(C_1)]_J\phi_0(C_2)\middle|\Phi_J\right\rangle\\&=\sum_{jN}e_{jN}\sum_{(\lambda\mu)\kappa}C_i^{N(\lambda\mu)\kappa J}C_j^{N(\lambda\mu)\kappa J}\mu_{(\lambda\mu)}^N R_{Nl_i}(a,\gamma),\\C_i^{N(\lambda\mu)\kappa J}&\equiv\langle(N,0)l_i,(\sigma,\tau)\rho_iL_i\|(\lambda\mu)\kappa J\rangle,\end{aligned} \tag{4·2·43}$$

where e_{jN} are obtained from

$$\chi_j(r)=\sum_N e_{jN}R_{Nl_j}(r,\gamma). \tag{4·2·44}$$

It should be noted that the SU_3 shell model wave functions Φ_J can be usually rewritten in the form of the RGM wave function due to the Bayman-Bohr theorem[72] (see also § 4.3) and so the calculational method like as Eqs. (4·2·20) and (4·2·43) is very useful also for those shell model wave functions.

4.3. Cluster model space

4.3.a. *Projection operator of Feshbach*

Any A-nucleon wave function $\hat{\Phi}_L$ can be broken up into two mutually

*) The normalization $\langle\Phi_L|\Phi_L\rangle=1$ means the normalization of e_N is $\sum_N e_N^2\mu_N=1$.

orthogonal parts as follows:

$$\hat{\Phi}_L = \mathcal{A}\{\chi_L(r)\, h_L\} + \hat{\Phi}_L{}^R, \quad h_L \equiv Y_{L0}(\hat{r})\,\phi_0(C_1)\,\phi_0(C_2). \tag{4·3·1}$$

$\hat{\Phi}_L{}^R$ satisfies

$$\langle h_L | \hat{\Phi}_L{}^R \rangle = 0. \tag{4·3·2}$$

The projection operator P_L which projects out of $\hat{\Phi}_L$ the component of two-cluster wave function $\mathcal{A}\{\chi_L(r)\, h_L\}$ as

$$P_L \hat{\Phi}_L = \mathcal{A}\{\chi_L(r)\, h_L\}, \tag{4·3·3}$$

has been obtained by Feshbach[73] as follows (see also Chap. II):

$$P_L = \frac{1}{q_{12}} \mathcal{A} \left\{ |h_L\rangle\langle h_L| + \sum_{\mu_\alpha \neq 0} \frac{1-\mu_\alpha}{\mu_\alpha} |\chi_L{}^\alpha h_L\rangle\langle \chi_L{}^\alpha h_L| \right\} \mathcal{A},$$

$$q_{12} \equiv \binom{A}{N_1} (1 + \delta_{C_1, C_2}). \tag{4·3·4}$$

Here $\chi_L{}^\alpha(r)$ and μ_α are the eigen-functions and eigen-values of the RGM norm kernel defined similarly to Eq. (4·1·8) by

$$\langle h_L | \mathcal{A}\{\chi_L{}^\alpha(r)\, h_L\} \rangle = (1 + \delta_{C_1 C_2})\, \mu_\alpha \chi_L{}^\alpha(r). \tag{4·3·5}$$

When the H.O. parameters of $\phi_0(C_1)$ and $\phi_0(C_2)$ are the same, we have the solutions of this eigen-value equation as was discussed in § 4.2, and so we have the explicit form of P_L.

According to the discussion of § 4.1, we know that the orthonormal basis wave functions $\Phi_{L\alpha}$ of the functional space spanned by the two-cluster wave functions of the form $\mathcal{A}\{\omega_L(r)\, h_L\}$ are given by

$$\Phi_{L\alpha} = \frac{1}{\sqrt{\mu_\alpha q_{12}}} \mathcal{A}\{\chi_L{}^\alpha(r)\, h_L\}. \tag{4·3·6}$$

We can easily check that

$$P_L = \sum_\alpha |\Phi_{L\alpha}\rangle\langle \Phi_{L\alpha}|. \tag{4·3·7}$$*)

When $\hat{\Phi}_L$ is normalizable and is normalized to unity $\langle \hat{\Phi}_L | \hat{\Phi}_L \rangle = 1$, it is important to evaluate the following quantity:

$$\sigma_L{}^2 \equiv \| P_L \hat{\Phi}_L \|^2 = \langle \hat{\Phi}_L | P_L | \hat{\Phi}_L \rangle \tag{4·3·8}$$

which tells us how much the clustering component is contained in $\hat{\Phi}_L$. By using Eq. (4·3·4) we obtain the formula to calculate $\sigma_L{}^2$ as

*) To prove Eq. (4.3.7) we need to use

$$\sum_\alpha \chi_L{}^\alpha(r)\, \chi_L{}^{\alpha *}(r') = \frac{\delta(r-r')}{rr'}.$$

This is safe at least when we are dealing the normalizable states.

$$\sigma_L^2 = S_L^2 + \sum_{\mu_\alpha \neq 0} \frac{1-\mu_\alpha}{\mu_\alpha} |\langle \chi_L^\alpha | y_L \rangle|^2 ,$$

$$y_L(r) \equiv \frac{1}{\sqrt{1+\delta_{c_1 c_2}}} \sqrt{\binom{A}{N_1}} \langle h_L | \hat{\Phi}_L \rangle , \quad S_L^2 \equiv \int_0^\infty dr \cdot r^2 |y_L(r)|^2 , \quad (4\cdot3\cdot9)$$

where y_L is the R.W.A. of $\hat{\Phi}_L$.

The σ_L^2 values for the deformed oscillator (anisotropic H.O.) model wave functions in ^{8}Be and ^{20}Ne are given in Ref. 14).

Here we introduce the notation K_L by

$$(1-K_L)\chi_L \equiv \langle h_L | \mathcal{A}_0 \{\chi_L(r) h_L\} \rangle , \quad \mathcal{A}_0 \equiv \frac{1}{1+\delta_{c_1 c_2}} \mathcal{A} . \quad (4\cdot3\cdot10)$$

K_L is usually called the exchange norm kernel, and is a bounded operator. The reason to introduce a factor $[1/(1+\delta_{c_1 c_2})]$ is to normalize the coefficient of the Dirac delta function operator 1 (an unbounded kernel) in Eq. (4·3·10) to unity. $(1-K_L)$ is the full norm kernel

$$\left\langle \frac{\delta(r-a)}{r^2} h_L \middle| \mathcal{A}_0 \left\{ \frac{\delta(r-b)}{r^2} h_L \right\} \right\rangle = \frac{\delta(a-b)}{ab} - K_L(a,b) . \quad (4\cdot3\cdot11)$$

By using the solutions of Eq. (4·3·5) we have

$$(1-K_L)(a,b) = \sum_\alpha \mu_\alpha \chi_L^\alpha(a) \chi_L^{\alpha *}(b) ,$$

$$K_L(a,b) = \sum_\alpha (1-\mu_\alpha) \chi_L^\alpha(a) \chi_L^{\alpha *}(b) . \quad (4\cdot3\cdot12)$$

With the use of the following definition,

$$(1-K_L)^{-n}(a,b) \equiv \sum_{\mu_\alpha \neq 0} \mu_\alpha^{-n} \chi_L^\alpha(a) \chi_L^{\alpha *}(b) , \quad n>0 , \quad (4\cdot3\cdot13)$$

we obtain

$$\langle (1-K_L)^{-1/2}(r,a) h_L | \mathcal{A}_0 \{(1-K_L)^{-1/2}(r,b) h_L\} \rangle = \frac{\delta(a-b)}{ab} . \quad (4\cdot3\cdot14)$$

This equation means that the following functions,[74),91)]

$$\Phi_L^a \equiv \frac{1}{\sqrt{q_{12}}} \mathcal{A} \{(1-K_L)^{-1/2}(r,a) h_L\} , \quad (4\cdot3\cdot15)$$

constitutes an orthonormal set

$$\langle \Phi_L^a | \Phi_L^b \rangle = \frac{\delta(a-b)}{ab} . \quad (4\cdot3\cdot16)^*$$

This set of functions is a complete set since we can easily prove the following relations:

$$P_L = \int da \cdot a^2 |\Phi_L^a\rangle\langle\Phi_L^a| = \frac{1}{q_{12}} \mathcal{A} \left\{ |h_L\rangle \frac{1}{1-K_L} \langle h_L| \right\} \mathcal{A} . \quad (4\cdot3\cdot17)$$

*) When the forbidden states χ_L^α with $\mu_\alpha=0$ are existent, this relation is valid within the space of the allowed functions $\chi_L^\alpha(a)$ or $\chi_L^\alpha(b)$ with $\mu_\alpha \neq 0$. Similarly Eq. (4·3·27) is valid for the allowed space. With use of the projection operator Λ of §5.1, the r.h.s. of Eqs. (4·3·16) and (4·3·27) are $\Lambda(a,b)$ and $\Lambda_{ij}(a_i,b_j)$, respectively.

The formal relation between $\Phi_{L\alpha}$ and $\Phi_L{}^a$ is

$$\Phi_L{}^a=\sum_\alpha \chi_L{}^{a*}(a)\Phi_{L,\alpha}\,. \tag{4·3·18}$$

With the use of the notation K_L we have

$$y_L=(1-K_L)\chi_L\,, \tag{4·3·19}$$

and if we define the following quantity,

$$\Omega_L(a)\equiv\langle\Phi_L{}^a|\hat{\Phi}_L\rangle=\frac{1}{\sqrt{1+\delta_{c_1c_2}}}\sqrt{\binom{A}{N_1}}\langle(1-K_L)^{-1/2}(r,a)\,h_L|\hat{\Phi}_L\rangle\,, \tag{4·3·20}$$

we get

$$\Omega_L=(1-K_L)^{-1/2}y_L=(1-K_L)^{1/2}\chi_L \tag{4·3·21}$$

and

$$\sigma_L{}^2=\langle\Omega_L|\Omega_L\rangle=\langle y_l|\,(1-K_L)^{-1}|y_L\rangle=\langle\chi_L|\,(1-K_L)\,|\chi_L\rangle. \tag{4·3·22}$$

Since $\sigma_L{}^2$ is the total probability of the clustering component in $\hat{\Phi}_L$, $\Omega_L(a)$ is the probability amplitude that the clusters C_1 and C_2 are located at the relative distance a. Thus $\Omega_L(a)$ can be said to be the relative wave function between clusters in the sense that $|\Omega_L(a)|^2$ can be interpreted as to be the probability density at the relative distance a. The importance of this relative wave function Ω_L has been emphasized by Saito and his coworkers[17] and by Fliessbach and his coworkers.[74] (See Chap. II.)

