

Multicluster Resonating-Group Method of s -Shell Cluster Systems

By

Yoshikazu FUJIWARA

Department of Physics, Kyoto University, Kyoto 606-01, Japan

Y.C. TANG

School of Physics, University of Minnesota, Minneapolis, MN 55455, USA

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Abstract

An analytic formulation of the multicluster resonating-group method (RGM) is presented for systems composed of any number of $(0s)$ -shell clusters. In this formulation, the construction of exchange integral kernels in the complex generator-coordinate space and the subsequent development to the RGM formalism is carried out in full generality with respect to the central, LS , and tensor two-nucleon forces of the Gaussian type and to the Coulomb interaction. Each term in the interaction kernel is classified not only by the modes in which nucleons are interchanged among clusters, but also by the interaction types which specify particular combinations of the complex generator-coordinate vectors involved in quadratic polynomials for Gaussian interaction factors. The interaction kernel involves spin-isospin factors in a concise way, the evaluation of which requires specification of spin-isospin coupling schemes for the particular system under consideration. In view of a practical application of the present formalism to the systems composed of one α -cluster and two $(0s)$ -shell clusters, the spin-isospin factors are derived in analytic form for any spin-isospin configurations of two s -shell clusters. The result is then extended to the case of the three-cluster kernels by employing the valence-orbital method. As an example of utilizing the resultant three-cluster RGM kernels, coupled-channel equations with three different types of two-cluster channels are formulated. These coupled-channel equations are then solved by a variational method employing Gaussian-type trial functions. The matrix elements of the resonating-group kernels with respect to angular-momentum coupled Gaussian basis functions are calculated easily with a new technique, which is specifically developed for this investigation by making use of the theory of double Gel'fand polynomials and transformation properties of the complex generator-coordinate kernels

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§1. Introduction and Summary

The resonating-group method (RGM), proposed by Wheeler [1] a long time ago, is a full microscopic framework which makes much account of cluster correlations in nuclear many-body problems. It is particularly suited to a unified description of bound-state, scattering and reaction problems, in which nuclear clusters are frequently natural building blocks of the total system and their dynamical interplay provides an essential role in many intricate nuclear phenomena, including structure changes from the shell-model-like to cluster structures. Once a combination of an appropriately large model space and an effective two-nucleon interaction is selected in view of physical considerations, there is no room for any phenomenological parameters in the RGM calculation, and the antisymmetrization due to the effect of the Pauli principle takes full account of cluster dynamics, resulting in a unique solution for the physical observables such as the bound-state energies and cross sections. Owing to these nice features, many detailed

calculations have been performed by using this method, especially in light nuclear systems. As for these enormous outgrowth within the last fifty years or so, a number of books [2], [3] and review articles [4]~[14] should be referred to.

In the RGM calculations, it is essential to choose an appropriately large model space that is spanned by a set of nonorthogonal basis functions representing various cluster configurations. There exist at present a number of many-channel calculations, as well as quite sophisticated single-channel calculations which take account of detailed properties of cluster internal functions. [15]~[76] We can categorize these into several groups. The first one is multiconfiguration RGM calculations performed especially by Hackenbroich and his collaborators, and later by Hofmann and his collaborators (see, e.g., refs. [15]~[33]). In the method of Hackenbroich, all necessary matrix elements of many-nucleon systems are directly calculated by successively applying the algebraic transformation formula of Gaussian integration, and all physical observables in the low-energy region are reasonably reproduced by adopting a wide model space spanned by many types of two-cluster configurations. The emphasis of these investigators is, however, on studying the level structures in the low-excitation region of light *p*-shell nuclei and the four-nucleon system. The second category is calculations by the method of pseudo-inelastic configurations, first performed by Thompson and Tang [34], [35] and subsequently by several authors [37]~[42]. The main idea of this method is as follows. In the deep inside of the nucleus or in the interaction region in a reaction process, clusters are usually distorted from the original free particles due to the interaction with the surrounding nucleons. This is called the specific distortion effect in ref. [3], and is particularly important in the low energy region, when clusters with low compressibility like the deuteron are involved. This effect is properly taken into account, if one introduces additional degree of freedom into the resonating-group trial functions and thereby improves the behavior of the compound system in the strongly interacting region. This can be attained either by adding into the formulation physical reaction channels as is done in the multiconfiguration RGM calculations or by employing the pseudo-state method in which pseudo-inelastic configurations are utilized to enlarge the model space. The main advantage of this method lies in its simplicity of formulation, because the kernel functions representing the couplings among various cluster configurations can be rather easily derived. Another important effect of the pseudo-inelastic configurations is to describe the direct breakup processes of clusters. The third one is the multiconfiguration and multichannel resonating-group calculations by the present authors [44]~[50], in which coupled-channel equations are derived by starting from an analytic formulation of a three-cluster RGM [51]. In this formulation, we can easily incorporate the following important effects : 1) the clustering effect of subsystems like $d + \alpha$ structure of ${}^6\text{Li}$; 2) inelastic excitations to the simple rotational partner of the ground state like $I = 2$ excited state of ${}^6\text{Li}$; 3) those to the states of intrinsic excitations such as $(3N + N)$ -like α^* state; 4) those to the pseudo-inelastic configurations; 5) effects of cluster-rearrangement configurations in reaction processes. Through detailed systematic investigations of differential and reaction cross sections in 6-, 7-, 8-, and 10-nucleon systems, the present authors have examined general characteristics of nuclear reactions, such as the essential features of internuclear interactions, important reaction

mechanisms and so on. For the interesting findings up to the present, a recent review article [50] should be referred to. Needless to say, this formulation has some restriction originating from dividing the total system into only three clusters. This is, in fact, a part of the motivations to extend this formalism to four- and more-cluster systems in the present paper. The fourth category is an attempt to solve 3-cluster systems directly either in the RGM formalism or in the generator-coordinate method (GCM). We should mention the very early variational RGM calculation of the 3α system by Fukushima and Kamimura [52], [53] and a GCM calculation by Uegaki, Okabe, Abe and Tanaka [54], [55]. Through an extensive study by Baye and his collaborators [56] ~ [63], it has been shown that the GCM is a suitable framework to incorporate many-cluster configurations in the microscopic cluster theory. By Descouvemont and Baye [64], [65] and also by Langanke and his collaborators [66] ~ [69], it is successfully applied to many nuclear reactions of astrophysical interest. For example, in the study of the 8-nucleon system in ref. [64], the folding procedure for the 2-cluster subsystem is employed to formulate the scattering problems for evaluating the astrophysical S -factors in ${}^7\text{Be}(p, \gamma){}^8\text{B}$ and ${}^7\text{Li}(n, \gamma){}^8\text{Li}$ reactions. A few ambitious attempts to take into account the three-body breakup processes and the effects of cluster excitations in the full microscopic 3-cluster formulations by the techniques of hyper-spherical harmonics and others are found in refs. [70] ~ [76].

The purpose of this paper is to present a mathematical formulation of the three-cluster RGM for systems composed of one α -cluster and two s -shell clusters, and thereby provide technical details for the multiconfiguration and multichannel resonating-group calculations by the present authors. In view of the recent rapid improvement of computer facilities, we will extend the applicability of the present formulations to more complicated systems such as four- and more-cluster systems. The only restriction is that the systems are composed of s -shell clusters described by translationally-invariant shell-model functions of the lowest configurations in harmonic-oscillator potential wells having a common width parameter ν . In contrast to the previous write-up [51], we will here discuss not only central forces but also LS , tensor and Coulomb interactions. The incorporation of these forces in the actual numerical calculations is a future project. If the system is only composed of spin-isospin saturated α -clusters, both of the normalization and interaction kernels are easily obtained from the standard techniques in terms of the Bloch-Brink wave functions [77]. In fact, even the system of an infinitely large number of α -clusters (α -matter) is discussed and the GCM kernels are elegantly expressed by using the Lambert series and the elliptic theta functions [78]. However, once the system has non-zero spin and isospin values, such a simple separation of the spatial and spin-isospin degrees of freedom is no longer possible. In such a case, one needs to handle a large number of analytic matrix inversions of large dimensionality corresponding to the nucleon number itself, which is still not easy even by using modern computer softwares for algebraic computations. Here we instead use another standard technique by the double-coset generator expansions, which was developed by Kramer and Seligman [79], [80]. A nice feature of this technique is that we only need to deal with the smallest number of independent terms for the exchange kernels from the very beginning and that it gives a complete procedure to calculate spin-isospin factors for