The projection operator of Feshbach can be similarly defined and calculated also for the complicated systems.[75),15),91),92] For the system with the wave functions of Eq. (4·1·1) we have

$$\begin{aligned}P&=\sum_{ij}\mathcal{A}_i'\left\{\delta_{ij}|\phi_i\rangle\langle\phi_j|+\sum_{\mu_\alpha\neq 0}\frac{1-\mu_\alpha}{\mu_\alpha}|\chi_i{}^\alpha\phi_i\rangle\langle\chi_j{}^\alpha\phi_j|\right\}\mathcal{A}_j'\\&=\sum_{ij}\mathcal{A}_i'\left\{|\phi_i\rangle\left(\frac{1}{1-K}\right)_{ij}\langle\phi_j|\right\}\mathcal{A}_j'\,,\end{aligned} \tag{4·3·23}$$

where μ_α and $\chi_i{}^\alpha$ are defined by Eq. (4·1·6) and K is defined by

$$\langle\mathcal{A}_i'\{\delta(\xi_i-a_i)\phi_i\}\,|\mathcal{A}_j'\{\delta(\xi_j-b_j)\phi_j\}\rangle=(1-K)_{ij}(a_i,b_j). \tag{4·3·24}$$

We can also express P as

$$P=\sum_\alpha|\Phi_\alpha\rangle\langle\Phi_\alpha|=\sum_i\int da_i|\Phi^{ia_i}\rangle\langle\Phi^{ia_i}|, \tag{4·3·25}$$

where Φ_α is defined by Eq. (4·1·7) and Φ^{ia_i} is defined by

$$\Phi^{ia_i}\equiv\sum_k\mathcal{A}_k'\{(1-K)_{ki}^{-1/2}(\xi_k,a_i)\,\phi_k\}. \tag{4·3·26}$$

$\{\Phi^{ia_i}\}$ constitutes an orthonormal basis set, satisfying

$$\langle \Phi^{ia_i} | \Phi^{jb_j} \rangle = \delta_{ij} \cdot \delta(a_i - b_i). \qquad (4\cdot3\cdot27)$$

4.3.b. *Norm kernel with unequal oscillator widths and almost forbidden states*

Here we discuss some aspects of norm kernel of the system of clusters, whose oscillator parameters are mutually different. The eigen-value problem of such system is no more solvable analytically in general, and we need to rely upon the numerical procedure. A characteristic difference of the case of unequal oscillator parameters from the case of equal ones is the disappearance of the forbidden states (F.S.) which are defined as the eigen-states of the norm kernel belonging to the zero eigen-value $\mu_\alpha = 0$.

When we use the reasonable values of the oscillator widths for clusters, the situation is not so much different from the case of equal oscillator widths and so we have the eigen-values μ_α which are very near zero and which approach to zero continuously if we continuously change the oscillator widths to the same limiting value $\nu = \nu_1 = \nu_2 = \cdots$. The eigen-functions belonging to these almost zero eigen-values are called the almost forbidden states (A.F.S.).[17] In order to catch the feeling we show some calculated examples. For the presentation of the calculated results we consider the dependence of the eigen-value μ_α on the oscillator parameters. The eigen-value μ_α is an overlap of the two wave functions and should therefore be dimensionless. When the system involves only one oscillator parameter ν whose dimension is fm^{-2}, μ_α cannot include ν in its expression in order to be dimensionless. Thus we know for the case where all the oscillator parameters of clusters are of the same value ν, the eigen-values μ_α do not depend on ν at all, as was in fact the case with the examples in § 4.2. The direct proof of this result is easy, if we notice the ν-dependence of the A-nucleon H.O. wave function Φ_α (which involves $\boldsymbol{X}_G$) is

$$\Phi_\alpha = \nu^{(3/4)A} \Phi_\alpha' (\sqrt{\nu}\boldsymbol{x}_1, \sqrt{\nu}\boldsymbol{x}_2, \cdots \sqrt{\nu}\boldsymbol{x}_A). \qquad (4\cdot3\cdot28)$$

The change of the integration variables from $\boldsymbol{x}_i$ to $\boldsymbol{y}_i \equiv \sqrt{\nu}\boldsymbol{x}_i$ in the calculation of the overlap of two such A-nucleon wave functions gives the expression of μ_α which does not include ν at all. If the two oscillator parameters ν_1 and ν_2 are involved in the system, μ_α can depend only on the dimensionless ratio (ν_1/ν_2). In Table III, we give the eigen-values*) μ_α of the systems, $\alpha + {}^{16}\mathrm{O}$ and $\alpha + {}^{40}\mathrm{Ca}$. The eigen-values $\mu_L{}^{\mathrm{AF}i}$ of the A.F.S. $\chi_L{}^{\mathrm{AF}i}$ are seen to be very small.

We below consider an illustrative system of two closed-shell clusters. The F.S. $\chi_L{}^{\mathrm{F}i}$ satisfy

$$\mathcal{A}\{\chi_L{}^{\mathrm{F}i}(r) h_L\} \equiv 0. \quad (i = 1 \sim n_L^{\mathrm{F}}) \qquad (4\cdot3\cdot29)$$

But for the A.F.S. $\chi_L{}^{\mathrm{AF}i}$, $\mathcal{A}\{\chi_L{}^{\mathrm{AF}i}(r) h_L\}$ no more vanish and so the corre-

*) These values are calculated by Dr. A. Tohsaki-Suzuki.

sponding normalized wave functions

$$\Phi_L^{\mathrm{AF}i} \equiv \frac{1}{\sqrt{\binom{A}{N_1}\mu_L^{\mathrm{AF}i}}} \mathcal{A}\{\chi_L^{\mathrm{AF}i}(r)\, h_L\}, \quad (i=1\sim n_L^F) \qquad (4\cdot3\cdot30)$$

are the members of the basis states of the cluster model space, as was discussed in § 4.1. Let us divide the eigen-functions into the A.F.S. $\chi_L^{\mathrm{AF}i}$ and other

Table III. Eigen-values of the norm kernels of the systems, (a) $^{16}O+\alpha$ and (b) $^{40}Ca+\alpha$, in the two cases of the equal and unequal oscillator widths of clusters. Superfices denote minus power of 10, for example, $0.3265^6=0.3265\times10^{-6}$.

(a) $^{16}O+\alpha$

N	$\nu_\alpha=\nu_o$	$\nu_\alpha/\nu_o=1.47$ L				
		0	2	4	6	8
0		0.3265^6				
2		0.1117^4	0.6202^5			
4		0.6617^3	0.2997^3	0.1773^3		
6		0.1345^1	0.1234^1	0.9913^2	0.6197^2	
8	0.2292	0.2391	0.2384	0.2366	0.2339	0.2302
10	0.5103	0.5131	0.5127	0.5119	0.5105	0.5088
12	0.7185	0.7163	0.7161	0.7159	0.7154	0.7147
14	0.8459	0.8424	0.8423	0.8422	0.8420	0.8418
16	0.9178	0.9146	0.9146	0.9146	0.9145	0.9144
18	0.9568	0.9545	0.9545	0.9545	0.9545	0.9544
20	0.9775	0.9760	0.9760	0.9760	0.9760	0.9760
22	0.9884	0.9875	0.9875	0.9875	0.9875	0.9875
24	0.9941	0.9935	0.9935	0.9935	0.9935	0.9935
26	0.9970	0.9966	0.9966	0.9966	0.9966	0.9966
N		1	3	5	7	9
1		0.1341^5				
3		0.4780^4	0.2784^4			
5		0.1431^2	0.1111^2	0.8070^3		
7		0.2726^1	0.2597^1	0.2370^1	0.2041^1	
9	0.3438	0.3518	0.3513	0.3505	0.3494	0.3479
11	0.6196	0.6179	0.6177	0.6174	0.6170	0.6164
13	0.7900	0.7861	0.7860	0.7858	0.7856	0.7854
15	0.8871	0.8834	0.8834	0.8833	0.8832	0.8831
17	0.9403	0.9375	0.9375	0.9375	0.9374	0.9374
19	0.9688	0.9669	0.9669	0.9669	0.9669	0.9669
21	0.9839	0.9827	0.9826	0.9826	0.9826	0.9826
23	0.9917	0.9910	0.9910	0.9910	0.9910	0.9910
25	0.9958	0.9953	0.9953	0.9953	0.9953	0.9953
27	0.9979	0.9976	0.9976	0.9976	0.9976	0.9976

(b) $^{40}Ca+\alpha$

N	$\nu_\alpha=\nu_{Ca}$	$\nu_\alpha/\nu_{Ca}=2.0$ L						
		0	2	4	6	8	10	12
0		0.1580^6						
2		0.6685^5	0.9303^5					
4		0.3433^4	0.3717^4	0.5443^4				
6		0.2892^3	0.3090^3	0.4123^3	0.3021^3			
8		0.2768^2	0.2836^2	0.2950^2	0.2758^2	0.1850^2		
10		0.2202^1	0.2167^1	0.2081^1	0.1924^1	0.1662^1	0.1266^1	
12	0.6914^1	0.1124	0.1117	0.1100	0.1073	0.1034	0.9809^1	0.9129^1
14	0.2641	0.2896	0.2890	0.2877	0.2856	0.2826	0.2787	0.2739
16	0.4751	0.4794	0.4790	0.4782	0.4768	0.4750	0.4726	0.4696
18	0.6479	0.6395	0.6392	0.6387	0.6379	0.6368	0.6354	0.6337
20	0.7728	0.7593	0.7592	0.7589	0.7585	0.7578	0.7570	0.7561
22	0.8571	0.8433	0.8432	0.8431	0.8428	0.8425	0.8420	0.8415
24	0.9117	0.8998	0.8997	0.8996	0.8995	0.8993	0.8991	0.8988
26	0.9462	0.9368	0.9367	0.9367	0.9366	0.9365	0.9363	0.9362
28	0.9676	0.9607	0.9605	0.9605	0.9604	0.9604	0.9603	0.9602
30	0.9806	0.9760	0.9757	0.9756	0.9755	0.9755	0.9755	0.9754
N		1	3	5	7	9	11	13
1		0.1547^5						
3		0.1309^4	0.2179^4					
5		0.9950^4	0.1219^3	0.1179^3				
7		0.8103^3	0.8838^3	0.9271^3	0.6984^3			
9		0.6611^2	0.6634^2	0.6520^2	0.5897^2	0.4371^2		
11		0.4331^1	0.4244^1	0.4074^1	0.3803^1	0.3400^1	0.2843^1	
13	0.1573	0.1924	0.1915	0.1896	0.1869	0.1832	0.1783	0.1722
15	0.3723	0.3858	0.3851	0.3838	0.3818	0.3791	0.3758	0.3716
17	0.5675	0.5641	0.5637	0.5628	0.5616	0.5600	0.5579	0.5555
19	0.7161	0.7043	0.7040	0.7035	0.7028	0.7018	0.7007	0.6993
21	0.8193	0.8052	0.8051	0.8048	0.8044	0.8039	0.8032	0.8025
23	0.8875	0.8744	0.8743	0.8742	0.8740	0.8737	0.8733	0.8729
25	0.9310	0.9203	0.9202	0.9201	0.9200	0.9198	0.9196	0.9194
27	0.9582	0.9500	0.9499	0.9499	0.9498	0.9497	0.9496	0.9495
29	0.9749	0.9690	0.9689	0.9689	0.9688	0.9688	0.9687	0.9687
31	0.9851	0.9813	0.9810	0.9809	0.9808	0.9808	0.9807	0.9807

normal states χ_L^{Nj}. In the limit of $\nu_1\to\nu_2$, $\chi_L^{AFi}\to\chi_L^{Fi}$ and $\chi_L^{Nj}\to\chi_L^{Aj}$, where χ_L^{Aj} are the allowed eigen-states belonging to the eigen-value $\mu_{Aj}\neq 0$ in the equal oscillator width limit. In this limiting process we also have $\{\binom{A}{N_1}\mu_L^{Nj}\}^{-1/2}\times\mathcal{A}\{\chi_L^{Nj}h_L\}\to\{\binom{A}{N_1}\mu_{Aj}\}^{-1/2}\mathcal{A}\{\chi_L^{Aj}h_L\}$. But, as for the states χ_L^{AFi} there are no corresponding limit states since $\mathcal{A}\{\chi_L^{Fi}h_L\}\equiv 0$. The limit states of Φ_L^{AFi} are out of the cluster model space composed of clusters with the common oscillator widths, since this space is spanned by the complete orthonormal

basis states $\{\binom{A}{N_1}\mu_{Aj}\}^{-1/2}\mathcal{A}\{\chi_L{}^{Aj}h_L\}$. This fact can be checked also in the following way[76]:

$$\lim_{\nu_1\to\nu_2}\langle h_L|\Phi_L{}^{\mathrm{AF}i}\rangle=\frac{1}{\sqrt{\binom{A}{N_1}}}\lim_{\nu_1\to\nu_2}\sqrt{\mu_L{}^{\mathrm{AF}i}}\chi_L{}^{\mathrm{AF}i}=0\,. \tag{4·3·31}$$

We expand $\chi_L{}^{\mathrm{AF}i}(r)$ in terms of $R_{NL}(r,\gamma)$ where $\gamma\equiv(N_1N_2/A)\nu_2$,

$$\chi_L{}^{\mathrm{AF}i}(r)=\sum_N C_{iN}R_{NL}(r,\gamma)\,.\quad(\sum_N|C_{iN}|^2=1) \tag{4·3·32}$$

C_{iN} satisfy

$$\lim_{\nu_1\to\nu_2}C_{iN}=0\quad\text{for}\quad N\geqq N_A\,, \tag{4·3·33}$$

where N_A is the lowest allowed number of the oscillator quanta in the equal oscillator width limit, namely for $N<N_A$, $\mu_N=0$ and for $N\geqq N_A$, $\mu_N\neq0$. Equation (4·3·33) is proved as follows:

$$\begin{aligned}0&=\lim_{\nu_1\to\nu_2}\mu_L{}^{\mathrm{AF}i}=\lim_{\nu_1\to\nu_2}\langle\chi_L{}^{\mathrm{AF}i}h_L|\mathcal{A}\{\chi_L{}^{\mathrm{AF}i}h_L\}\rangle\\&=\lim_{\nu_1\to\nu_2}\sum_{N_1N_2}C^*_{iN_1}C_{iN_2}\langle R_{N_1L}(r,\gamma)h_L|\mathcal{A}\{R_{N_2L}(r,\gamma)h_L\}\rangle\\&=\sum_N(\lim_{\nu_1\to\nu_2}|C_{iN}|^2)\cdot\mu_N\,.\end{aligned} \tag{4·3·34}$$

By Eq. (4·3·32) we have

$$\begin{aligned}\Phi_L{}^{\mathrm{AF}i}&=\sum_N C_{iN}\sqrt{\frac{\delta_{NL}}{\mu_L{}^{\mathrm{AF}i}}}\Phi_{NL}\,,\\\Phi_{NL}&\equiv\left\{\binom{A}{N_1}\delta_{NL}\right\}^{-1/2}\mathcal{A}\{R_{NL}(r,\gamma)h_L\}\,,\end{aligned} \tag{4·3·35}$$

where δ_{NL} is defined by

$$\delta_{NL}\equiv\langle R_{NL}(r,\gamma)h_L|\mathcal{A}\{R_{NL}(r,\gamma)h_L\}\rangle, \tag{4·3·36}$$

by which $\|\{\binom{A}{N_1}\delta_{NL}\}^{-1/2}\mathcal{A}\{R_{NL}h_L\}\|=1$. The values of $\lim_{(\nu_1\to\nu_2)}C_{iN}\sqrt{\delta_{NL}/\mu_L{}^{\mathrm{AF}i}}$ cannot be singular since $\|\Phi^{\mathrm{AF}i}\|=\|\Phi_{NL}\|=1$, namely,

$$\lim_{\nu_1\to\nu_2}C_{iN}\sqrt{\frac{\delta_{NL}}{\mu_L{}^{\mathrm{AF}i}}}=0\quad\text{or finite.} \tag{4·3·37}$$

In order to see $\lim_{(\nu_1\to\nu_2)}\Phi_{NL}$, we expand $\phi_0(C_1,\nu_1)$ as follows:

$$\begin{aligned}\phi_0(C_1,\nu_1)&=\sum_n(\nu_1-\nu_2)^n\phi_0{}^{(n)}(C_1,\nu_2)\,,\\\phi_0{}^{(n)}(C_1,\nu_2)&=\frac{1}{n!}(\partial/\partial\nu_2)^n\phi_0(C_1,\nu_2)\,.\end{aligned} \tag{4·3·38}$$

We notice the $\phi_0{}^{(n)}(C_1,\nu_2)$ has at most $2n$-$\hbar\omega_2$ higher quanta than $\phi_0(C_1,\nu_2)$ ($\nu_2=m\omega_2/2\hbar$). The reason is easily understood from the form of the H.O.

shell model wave function $\phi_0(C_1, \nu_2)$

$$\phi_0(C_1, \nu_2) = \nu_2^{(3/4)(N_1-1)} \times \begin{pmatrix} \text{polynomial of } \sqrt{\nu_2}x_i \\ \text{whose degree is } n \end{pmatrix} \times \exp\left(-\nu_2 \sum_{i \in C_1} (\boldsymbol{x}_i - \boldsymbol{X}_1)^2\right). \tag{4·3·39}$$

By inserting Eq. (4·3·37) into Φ_{NL}, we have

$$\mathcal{A}\{R_{NL}(r, \gamma) h_L\} = \sum_{2n+\overline{N} \geq N_A} (\nu_1 - \nu_2)^n \mathcal{A}\{R_{NL}(r, \gamma) h_L{}^{(n)}(\nu_2)\},$$

$$\delta_{NL} = (\nu_1 - \nu_2)^{(N_A-N)} OV_{NL}\left(\frac{N_A - N}{2}\right) + \sum \begin{pmatrix} \text{higher power of} \\ (\nu_1 - \nu_2) \text{ than } ((N_A-N)/2) \end{pmatrix},$$

$$h_L{}^{(n)}(\nu_2) \equiv Y_{L0}(\hat{r}) \phi_0{}^{(n)}(C_1, \nu_2) \phi_0(C_2, \nu_2),$$

$$OV_{NL}(n) = \langle R_{NL}(r, \gamma) h_L{}^{(n)}(\nu_2) | \mathcal{A}\{R_{NL}(r, \gamma) h_L{}^{(n)}(\nu_2)\} \rangle . \tag{4·3·40}$$

Thus we get

$$\lim_{\nu_1 \to \nu_2} \Phi_{NL} = \frac{1}{\sqrt{\binom{A}{N_1} OV_{NL}(n_0)}} \mathcal{A}\{R_{NL}(r, \gamma) h_L{}^{(n_0)}(\nu_2)\},$$

$$n_0 = (N_A - N)/2 . \tag{4·3·41}$$

If $OV_{NL}((N_A-N)/2) = 0$ and $OV_{NL}((N_A-N)/2+1) \neq 0$, we only need to put $n_0 = (N_A-N)/2+1$ in Eq. (4·3·41). From Eqs. (4·3·33), (4·3·37) and (4·3·41), we know that the limit states $\lim_{(\nu_1 \to \nu_2)} \Phi_L{}^{\mathrm{AF}i}$ generally have the same total number of the oscillator quanta as the lowest basis state of the cluster model space, $\{\binom{A}{N_1} \mu_{N_A}\}^{-1/2} \mathcal{A}\{R_{N_AL}(r, \gamma) \phi_0(C_1, \nu_2) \phi_0(C_2, \nu_2)\}$, if $OV_{NL}((N_A-N)/2) \neq 0$ for some $N \leqq N_A$ for which $\lim_{(\nu_1 \to \nu_2)} C_{iN} (\delta_{NL}/\mu_L{}^{\mathrm{AF}i})^{1/2} \neq 0$. Namely, for example, for $\alpha + {}^{16}\mathrm{O}$ system, the limit states of $\Phi_L{}^{\mathrm{AF}i}$ are expected to be of the $(\mathrm{sd})^4$ configuration, under the above mentioned conditions.

For more detailed discussion of A.F.S. especially in the dynamical problems, related to the Levinson theorem, the foundation of OCM and others, see Chap. II and also Refs. 17), 76).

4.3.c. *Relation of the cluster model states with the shell model states*

The inter-relation between cluster model space and shell model space has long been discussed by many authors. Wildermuth[36] and Sheline,[77] Bayman and Bohr,[72] and Horie[78] have investigated the relation between the RGM wave functions with the H.O. relative wave functions (which may be called the Wildermuth wave functions) and the shell model wave functions. When the number of the H.O. quanta of the relative wave function is small, seemingly different wave functions of the cluster model and the SU_3 shell model were found to be equivalent. This is due to the Pauli principle. We are now able to construct the (orthonormal) basis wave functions of the various cluster model spaces, which are classified by the H.O. quanta and SU_3 labels. The

comparison of the two model spaces have shown that many important shell model configurations are contained in the cluster model space, as is displayed for example, in Ref. 15) and Table IV. In the $^{12}C+\alpha$ system in Ref. 15), the cluster model state with $N=4$, $(\lambda, \mu)=(0, 0)$ is just the closed-shell state, the ones with $N=5$, $(\lambda, \mu)=(2, 1)$ are the $1p$-$1h$ $(T=0)$ states, the ones with $N=8$, $(\lambda, \mu)=(8, 4)$ are the most deformed $4p-4h$ states and so on. In the case of the $^{12}C+2\alpha$ system of Table IV, the states with $N=12$, $(\lambda, \mu)=(8, 0)$, $(4, 2)$, $(0, 4)$ are equivalent to the shell model states $(sd)^4[4]$, $(\lambda, \mu)=(8, 0)$, $(4, 2)$, $(0, 4)$, the ones with $N=13$, $(\lambda, \mu)=(8, 2)$ are the so-called $0p$-hole states with $(8, 2)$ symmetry and so on.

On the other hand Perring and Skyrme,[79] and Brink[18] have discussed the connection of the shell model wave functions with the cluster model wave functions with geometrical cluster arrangements. In the case of Brink model, the cluster model wave functions are the GCM ones discussed in § 2. The Brink wave functions or the generating wave functions of GCM use the coherent states of the H.O. quanta for the relative motion (see § 2.1.b) in contrast to the Wildermuth wave functions with definite number of H.O. quanta. Brink has showed how the normalized cluster intrinsic states with various geometrical configurations are connected with the intrinsic states of the SU_3 shell model wave functions of the ground or many-particle many-hole states in the limit of vanishing GC, $\boldsymbol{S}_i \to 0$. To see the limits, the H.O. expansion of $\Gamma(\boldsymbol{\xi}_i, \boldsymbol{S}_i, \gamma_i)$ (or equivalently power series expansion with respect to $\boldsymbol{S}_i$ of $\Gamma(\boldsymbol{\xi}_i, \boldsymbol{S}_i, \gamma_i)$) is useful. For details especially about the limiting process of the orthogonal single-particle orbitals in the cluster intrinsic states, see Ref. 18). (See also Refs. 80) and 81).)