arbitrary systems in terms of shell-model-like cfp expansions. These authors use the expansions even for the spatial part [82], but we rather use simpler Brink techniques to handle this continuous degree of freedom. Each term in the interaction kernel is classified not only by the modes in which nucleons are interchanged among clusters, but also by the interaction types which specify particular combinations of the complex generator-coordinate vectors involved in quadratic polynomials for Gaussian interaction factors. These kernels have very simple structure for a clear separation of spin-isospin factors and factorization of each term into the normalization, the central-Gaussian, and the noncentral factors. By considering these kernels in the complex generator-coordinate space, the subsequent transformation to the RGM kernels and evaluation of the matrix elements for Gaussian-type trial functions are carried out in full generality irrespective of the number of clusters.

Although the procedure to evaluate the spin-isospin factors is straightforward, we need to specify spin-isospin coupling schemes for practical calculations of these factors. Even in 3-cluster systems, this process becomes fairly cumbersome for general spin-isospin configurations. On the other hand, the systems we are concerned with usually contain at least one α -cluster, and hence a full generality of the spin-isospin configurations for 2-cluster subsystems is practically good enough for the description of 3-cluster systems. In this paper, we will analytically derive the spin-isospin factors in the interaction kernels for any spin-isospin configurations of two ($0s$)-shell clusters, and the result is then generalized to the case of 3-cluster kernels in the generator-coordinate space, employing the valence-orbital method [83]. A computer-aided algebraic computation of these spin-isospin factors for arbitrary systems is certainly a promising future direction to proceed.

Once the kernel functions are thus derived in the GCM or RGM representation, the next important problem is how to solve these n -cluster integro-differential equations. In principle, we should be able to formulate Faddeev-type connected-kernel equations which take into account correct asymptotic behavior of many-cluster systems. However, a complete treatment of breakup processes is not yet accomplished even in the Faddeev formalism for systems of structureless particles. In this paper, we only give a possible application of the n -cluster RGM formalism, which is practically feasible and still physically meaningful. Namely, we discuss 3-cluster systems composed of one α -cluster and two ($0s$)-shell clusters, and formulate coupled-channel equations with three different types of two-cluster kernels. We assume appropriate relative-motion functions for 2-cluster subsystems composed of any pairs of the three clusters. In practice, these relative-motion functions are selected according to a variational procedure constrained by relevant experimental information such as the root-mean-square radius or the charge form-factor data. These coupled-channel equations are then solved by the variational method, employing Gaussian-type trial functions [85]. Through this procedure, we can investigate the effect of channel couplings due to the cluster rearrangement, as well as the effect of clustering in the sophisticated channel wave functions. We can even incorporate the effect of cluster breakup in an approximate way, by introducing the pseudo-state configurations for the subsystems [84].

The variational method for coupled-channel problems is extensively discussed by

Kamimura [85], and has been used by many authors. In the application to multicluster problems, it is crucial to have concise expressions of RGM matrix elements for efficiently calculating the huge number of them, since the main computation time is spent for this part. Such expressions are known to be obtained by using Gaussian-type basis functions, by which another tedious process of angular-momentum projection is also greatly simplified. We have developed in Appendix B of ref. [43] a new technique to calculate Gaussian matrix elements for RGM kernels, directly starting from the GCM kernels. This technique requires the transformation formula from GCM to RGM kernels, which is easily obtained through the Bargmann integrals in the complex generator-coordinate space. We have applied this technique to central matrix elements of 3-cluster systems in ref. [51], and have obtained a concise expression which contains only one simple Clebsch-Gordan (C-G) coefficient for the angular-momentum projection. Here we combine this technique with the theory of double Gel'fand polynomials [86] developed for the multiplicity-free problems in the representation theory of unitary groups. Instead of taking the infinity limit of the RGM argument variables as is done in refs. [43] and [51], we employ a simple reduction rule from 3-dimensional complex variables to 2-dimensional ones. This rule converts the process of calculating the RGM matrix elements with respect to the angular-momentum coupled Gaussian basis functions into that of expanding the generating functions in terms of two-row type $SU_2 \times SU_{n-1}$ double Gel'fand polynomials. Since the necessary SU_{n-1} C-G coefficients are all expressed by the angular-momentum Wigner coefficients, this new technique corresponds to a transparent bookkeeping of the complicated angular-momentum projections of the many-cluster systems in the quasi-spin or quasi- SU_{n-1} space.