§ 5. Calculation of OCM operators

5.1. OCM operators

The framework of the orthogonality condition model (OCM) of Saito[60] demands to calculate the projection operator onto the allowed states and the effective potentials between clusters.

For the system with the wave functions of Eq. (4·1·1), the OCM equation is (see Chap. II)

$$\sqrt{1-K}(E-T-V_{\text{eff}})\sqrt{1-K}\{\chi_l\}=0\,, \qquad (5\cdot1\cdot1)$$

namely

$$\sum_{jkl}(\sqrt{1-K})_{ij}(E-T-V_{\text{eff}})_{jk}(\sqrt{1-K})_{kl}\chi_l=0\,, \qquad (5\cdot1\cdot2)$$

where $(E-T)$ is diagonal; $(E-T)_{jk}=(E_j-T_j)\cdot\delta_{jk}$. If we introduce $\{\Omega_k\}$ by (see Eq. (4·3·20)),

$$\{\Omega_k\} = \sqrt{1-K}\{\chi_l\}, \tag{5·1·3}$$

we can rewrite Eq. (5·1·1) as

$$\Lambda(E-T-V_{\text{eff}})\Lambda\{\Omega_l\} = 0, \tag{5·1·4}$$

where Λ is the projection operator onto allowed states,

$$\Lambda = \sum_{\mu_\alpha \neq 0} |\{\chi_k{}^\alpha\}\rangle\langle\{\chi_l{}^\alpha\}|. \tag{5·1·5}$$

Equation (5·1·1) means to approximate the RGM kernel of the Hamiltonian H as follows:[17),82),83),92)]

$$\begin{aligned}&\langle \mathcal{A}_i'\{\delta(\xi_i-a_i)\phi_i\}|(H-\widehat{E}_i\delta_{ij})|\mathcal{A}_j'\{\delta(\xi_j-b_j)\phi_j\}\rangle \\ &\quad\approx\{\sqrt{1-K}(T+V_{\text{eff}})\sqrt{1-K}\}_{ij}(a_i,b_j), \\ &\widehat{E}_i = \text{internal binding energy of the } i\text{-channel.}\end{aligned} \tag{5·1·6}$$

The knowledge of the solution of the eigen-value problem of the norm kernel is sufficient to construct the operators $\sqrt{1-K}$ or Λ. But when we treat the complicated systems like as the channel coupling systems and the multi-cluster systems, the eigen-value problem of the norm kernel becomes fairly tedious to solve. The purpose of this section is to give the methods[63)] of the construction of the operator Λ which avoid solving the eigen-value problem of the norm kernel. The oscillator parameters of the clusters are assumed to be the same mutually.

As for the effective interaction V_{eff}, it is usually assumed and sometimes checked by comparing with the results of the RGM (or GCM) calculations that the RGM direct interaction kernel can give a good approximation to V_{eff} if we introduce suitable modification if necessary. The evaluation methods of the RGM direct interaction kernel are discussed in § 3 and so we do not enter this problem of the direct potential here. Recently Friedrich and Canto[84)] have searched V_{eff} in the two closed-shell cluster systems assuming the superposition of the several range Gaussian potentials for the form of V_{eff}. The parameters of V_{eff} are so determined as to make the approximation of Eq. (5·1·6) as good as possible. In actual calculation they utilize the GCM matrix elements of both the sides of Eq. (5·1·6). We here study a little how good the approximation of Eq. (5·1·6) is for the case of the kinetic energy operator in the two closed-shell cluster systems. The exact kernel in the H.O. representation is given in Eq. (4·2·5), while we have

$$\langle V_{Nl}\sqrt{1-K}\,T_r\sqrt{1-K}V_{N'l}\rangle = \sqrt{\mu_N\mu_{N'}}\langle V_{Nl}T_rV_{N'l}\rangle. \tag{5·1·7}$$

Thus we know that for $N=N'$ our approximation gives an exact answer while for $N=N'+2$ the error of the approximation is

$$(1-\sqrt{\mu_{N-2}/\mu_N})\times\sqrt{\mu_N\mu_{N-2}}(\hbar\omega/4)\sqrt{(N-l)(N+l+1)},$$

which is small if μ_N changes slowly as a function of N.

5.2. Construction of the allowed states

5.2.a. *Two-cluster system*

The allowed states of the single channel two-cluster system can be known usually with ease without explicitly solving the eigen-value problem of the norm kernel. Let us denote by $N(A)$ the lowest possible total number of the H.O. quanta of the A-nucleon H.O. wave function. Since the total number of the H.O. quanta of $\mathcal{A}\{V_{Nlm}(r,\gamma)\phi_0(C_1)\phi_0(C_2)\}$ is $N+N(C_1)+N(C_2)$, N should be $N\geqq Nd$, where $Nd\equiv N(A)-N(C_1)-N(C_2)$, for V_{Nlm} to be an allowed state. ($N(C_i)$ is the total number of the H.O. quanta of $\phi_0(C_i)$ as was defined in Eq. (4·2·6)). Thus, the condition $N\geqq Nd$ is a necessary condition for V_{Nlm} to be allowed. Usually this condition $N\geqq Nd$ is also a sufficient one for the allowed states. We know some cases where this condition is insufficient, but even then with some more careful examination, we usually get a correct sufficient condition for the allowed states. For example, Nd of $^{16}O+^{16}O$ is 20, while the correct condition for V_{Nlm} to be allowed is $N\geqq 24$. The reason why $N=20, 22$ are forbidden numbers is easily given by considering the conservation of the number of the H.O. quanta in each x, y and z direction. As another example, Nd of $3N+N$ system with $T=0$ is 0, but V_{Nlm} with $N=1$ is forbidden. The reason is that the 1-$\hbar\omega$ excited states with $T=0$ in ^{4}He do not exist except the spurious state of the C.M. excitation.

When we treat the channel coupling two-cluster system, we have no more simple method as above to determine what states are allowed. So we need to solve the eigen-value problem of the norm kernel in general. In § 5.2.b, however, we will find that we have a method, for some kind of the channel coupling two-cluster systems, to construct the allowed states, which avoids calculating the norm kernel and solving it.

5.2.b. *Multi-cluster system*

First we consider the case where all the constituent clusters are SU_3 scalar. As a general property of the eigen-function of the norm kernel with non-zero eigen-value ($\mu_\alpha\neq 0$), we notice that they are orthogonal to all the "two-cluster forbidden states" between any two constituent clusters. Let $V_k^F(\boldsymbol{t}_{ij})$ be any two-cluster forbidden state between clusters C_i and C_j, satisfying $\mathcal{A}\{V_k^F(\boldsymbol{t}_{ij})\phi_0(C_i)\phi_0(C_j)\}\equiv 0$, where $\boldsymbol{t}_{ij}\equiv\boldsymbol{X}_i-\boldsymbol{X}_j$. Since there follows

$$\mathcal{A}\{V_k^F(\boldsymbol{t}_{ij})\phi_0(C_1)\cdots\phi_0(C_n)\}\equiv 0\,, \tag{5·2·1}$$

by combining this with

$$\langle\phi_0(C_1)\cdots\phi_0(C_n)|\mathcal{A}\{\chi^\alpha\phi_0(C_1)\cdots\phi_0(C_n)\}\rangle=\mu_\alpha\chi^\alpha\,, \tag{5·2·2}$$

we get

$$0\equiv\langle V_k^F(\boldsymbol{t}_{ij})\phi_0(C_1)\cdots\phi_0(C_n)|\mathcal{A}\{\chi^\alpha\phi_0(C_1)\cdots\phi_0(C_n)\}\rangle$$

$$=\mu_\alpha\langle V_k^F(\boldsymbol{t}_{ij})|\chi^\alpha\rangle, \qquad (5\cdot2\cdot3)$$

which means that for $\mu_\alpha\neq0$, $\langle V_k^F(\boldsymbol{t}_{ij})|\chi^\alpha\rangle=0$. We introduce the notation $N^F(i,j)$ which expresses the set of all the forbidden numbers of the H.O. quanta between clusters C_i and C_j; namely for $N\in N^F(i,j)$, $\mathcal{A}\{V_{Nlm}(\boldsymbol{t}_{ij})\phi_0(C_i)\times\phi_0(C_j)\}\equiv0$.

Now let us define a functional space H_n', which is spanned by the multi-cluster relative wave functions that are orthogonal to all the two-cluster forbidden states $V_k^F(\boldsymbol{t}_{ij})$ between any two constituent clusters. If we denote by H_n the space spanned by all the allowed states (or eigen-functions with $\mu_\alpha\neq0$), the above argument shows that this space H_n is contained in H_n'; $H_n\subset H_n'$. We here introduce a hypothesis[63] that $H_n=H_n'$. This hypothesis was shown to be true for 3α and $^{16}\mathrm{O}+2\alpha$ systems by constructing H_n and H_n' explicitly and then by comparing them. What we discuss here is the construction method of H_n', which, according to this hypothesis, is equivalent to the construction of the allowed states.

Even if $H_n\neq H_n'$, the space H_n' has its own significance. To solve the many-body Schrödinger equation within the space H_n' where the interaction operator is given by the sum of pair interactions between clusters $\sum_{i>j}V_{\mathrm{eff}}^{(ij)}(\boldsymbol{t}_{ij})$, namely to solve

$$\Lambda'(E-T-\textstyle\sum_{i>j}V_{\mathrm{eff}}^{(ij)}(\boldsymbol{t}_{ij}))\Lambda'\Omega'=0 \qquad (5\cdot2\cdot4)$$

with Λ' denoting the projection operator onto H_n', is just equivalent to solving the many-body Schrödinger equation where the interaction process between any two constituent clusters is described by the two-cluster OCM, $\Lambda_{ij}(E-T_{ij}-V_{\mathrm{eff}}^{(ij)}(\boldsymbol{t}_{ij}))\Lambda_{ij}\Omega_{ij}=0$.[63,85,86]

Neudatchin and his coworkers[87] have proposed a method to treat Eq. (5·2·4) which does not construct Λ' explicitly. They introduce pseudo potentials $\lambda\sum_k|V_k^F(\boldsymbol{t}_{ij})\rangle\langle V_k^F(\boldsymbol{t}_{ij})|$ in addition to the original interaction $V_{\mathrm{eff}}^{(ij)}(\boldsymbol{t}_{ij})$ for each pair (i,j) and solve the many-body Schrödinger equation without Λ'. The stable finite solutions in letting $\lambda\to\infty$ are the desired answer whose wave functions are surely orthogonal to all the two-cluster forbidden states.*)

Our construction method[63] of the basis states of H_n' of n-cluster system is based on the concept of the "coefficient of fractional parentage" (cfp). We first construct the basis states of H_3' of three-cluster system on the basis of the knowledge of the two-cluster allowed states. Then we construct the basis states of H_4' of four-cluster system using the knowledge of H_3', and so on.

We expand the state $\chi_{J\alpha}(n)$ of H_n' by the basis states $\chi_{L\beta}(n-1)$ of H_{n-1}' as follows:

$$\chi_{J\alpha}(n)=\sum_{L\beta N_1l_1}C^{(n)}(J\alpha|L\beta N_1l_1)[V_{N_1l_1}(\boldsymbol{s}_n)\chi_{L\beta}(n-1)]_J,$$

*) The same idea as that of Neudatchin et al. has also been proposed by Saito et al. The point of this method is how to get the numerical stability of the practical calculation in letting $\lambda\to\infty$.

$$\boldsymbol{s}_n \equiv \boldsymbol{X}_n - \boldsymbol{X}_G(n-1), \tag{5·2·5}$$

where $\boldsymbol{X}_n$ and $\boldsymbol{X}_G(n-1)$ are the center-of-mass (C.M.) coordinates of the n-th cluster and $(n-1)$-cluster system, respectively. Since all the basis states $\chi_{L\beta}(n-1)$ of H'_{n-1} are assumed to be already known, our task is to calculate the cfp $C^{(n)}(J\alpha|L\beta N_1 l_1)$. The cfp are determined by the orthogonality condition of $\chi_{J\alpha}(n)$ to all the two-cluster forbidden states between constituent two clusters. In $\chi_{L\beta}(n-1)$, all the two-cluster forbidden states between any two clusters in the $(n-1)$-cluster system are already eliminated, and so what is remained to do is the elimination of the two-cluster forbidden states between the n-th cluster C_n and the cluster $C_i\,(1\leqq i\leqq n-1)$ in the $(n-1)$-cluster system. For this purpose we expand $\chi_{L\beta}(n-1)$ by the basis states $\chi_{P\gamma}(n-2)$ of H'_{n-2} of the $(n-2)$-cluster system just as in Eq. (5·2·5) with the use of the cfp $C_i^{(n-1)}(L\beta|P\gamma N_2 l_2)$ which are assumed to be already known; $\chi_{L\beta}(n-1) = \sum_{P\gamma N_2 l_2} C_i^{(n-1)}(L\beta|P\gamma N_2 l_2)\,[V_{N_2 l_2}(\boldsymbol{s}_i)\,\chi^i_{P\gamma}(n-2)]_L$ where $\boldsymbol{s}_i \equiv \boldsymbol{X}_i - \boldsymbol{X}_G^{\,i}(n-2)$, $1\leqq i\leqq n-1$ with $\boldsymbol{X}_G^{\,i}(n-2)$ denoting the C.M. coordinate of the $(n-2)$-cluster system composed of the clusters $C_j\,(1\leqq j\leqq n-1)$ except C_i. Then $\chi_{J\alpha}(n)$ can be written as follows:

$$\begin{aligned}
\chi_{J\alpha}(n) &= \sum_{L\beta N_1 l_1} C^{(n)}(J\alpha|L\beta N_1 l_1) \sum_{P\gamma N_2 l_2} C_i^{(n-1)}(L\beta|P\gamma N_2 l_2) \\
&\quad \times [V_{N_1 l_1}(\boldsymbol{s}_n)\,[V_{N_2 l_2}(\boldsymbol{s}_i)\,\chi^i_{P\gamma}(n-2)]_L]_J \\
&= \sum_{\substack{L\beta N_1 l_1 \\ P\gamma N_2 l_2}} C^{(n)}(J\alpha|L\beta N_1 l_1)\, C_i^{(n-1)}(L\beta|P\gamma N_2 l_2) \sum_Q \sqrt{(2L+1)\,(2Q+1)} \\
&\quad \times W(l_1 l_2 JP; QL)\,[V^{N_1 N_2}_{l_1 l_2 Q}(\boldsymbol{s}_n, \boldsymbol{s}_i)\,\chi^i_{P\gamma}(n-2)]_J,
\end{aligned} \tag{5·2·6}$$

where $V^{N_1 N_2}_{l_1 l_2 Q}$ is defined in Eq. (4·1·43). By using the Talmi-Moshinsky-Smirnov (TMS) coefficient we express $V^{N_1 N_2}_{l_1 l_2 Q}(\boldsymbol{s}_n, \boldsymbol{s}_i)$ of $\boldsymbol{s}_n$, $\boldsymbol{s}_i$ coordinates by the linear combination of the H.O. functions of the coordinates $\boldsymbol{s}_{ni} \equiv (M_n \boldsymbol{X}_n + M_i \boldsymbol{X}_i)/(M_n + M_i) - \boldsymbol{X}_G^{\,i}(n-2)$ and $\boldsymbol{t}_{ni} \equiv \boldsymbol{X}_n - \boldsymbol{X}_i$ as $V^{N_1 N_2}_{l_1 l_2 Q}(\boldsymbol{s}_n, \boldsymbol{s}_i) = \sum_{N_3 l_3 N_4 l_4} \times \langle N_1 l_1 N_2 l_2 | N_3 l_3 N_4 l_4, Q\rangle_{\theta_i} \cdot V^{N_3 N_4}_{l_3 l_4 Q}(\boldsymbol{s}_{ni}, \boldsymbol{t}_{ni})$ where θ_i is the angle of the TMS transformation $(\boldsymbol{s}_n, \boldsymbol{s}_i) \to (\boldsymbol{s}_{ni}, \boldsymbol{t}_{ni})$ which is shown in Fig. 1. Then by putting zero every coefficient of $[V^{N_3 N_4}_{l_3 l_4 Q}(\boldsymbol{s}_{ni}, \boldsymbol{t}_{ni})\,\chi^i_{P\gamma}(n-2)]_J$ with $N_4 \in N^F(n, i)$, in order to guarantee the orthogonality of $\chi_{J\alpha}(n)$ to $V_{N_4 l_4}(\boldsymbol{t}_{ni})$ with $N_4 \in N^F(n, i)$, we get

$$\begin{aligned}
&\sum_{\substack{L\beta N_1 l_1 \\ N_2 l_2}} C^{(n)}(J\alpha|L\beta N_1 l_1)\, C_i^{(n-1)}(L\beta|P\gamma N_2 l_2) \sqrt{(2L+1)\,(2Q+1)} \\
&\quad \times W(l_1 l_2 JP; QL)\langle N_1 l_1 N_2 l_2 | N_3 l_3 N_4 l_4, Q\rangle_{\theta_i} = 0,
\end{aligned} \tag{5·2·7}$$

where $N_4 \in N^F(n,i)$, $1\leqq i\leqq n-1$, and P, γ, Q, N_3, l_3, l_4 are arbitrary possible values. Equation (5·2·7) shows that the cfp $C^{(n)}(J\alpha|L\beta N_1 l_1)$ of the n-cluster system are calculable successively from the knowledge of the cfp $C_i^{(n-1)}(L\beta|P\gamma N_2 l_2)$ of the $(n-1)$-cluster systems. The solutions $C^{(n)}(J\alpha|L\beta N_1 l_1)$ of

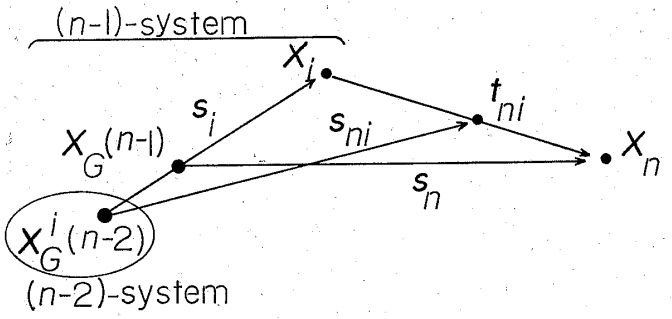

Fig. 1. Internal coordinates. $\boldsymbol{X}_G{}^i(n-2)$ is the C.M. coordinate of $(n-2)$ clusters excluding i-th and n-th clusters. $\boldsymbol{X}_G(n-1)$ is the C.M. coordinate of $(n-1)$ clusters except n-th cluster. $\boldsymbol{s}_n \equiv \boldsymbol{X}_n - \boldsymbol{X}^G(n-1)$, $\boldsymbol{s}_i \equiv \boldsymbol{X}_i - \boldsymbol{X}_G{}^i(n-2)$, are related to $\boldsymbol{t}_{ni} \equiv \boldsymbol{X}_n - \boldsymbol{X}_i$, $\boldsymbol{s}_{ni} \equiv (M_n\boldsymbol{X}_n + M_i\boldsymbol{X}_i)/(M_n+M_i) - \boldsymbol{X}_G{}^i(n-2)$ by the TMS transformation of the angle θ_i.

Eq. (5·2·7) are obtained as the eigen-vectors with the eigen-value $q_\alpha = 0$ of the following secular equation,

$$\sum_{L\beta N_1 l_1} Q^{(n)}(L'\beta' N_1' l_1' | L\beta N_1 l_1) C^{(n)}(J\alpha | L\beta N_1 l_1) = q_\alpha C^{(n)}(J\alpha | L'\beta' N_1' l_1'),$$

$$Q^{(n)}(L'\beta' N_1' l_1' | L\beta N_1 l_1) \equiv \sum_{i=1}^{n-1} \sum_{\substack{P\gamma Q N_2 l_3 l_4 \\ N_4 \in N^F(n,i)}} \omega(iP\gamma Q l_3 l_4 N_4 | L'\beta' N_1' l_1') \times \omega(iP\gamma Q l_3 l_4 N_4 | L\beta N_1 l_1),$$

$$\omega(iP\gamma Q l_3 l_4 N_4 | L\beta N_1 l_1) \equiv \sqrt{(2L+1)(2Q+1)} \sum_{N_2 l_2} C_i^{(n-1)}(L\beta | P\gamma N_2 l_2) \times W(l_1 l_2 JP; QL) \langle N_1 l_1 N_2 l_2 | N_3 l_3 N_4 l_4, Q \rangle_{\theta_i}. \qquad (5\cdot2\cdot8)$$

It is easy to show that the matrix elements $Q^{(n)}(L'\beta' N_1' l_1' | L\beta N_1 l_1)$ are just the matrix elements of the operator $Q^{(n)}$ defined in Eq. (5·2·9) by the functions $[V_{N_1 l_1}(\boldsymbol{s}_n)\chi_{L\beta}(n-1)]_J$ with fixed J;

$$Q^{(n)} \equiv \sum_{i=1}^{n-1} \sum_{N_4 \in N^F(n,i),\, l_4, m_4} |V_{N_4 l_4 m_4}(\boldsymbol{t}_{ni})\rangle\langle V_{N_4 l_4 m_4}(\boldsymbol{t}_{ni})|. \qquad (5\cdot2\cdot9)$$

Clearly $Q^{(n)}$ preserves the number of the H.O. quanta. So if $\chi_{L\beta}(n-1)$ have the definite number of the H.O. quanta, $\chi_{J\alpha}(n)$ also have the definite number of H.O. quanta.

The fact that the TMS (Talmi-Moshinsky-Smirnov) transformation preserved the Elliott SU_3 symmetry makes it possible to classify the elements of H_n' space by SU_3 group.[63),85),86)] Moreover what is important is that the introduction of SU_3 group greatly simplifies the construction process of the basis states of H_n' described above. We show this slightly in detail in the case of the three-cluster system. The cfp expansion of the basis states $\chi_{N(\lambda,\mu)\kappa J,p}$ of H_3' is written as

$$\chi_{N(\lambda,\mu)\kappa J,p} = \sum_{N_2 \in N^F(1,2)} \hat{A}_{p,N_2}^{N(\lambda,\mu)}(2)\, V_{N_1 N_2}^{N(\lambda,\mu)\kappa J}(\boldsymbol{s}_3, \boldsymbol{t}_{12}), \qquad (5\cdot2\cdot10)$$

where the cfp $\hat{A}^{N(\lambda,\mu)}_{p,N_2}(2)$ are to be identical with $A^{N(\lambda,\mu)}_{p,N_2}$ of Eq. (4·1·44) if $H_3'=H_3$, and $\boldsymbol{s}_3\equiv\boldsymbol{X}_3-(M_1\boldsymbol{X}_1+M_2\boldsymbol{X}_2)/(M_1+M_2)$. $V^{N(\lambda,\mu)\kappa J}_{N_1N_2}$ are defined in Eq. (4·1·43) and they transform under the TMS transformation as follows:

$$V^{N(\lambda,\mu)\kappa J}_{N_1N_2}(\boldsymbol{s}_3,\boldsymbol{t}_{12})=\sum_{N_3+N_4=N}\langle N_3N_4|N_1N_2,(\lambda,\mu)\rangle_{\theta_i}V^{N(\lambda,\mu)\kappa J}_{N_3N_4}(\boldsymbol{s}_i,\boldsymbol{t}_{jk}),\quad(5\cdot2\cdot11)$$

where $(i,j,k)=(1,2,3)$ or $(2,3,1)$ and θ_i is the angle of TMS transformation $(\boldsymbol{s}_3,\boldsymbol{t}_{12})\to(\boldsymbol{s}_i,\boldsymbol{t}_{jk})$. The reduced TMS coefficients $\langle N_3N_4|N_1N_2,\ (\lambda,\mu)\rangle_{\theta_i}$ do not depend on κ and J due to the SU_3 scalar property of TMS transformation. We substitute Eq. (5·2·11) into Eq. (5·2·10) and put zero every coefficient of $V^{N(\lambda,\mu)\kappa J}_{N_3N_4}(\boldsymbol{s}_i,\boldsymbol{t}_{jk})$ with $N_4\in N^F(j,k)$. This gives us the orthogonality equation of $\chi_{N(\lambda,\mu)\kappa J,p}$ to the two-cluster forbidden states $V_{N_4l_4m_4}(\boldsymbol{t}_{jk})$ with $N_4\in N^F(jk)$,

$$\sum_{N_2\notin N^F(1,2)}\hat{A}^{N(\lambda,\mu)}_{p,N_2}(2)\langle N_3N_4|N_1N_2,\ (\lambda,\mu)\rangle_{\theta_i}=0\,,\qquad(5\cdot2\cdot12)$$

where $N_4\in N^F(j,k)$, $(i,j,k)=(1,2,3)$, $(2,3,1)$. Equation (5·2·12) shows that $\hat{A}^{N(\lambda,\mu)}_{p,N_2}(2)$ do not depend on κ and J since $\langle N_3N_4|N_1N_2,\ (\lambda,\mu)\rangle_{\theta_i}$ do not depend on κ and J. To solve Eq. (5·2·12) is equivalent to obtaining the eigen-vectors with the zero eigenvalue $q_p=0$ of the following secular equation,

$$\sum_{N_2\notin N^F(1,2)}Q^{N(\lambda,\mu)}(N_1'N_2'|N_1N_2)\,\hat{A}^{N(\lambda,\mu)}_{p,N_2}(2)=q_p\hat{A}^{N(\lambda,\mu)}_{p,N_2'}(2),$$

$$Q^{N(\lambda,\mu)}(N_1'N_2'|N_1N_2)\equiv\sum_{i=1}^{2}\sum_{N_4\in N^F(j,k)}\langle N_3N_4|N_1'N_2',\ (\lambda,\mu)\rangle_{\theta_i}$$
$$\times\langle N_3N_4|N_1N_2,\ (\lambda,\mu)\rangle_{\theta_i}\,.\qquad(5\cdot2\cdot13)$$

We can easily show that $Q^{N(\lambda,\mu)}(N_1'N_2'|N_1N_2)$ are just the matrix elements of the operator $Q^{(3)}$ of Eq. (5·2·9) with $n=3$ by the functions $V^{N(\lambda,\mu)\kappa J}_{N_1N_2}(\boldsymbol{s}_3,\boldsymbol{t}_{12})$ with $N_2\notin N^F(1,2)$, $N_1+N_2=N$.

What are necessary for the practical treatment of the above procedure in SU_3 scheme are the simple and rapid evaluation of the SU_3 C-G coefficients $\langle(N_1\,0)\,l_1\,(N_2\,0)\,l_2\|\,(\lambda,\mu)\kappa J\rangle$ and the reduced TMS coefficients $\langle N_3N_4|N_1N_2,\ (\lambda,\mu)\rangle_\theta$. An answer to this problem is given by the quasi-spin $\boldsymbol{S}$ introduced by Bargmann and Moshinsky,[88]

$$S_+\equiv\boldsymbol{a}^\dagger(\boldsymbol{s}_3)\cdot\boldsymbol{a}(\boldsymbol{t}_{12}),\ S_-\equiv(S_+)^\dagger,\ S_z\equiv\tfrac{1}{2}(\boldsymbol{a}^\dagger(\boldsymbol{s}_3)\cdot\boldsymbol{a}(\boldsymbol{s}_3)-\boldsymbol{a}^\dagger(\boldsymbol{t}_{12})\cdot\boldsymbol{a}(\boldsymbol{t}_{12}))\,,$$
$$[S_+,S_-]=2S_z,\ \ [S_z,S_\pm]=\pm S_\pm\,,\qquad(5\cdot2\cdot14)$$

where $\boldsymbol{a}^\dagger(\boldsymbol{v})$ is the creation operator of the H.O. quanta of the coordinate $\boldsymbol{v}$; $\boldsymbol{a}^\dagger(\boldsymbol{v})=\sqrt{\gamma}\,(\boldsymbol{v}-(1/2\gamma)\,\partial/\partial\boldsymbol{v})$. By using the SU_3-scalar property of $\boldsymbol{S}$, we can easily show the following relations,[89]

$$\boldsymbol{S}^2V^{N(\lambda,\mu)\kappa J}_{N_1N_2}(\boldsymbol{s}_3,\boldsymbol{t}_{12})=j(j+1)\,V^{N(\lambda,\mu)\kappa J}_{N_1N_2}(\boldsymbol{s}_3,\boldsymbol{t}_{12}),$$
$$S_\pm V^{N(\lambda,\mu)\kappa J}_{N_1N_2}(\boldsymbol{s}_3,\boldsymbol{t}_{12})=\sqrt{(j\mp m)\,(j\pm m+1)}\,V^{N(\lambda,\mu)\kappa J}_{N_1\pm1,N_2\mp1}(\boldsymbol{s}_3,\boldsymbol{t}_{12}),$$
$$j=\lambda/2\,,\quad m=(N_1-N_2)/2\,.\qquad(5\cdot2\cdot15)$$

From this we obtain

$$\frac{1}{2}\sqrt{(\lambda\mp N_1\pm N_2)(\lambda\pm N_1\mp N_2+2)}\langle(N_1\pm1,0)l_1,\ (N_2\mp1,0)l_2\|(\lambda,\mu)\kappa J\rangle$$
$$=\sum_{l_1'l_2'}\langle(N_1,0)l_1',\ (N_2,0)l_2'\|(\lambda,\mu)\kappa J\rangle\langle V^{N_1\pm1,N_2\mp1}_{l_1l_2J}|S_\pm|V^{N_1N_2}_{l_1'l_2'J}\rangle,$$

$$\langle V^{N_1+1,N_2-1}_{l_1l_2J}|S_+|V^{N_1N_2}_{l_1'l_2'J}\rangle=(-)^{l_1+l_2'+J+1}W(l_1l_2l_1'l_2';J1)$$
$$\times\langle V_{N_1+1,l_1}\|a^\dagger\|V_{N_1,l_1'}\rangle\langle V_{N_2,l_2'}\|a^\dagger\|V_{N_2-1,l_2}\rangle,$$

$$\langle V_{N+1,l}\|a^\dagger\|V_{N,l'}\rangle=\begin{cases}\sqrt{(N+l'+3)(l'+1)}, & l=l'+1,\\ \sqrt{(N-l'+2)l'}, & l=l'-1,\end{cases}\qquad(5\cdot2\cdot16)$$

which we can use as the recursion formula to calculate the reduced C-G coefficients. The TMS coefficients are given simply by the familiar rotation matrix as[89]

$$\langle N_3N_4|N_1N_2,\ (\lambda,\mu)\rangle_\theta=d^j_{m'm}(\theta)\equiv\langle jm'|e^{-i\theta J_y}|jm\rangle,$$
$$j=\lambda/2,\ m'=(N_3-N_4)/2,\ m=(N_1-N_2)/2,\qquad(5\cdot2\cdot17)$$

which is due to the following relation,

$$e^{i\theta_iS_y}\begin{pmatrix}\boldsymbol{a}^\dagger(\boldsymbol{s}_3)\\ \boldsymbol{a}^\dagger(\boldsymbol{t}_{12})\end{pmatrix}e^{-i\theta_iS_y}=\begin{pmatrix}\cos\frac{\theta_i}{2} & -\sin\frac{\theta_i}{2}\\ \sin\frac{\theta_i}{2} & \cos\frac{\theta_i}{2}\end{pmatrix}\begin{pmatrix}\boldsymbol{a}^\dagger(\boldsymbol{s}_3)\\ \boldsymbol{a}^\dagger(\boldsymbol{t}_{12})\end{pmatrix}=\begin{pmatrix}\boldsymbol{a}^\dagger(\boldsymbol{s}_i)\\ \boldsymbol{a}^\dagger(\boldsymbol{t}_{jk})\end{pmatrix},\qquad(5\cdot2\cdot18)$$

where $\cos\theta_i/2=-\sqrt{M_iM_3/(M_1+M_2)(M_j+M_k)}$ and
$\sin\theta_i/2=\varepsilon_i\sqrt{M_j(M_1+M_2+M_3)/(M_1+M_2)(M_j+M_k)}$ with $\varepsilon_1=-1$ and $\varepsilon_2=+1$. For more detailed discussion and applications of the above mentioned procedure, see Ref. 63).

Our method described above to construct the allowed states of the system composed of the many SU_3-scalar clusters can be utilized to construct the allowed states of some kind of coupled channel systems including non-SU_3-scalar clusters. For the sake of explanation, we consider $^{20}\mathrm{Ne}+\alpha$ system where the ground band states of ^{20}Ne are described by the SU_3 shell model configuration $(\mathrm{sd})^4[4](8,0)$. The point of our method is to use the fact that this shell model wave function $\phi_L(^{20}\mathrm{Ne})$ is equivalent to the two-cluster wave function $1/\sqrt{\binom{20}{4}\mu_8}\mathcal{A}\{V_{8L}(\boldsymbol{t}_{O\alpha})\phi_0(^{16}\mathrm{O})\phi_0(\alpha)\}$. From the discussion of § 4.1.c, the orthonormal basis wave functions of this $^{20}\mathrm{Ne}+\alpha$ system should have definite SU_3 symmetry as

$$\Phi^N_{(\lambda,\mu)}=\frac{1}{\sqrt{\binom{24}{4}\mu^N_{(\lambda,\mu)}}}\mathcal{A}\{[V_{(N,0)}(\boldsymbol{r},\gamma)\phi_{(8,0)}(^{20}\mathrm{Ne})]_{(\lambda,\mu)\kappa J}\phi_0(\alpha)\}$$
$$=(\mathrm{const})\,\mathcal{A}\{V^{N+8(\lambda,\mu)\kappa J}_{N,8}(\boldsymbol{r},\boldsymbol{t}_{O\alpha})\phi_0(^{16}\mathrm{O})\phi_0(\alpha)\phi_0(\alpha)\}.\qquad(5\cdot2\cdot19)$$

For the allowed symmetry (λ, μ), $\mathcal{A}\{V^{N+8,(\lambda,\mu)K J}_{N,8}\phi_0(^{16}\mathrm{O})\phi_0(\alpha)\phi_0(\alpha)\}$ cannot vanish. This requires that $V^{N+8,(\lambda,\mu)K J}_{N,8}$ should have non-vanishing overlap with at least one allowed state of the three SU_3-scalar cluster system of $^{16}\mathrm{O}+\alpha+\alpha$. This condition for $V^{N+8,(\lambda,\mu)K J}_{N,8}$ is not only necessary but also sufficient for the symmetry (λ, μ) to be allowed in the $^{20}\mathrm{Ne}+\alpha$ system. From the form of $\chi_{N(\lambda,\mu)K J,p}$ of Eq. (5·2·10), we see that if the cfp $\hat{A}^{N+8,(\lambda,\mu)}_{p,N_2=8}(2)$ is non-zero at least for one p the symmetry (λ, μ) is an allowed quantum number in the $^{20}\mathrm{Ne}+\alpha$ system. Thus we can determine what (λ, μ) are allowed in some kind of the channel coupled systems without calculating the norm kernel and without solving the eigen-value problem of it.

Finally we discuss below the general construction procedure[90] of the allowed states of the multi-cluster system which includes non-SU_3-scalar clusters. We explain in the case of three-cluster system in which the cluster C_1 is described by a non-SU_3-scalar wave function with SU_3 symmetry (σ_0, τ_0) while C_2 and C_3 are SU_3-scalar. From the investigation of § 4.1.c, we know that we have three sets $N^A(1, i)$, $N^{PF}(1, i)$, $N^F(1, i)$ to which we classify the number of the H.O. quanta of the relative wave function between clusters C_1 and C_i $(i=2, 3)$. For $N\in N^A(1, i)$, $\mathcal{A}\{[V_{(N,0)}(\boldsymbol{t}_{1i})\phi_{(\sigma_0,\tau_0)}(C_1)]_{(\lambda,\mu)K J}\phi(C_i)\}$ with any (λ, μ) resulting from $(N, 0)\times(\sigma_0, \tau_0)$ are allowed (or non-vanishing), while for $N\in N^F(1, i)$ all (λ, μ) are forbidden, and for $N\in N^{PF}(1, i)$, (λ, μ) are divided into allowed and forbidden. In the case of $^{12}\mathrm{C}+\alpha$, $N^A(^{12}\mathrm{C}, \alpha)=\{N; N\geqq 8\}$, $N^{PF}(^{12}\mathrm{C}, \alpha)=\{N; 7\geqq N\geqq 4\}$ and $N^F(^{12}\mathrm{C}, \alpha)=\{N; N\leqq 3\}$. First we regard $N^{PF}(1, i)$ as if it were contained in $N^A(1, i)$ and construct the quasi-allowed state $\chi_{N(\sigma,\tau)\rho P,p}$ exactly following the prescription discussed above for the three SU_3-scalar cluster system. The truely-allowed three-cluster state $Z_{N(\lambda,\mu)K J,r}$ can be expanded by using these $\chi_{N(\sigma,\tau)\rho P,p}$ as follows:

$$Z_{N(\lambda,\mu)K J,r}=\sum_{(\sigma,\tau),p} H^{N(\lambda,\mu)}_{r,(\sigma,\tau)p}[\chi_{N(\sigma,\tau),p}\phi_{(\sigma_0,\tau_0)}(C_1)]_{(\lambda,\mu)K J}\,, \qquad (5\cdot2\cdot20)$$

where $[\chi_{(\sigma,\tau)}\phi_{(\sigma_0,\tau_0)}]_{(\lambda,\mu)}$ denotes the SU_3 vector coupling $(\sigma, \tau)\times(\sigma_0, \tau_0)\to(\lambda, \mu)$. The coefficients $H^{N(\lambda,\mu)}_{r,(\sigma,\tau)p}$ are determined by requiring the orthogonality of $Z_{N(\lambda,\mu)K J,r}$ to the two-cluster forbidden states $[V_{(N_2,0)}(\boldsymbol{t}_{1i})\phi_{(\sigma_0,\tau_0)}(C_1)]_{(\sigma',\tau')}$ with $N_2\in N^{PF}(1, i)$, $(\sigma', \tau')\in W_{N_2}(1, i)$ which are regarded as if they were allowed in constructing $\chi_{N(\sigma,\tau)\rho P,p}$. By the notation $W_{N_2}(1, i)$, we mean the set composed of those (σ', τ') which gives the forbidden state $[V_{(N_2,0)}(\boldsymbol{t}_{1i})\phi_{(\sigma_0,\tau_0)}(C_1)]_{(\sigma',\tau')}$ for $N_2\in N^{PF}(1, i)$, namely $\mathcal{A}\{[V_{(N_2,0)}(\boldsymbol{t}_{1i})\phi_{(\sigma_0,\tau_0)}(C_1)]_{(\sigma',\tau')\rho' P'}\phi_0(C_i)\}\equiv 0$. The equation to determine $H^{N(\lambda,\mu)}_{r,(\sigma,\tau)p}$ is therefore

$$\sum_{(\sigma,\tau)p} H^{N(\lambda,\mu)}_{r,(\sigma,\tau)p}X_i((\sigma, \tau), p, N_2, (\sigma', \tau'))=0\,,$$

$$X_i((\sigma, \tau), p, N_2, (\sigma', \tau'))$$

$$\equiv\hat{A}^{N(\sigma,\tau)}_{p,N_2}(i)\,U((N_1, 0)(N_2, 0)(\lambda, \mu)(\sigma_0, \tau_0); (\sigma, \tau)(\sigma', \tau'))\,,$$

$$\text{for } N_2 \in N^{PF}(1,i),\ (\sigma',\tau') \in W_{N_2}(1,i),\ (i=2,3) \qquad (5\cdot2\cdot21)$$

where $\hat{A}^{N(\sigma,\tau)}_{p,N_2}(i=3)$ are the cfp of the expansion of $\chi_{N(\sigma,\tau)\rho P,p}$ by $V^{N(\sigma,\tau)\rho P}_{N_1,N_2}(\boldsymbol{s}_2,\boldsymbol{t}_{13})$ while $\hat{A}^{N(\sigma,\tau)}_{p,N_2}(i=2)$ are by $V^{N(\sigma,\tau)\rho P}_{N_1,N_2}(\boldsymbol{s}_3,\boldsymbol{t}_{12})$ like as in Eq. (5·2·10). $U((N_1,0)\times(N_2,0)(\lambda,\mu)(\sigma_0,\tau_0);(\sigma,\tau)(\sigma',\tau'))$ are the SU_3 recoupling coefficient defined by

$$\begin{aligned}&[[(N_1,0)(N_2,0)]_{(\sigma,\tau)}(\sigma_0,\tau_0)]_{(\lambda,\mu)}\\&\quad=\sum_{(\sigma'\tau')}U((N_1,0)(N_2,0)(\lambda,\mu)(\sigma_0,\tau_0);(\sigma,\tau)(\sigma',\tau'))\\&\qquad\times[(N_1,0)[(N_2,0)(\sigma_0,\tau_0)]_{(\sigma',\tau')}]_{(\lambda,\mu)}\,.\end{aligned}\qquad(5\cdot2\cdot22)$$

(Here the multiplicity of (λ,μ) is assumed to be one for simplicity. This is true when (σ_0,τ_0) is either $(\sigma_0,0)$ or $(0,\tau_0)$.) Equation (5·2·21) is equivalent to finding the eigen-vector $H^{N(\lambda,\mu)}_{r,(\sigma,\tau)p}$ with eigen-value $q_r=0$ of the following equation,

$$\begin{aligned}&\sum_{(\sigma,\tau)p}Q^{N(\lambda,\mu)}((\bar{\sigma},\bar{\tau})\bar{p}|(\sigma,\tau)p)H^{N(\lambda,\mu)}_{r,(\sigma,\tau)p}=q_rH^{N(\lambda,\mu)}_{r,(\bar{\sigma},\bar{\tau})\bar{p}}\,,\\&Q^{N(\lambda,\mu)}((\bar{\sigma},\bar{\tau})\bar{p}|(\sigma,\tau)p)\equiv\sum_{i=2,3}\sum_{\substack{N_2\in N^{PF}(1,i)\\(\sigma',\tau')\in W_{N_2}(1,i)}}X_i((\bar{\sigma},\bar{\tau})\bar{p},N_2,(\sigma',\tau'))\\&\qquad\qquad\times X_i((\sigma,\tau),p,N_2,(\sigma',\tau'))\,.\end{aligned}\qquad(5\cdot2\cdot23)$$

We give in Table IV as an example of application, the allowed states of $^{12}C+\alpha+\alpha$ system where ^{12}C is described by the SU_3 shell model wave function with (0, 4) symmetry and is allowed to be excited to the ground band member states 2^+ and 4^+.

Table IV. SU_3 classification of the allowed states (of H_3') of the $^{12}C+2\alpha$ system.

N	$(\lambda,\mu)^n$
12	(8, 0)(4, 2)(0, 4)
13	(9, 0)(8, 2)(7, 1)(6, 3)(5, 2)^2(4, 4)(3, 3)^2(2, 5)(1, 4)
14	(11, 1)(10, 0)^3(9, 2)^2(8, 1)^3(8, 4)(7, 3)^3(6, 2)^5(6, 5)(5, 4)^3 (4, 3)^3(4, 6)^2(3, 5)^2(2, 4)^3(1, 6)(0, 8)
15	(12, 1)^2(11, 0)^5(11, 3)(10, 2)^4(9, 1)^6(9, 4)^2(8, 3)^5(7, 2)^7(8, 6)(7, 5)^3(6, 4)^5 (5, 3)^6(6, 7)(5, 6)^3(4, 5)^4(3, 4)^4(4, 8)(3, 7)^2(2, 6)^2(1, 5)^2(2, 9)(1, 8)(0, 7)

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Appendix

A.1. Proof of Jacobi formula Eq. (2·2·7)

We note the following relation,

$$\begin{vmatrix} c_{k_1l_1} & \cdots & c_{k_rl_1} \\ \vdots & & \vdots \\ c_{k_1l_r} & \cdots & c_{k_rl_r} \end{vmatrix} = \begin{vmatrix} c_{k_1l_1} & \cdots & c_{k_rl_1} & c_{p_1l_1} & \cdots & c_{p_{n-r},l_1} \\ \vdots & & \vdots & \vdots & & \vdots \\ c_{k_1l_r} & \cdots & c_{k_rl_r} & c_{p_1l_r} & \cdots & c_{p_{n-r},l_r} \\ & & & 1 & & \\ & 0 & & & \ddots & \\ & & & 0 & & 1 \end{vmatrix},$$

$$c_{ij} \equiv (\det \cdot a)\,(a^{-1})_{ji}, \tag{A·1}$$

where $(p_1, p_2, \cdots, p_{n-r})$ are the numbers which are left after subtracting the set of numbers $(k_1, k_2, \cdots, k_r)$ from $(1, 2, \cdots, n)$ and satisfy $p_1 < p_2 < \cdots < p_{n-r}$. Next we consider the determinant

$$\begin{vmatrix} a_{k_1l_1} & \cdots & a_{k_1l_r} & a_{k_1q_1} & \cdots & a_{k_1q_{n-r}} \\ \vdots & & \vdots & \vdots & & \vdots \\ a_{k_rl_1} & \cdots & a_{k_rl_r} & \vdots & & \vdots \\ a_{p_1l_1} & \cdots & \cdots & a_{p_1q_1} & \cdots & a_{p_1q_{n-r}} \\ \vdots & & & \vdots & & \vdots \\ a_{p_{n-r}l_1} & \cdots & \cdots & a_{p_{n-r}q_1} & \cdots & a_{p_{n-r}q_{n-r}} \end{vmatrix}, \tag{A·2}$$

where $(q_1, q_2, \cdots, q_{n-r})$ are the numbers which are left after subtracting $(l_1, l_2, \cdots, l_r)$ from $(1, 2, \cdots, n)$ and satisfy $q_1 < q_2 < \cdots < q_{n-r}$. Clearly this determinant is equal to $\varepsilon\binom{1\cdots r\ r+1\cdots n}{k_1\cdots k_r\ p_1\cdots p_{n-r}} \times \varepsilon\binom{1\cdots r\ r+1\cdots n}{l_1\cdots l_r\ q_1\cdots q_{n-r}} \cdot \det\{a_{ij}\}$, $\varepsilon(P)$ denoting the signature of the permutation P. By multiplying the two determinants of Eqs. (A·1) and (A·2) and by using Eq. (2·2·5) we obtain

$$\begin{vmatrix} c_{k_1l_1} & \cdots & c_{k_rl_1} \\ \vdots & & \vdots \\ c_{k_1l_r} & \cdots & c_{k_rl_r} \end{vmatrix} \cdot \varepsilon\begin{pmatrix} 1 & \cdots & r & r+1 & \cdots & n \\ k_1 & \cdots & k_r & p_1 & \cdots & p_{n-r} \end{pmatrix} \cdot \varepsilon\begin{pmatrix} 1 & \cdots & r & r+1 & \cdots & n \\ l_1 & \cdots & l_r & q_1 & \cdots & q_{n-r} \end{pmatrix} \cdot \det\{a_{ij}\}$$

$$= \begin{vmatrix} \det\cdot a & & & & \\ & \det\cdot a & 0 & & \\ & & \ddots & & \\ 0 & & & 0 & \\ & & \det\cdot a & & \\ a_{p_1 l_1} & \cdots\cdots & a_{p_1 q_1} & \cdots\cdots & a_{p_1 q_{n-r}} \\ \vdots & & \vdots & & \vdots \\ a_{p_{n-r} l_1} & \cdots\cdots & a_{p_{n-r} q_1} & \cdots\cdots & a_{p_{n-r} q_{n-r}} \end{vmatrix}$$

$$= (\det\cdot a)^r \cdot B\begin{pmatrix} k_1 \cdots\cdots k_r \\ l_1 \cdots\cdots l_r \end{pmatrix}, \qquad (A\cdot 3)$$

where we used the fact

$$B\begin{pmatrix} k_1 \cdots\cdots k_r \\ l_1 \cdots\cdots l_r \end{pmatrix} = \begin{vmatrix} a_{p_1 q_1} & \cdots\cdots & a_{p_1 q_{n-r}} \\ \vdots & & \vdots \\ a_{p_{n-r} q_1} & \cdots\cdots & a_{p_{n-r} q_{n-r}} \end{vmatrix}, \qquad (A\cdot 4)$$

which is evident from the definition of $B\binom{k_1 \cdots k_r}{l_1 \cdots l_r}$. By using the relations

$$\varepsilon\begin{pmatrix} 1 \cdots\cdots r & r+1 \cdots\cdots n \\ k_1 \cdots\cdots k_r & p_1 \cdots\cdots p_{n-r} \end{pmatrix} = (-)^{\sum_{i=1}^{r}(i+k_i)},$$

$$\varepsilon\begin{pmatrix} 1 \cdots\cdots r & r+1 \cdots\cdots n \\ l_1 \cdots\cdots l_r & q_1 \cdots\cdots q_{n-r} \end{pmatrix} = (-)^{\sum_{i=1}^{r}(i+l_i)}, \qquad (A\cdot 5)$$

which are proved in Appendix A. 2, we get from Eq. (A·3) the desired formula

$$B\begin{pmatrix} k_1 \cdots\cdots k_r \\ l_1 \cdots\cdots l_r \end{pmatrix} = (\det\cdot a)^{-r+1} \cdot (-)^{\sum_{i=1}^{r}(k_i+l_i)} \cdot \begin{vmatrix} c_{k_1 l_1} & \cdots\cdots & c_{k_r l_1} \\ \vdots & & \vdots \\ c_{k_1 l_r} & \cdots\cdots & c_{k_r l_r} \end{vmatrix}$$

$$= (\det\cdot a) \cdot (-)^{\sum_{i=1}^{r}(k_i+l_i)} \cdot \begin{vmatrix} (a^{-1})_{l_1 k_1} & \cdots\cdots & (a^{-1})_{l_1 k_r} \\ \vdots & & \vdots \\ (a^{-1})_{l_r k_1} & \cdots\cdots & (a^{-1})_{l_r k_r} \end{vmatrix}. \qquad (A\cdot 6)$$

A.2. Sign of permutation $\binom{1 \cdots\cdots r \quad r+1 \cdots\cdots n}{k_1 \cdots k_r \quad p_1 \cdots p_{n-r}}$

The sign $\varepsilon(P)$ of the permutation $P \equiv \binom{1 \cdots\cdots n}{p_1 \cdots p_n}$ can be calculated by knowing the number of inversion $I(p_i)$ for each number p_i which is defined as the number of letters p_j which satisfies $j>i$ and $p_j<p_i$ (namely which locates to the right of p_i and is smaller than p_i). The relation

$$\varepsilon(P) = (-)^{\sum_{i=1}^{n} I(p_i)} \qquad (A\cdot 7)$$

can be proved as follows; Consider the process to put back the numbers $(p_1, p_2, \cdots, p_n)$ to the original order $(1, 2, \cdots, n)$. Let p_{i_1} be $p_{i_1}=n$. In order to put back p_{i_1} to the original position, we need $(n-i_1)$-time transpositions and this number $(n-i_1)$ is just the number of inversion for $p_{i_1}=n$,

namely $I(p_{i_1})=n-i_1$ since all the letters locating to the right of $p_{i_1}=n$ are smaller than $p_{i_1}=n$. After putting back $p_{i_1}=n$ to the original position, we recalculate the number of inversions for the remaining letters $p_j\neq p_{i_1}=n$. Quite clearly $I(p_j)$ (for $p_j\neq p_{i_1}=n$) receive no change at all. Now let p_{i_2} be $p_{i_2}=n-1$, and we put it back to the original position by $I(p_{i_2})$-time transpositions. After putting back p_{i_1} and p_{i_2} to their original positions we know again that the numbers of inversion for the remaining p_j ($p_j\neq p_{i_1}$, $p_j\neq p_{i_2}$) receive no change at all also. Repeating the same process, the numbers $(p_1, p_2, \cdots, p_n)$ are put back to their original order $(1, 2, \cdots, n)$ after $(\sum_{i=1}^{n} I(p_i))$-time transpositions. Thus Eq.(A·7) is proved.

Now consider the permutation

$$P\equiv\begin{pmatrix}1\cdots\cdots r & r+1\cdots\cdots n\\ k_1\cdots\cdots k_r & p_1\cdots\cdots p_{n-r}\end{pmatrix},$$
$$k_1<k_2<\cdots<k_r;\ p_1<p_2<\cdots<p_{n-r}. \qquad (A\cdot 8)$$

Clearly the numbers of inversion for p_i ($i=1\sim n-r$) are all zero; $I(p_i)=0$, $i=1\sim n-r$. For each k_i there are (k_i-1) letters (namely $1, 2, \cdots, k_i-1$) which are smaller than k_i. Among these (k_i-1) letters $(i-1)$ letters are located to the left of k_i (namely $k_1, k_2, \cdots, k_{i-1}$), and so we obtain $I(k_i)=(k_i-1)-(i-1)=k_i-i$. From Eq. (A·7) we therefore obtain

$$\varepsilon(P)=(-)^{\sum_{i=1}^{r}(i+k_i)}. \qquad (A\cdot 9)$$

By using Eq. (A·9) we can prove the Laplace expansion given in Eq. (2·2·2). First we note

$$\det\{a_{ij}\}=\varepsilon\begin{pmatrix}1\cdots\cdots r & r+1\cdots\cdots n\\ l_1\cdots\cdots l_r & q_1\cdots\cdots q_{n-r}\end{pmatrix}\cdot I,$$
$$I\equiv\begin{vmatrix}a_{1l_1}\cdots\cdots a_{1l_r} & a_{1q_1}\cdots\cdots a_{1q_{n-r}}\\ \vdots\quad\quad\vdots & \vdots\quad\quad\vdots\\ a_{nl_1}\cdots\cdots a_{nl_r} & a_{nq_1}\cdots\cdots a_{nq_{n-r}}\end{vmatrix}. \qquad (A\cdot 10)$$

Next we use the relation of Eq. (2·2·21), which gives us

$$I=\sum_{(k_1<k_2<\cdots<k_r)}\varepsilon\begin{pmatrix}1\cdots\cdots r & r+1\cdots\cdots n\\ k_1\cdots\cdots k_r & p_1\cdots\cdots p_{n-r}\end{pmatrix}\cdot\begin{vmatrix}a_{k_1l_1}\cdots\cdots a_{k_1l_r}\\ \vdots\quad\quad\vdots\\ a_{k_rl_1}\cdots\cdots a_{k_rl_r}\end{vmatrix}\cdot\begin{vmatrix}a_{p_1q_1}\cdots\cdots a_{p_1q_{n-r}}\\ \vdots\quad\quad\vdots\\ a_{p_{n-r}q_1}\cdots\cdots a_{p_{n-r}q_{n-r}}\end{vmatrix}. \qquad (A\cdot 11)$$

Thus by Eq. (A·9) we have proved Eq. (2·2·2) for the case of $\sum=\sum_{(k_1<k_2<\cdots<k_r)}$. The proof of Eq. (2·2·2) in the case of $\sum=\sum_{(l_1<l_2<\cdots<l_r)}$ is similar and evident.

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