Finally, a brief comment may be useful to clarify the characteristics of our approach. The present many-cluster formalism is entirely analytic. This implies that we treat explicitly kernel expressions in the RGM or GCM formalism for a definite multicluster model space, and try to connect the complex many-body nature of nucleon systems to various properties of the kernels which completely determine the relative motion between clusters. Therefore, it is possible in our approach to examine the properties of the kernels in terms of nucleon-exchange modes and interaction types, and also to study the relationship of the multicluster kernels with coupling kernels in the coupled-channel formalism and with the kernels of subsystems in cases where subsystems of many clusters are approximately described by harmonic-oscillator shell-model wave functions. These studies are important, in order to clarify such interesting microscopic effects as nucleon-exchange effects, distortion effects, channel-coupling effects, clustering effects, and other effects in various reaction processes. The completely analytic character of the formulation makes it necessary to restrict to some extent the range and the nature of systems that can be readily treated. On the other hand, it also results in the practical advantage that the requirement of computational facilities is greatly reduced.

Another important nature of our approach is that our two-cluster coupled-channel RGM equations are derived as a result of an approximation to the three-cluster RGM equation. Thus, if one wishes to elucidate the foundation of such a coupled-channel approximation, one only needs to investigate the properties of the three-cluster RGM equation itself in much more detail. Although all necessary three-cluster kernels is de-

rived in this paper, no investigation has yet been made concerning the problem of which kind of three-cluster equations one should solve for the microscopic 3-cluster systems, in order to insure a correct dynamical behavior for the relative motions among three clusters in the sense of a three-body Faddeev-type theory. With a complete formulation of the three-cluster RGM, one should be able to incorporate in a natural way the three-cluster breakup effect, as well as the channel-coupling effect of two-cluster channels. In this context, one might need to pay special attention to semi-direct potentials resulting from partial antisymmetrization of 2-cluster subsystems in the framework of a correct three-cluster RGM theory, since such potentials have never been directly treated in any three-body formalism of structureless particles. Recently, Schmid and other authors [87]~ [91] have discussed the relationship between three-cluster forces and the elementary-particle concept of clusters, by introducing a certain type of off-shell transformation in the three-cluster RGM equation. The approach developed in this investigation might give some helpful hints as to how one could proceed with such a theoretical investigation of three-cluster systems.

The organization of this paper is as follows. In §2, we first outline the coupled-channel formulation of 3-cluster systems, which employ the $n=3$ case of the following n -cluster RGM formalism. In §3, the structure of the n -cluster RGM kernels for systems of $(0s)$ -shell clusters is clarified. After a short comment on general procedure to evaluate GCM kernels, double-coset generator expansion of the antisymmetrization operator is introduced and employed to evaluate interaction kernels for central, LS , tensor interactions, and for the Coulomb interaction as well. Each term in the interaction kernel is classified not only by the exchange modes of nucleons, but also by the interaction types which involve somewhat increasing complexity for larger number of clusters. In particular, for 3-cluster systems, it is shown that 3-cluster interaction types are specified by a slight extension of simple 2-cluster interaction types, together with a particular set of Jacobi coordinates which specifies the positions of clusters directly involved in the particular two-nucleon matrix element under consideration. This classification scheme of the 3-cluster interaction types is particularly convenient, when we discuss the transformation properties of the coefficients of the GCM kernels for rearrangements of the Jacobi coordinates. In §4, a few explicit examples of spin-isospin factors are given for arbitrary spin-isospin configurations of 2-clusters and for 3-cluster systems which involve one α -cluster and two $(0s)$ -shell clusters. The 2-cluster case follows the general procedure, which is in principle applicable to systems of any number of $(0s)$ -shell clusters. On the other hand, a simpler valence-orbital method is employed for the particular 3-cluster systems considered, in which we can take full advantage of the spin-isospin saturated nature of the α -cluster. The last two sections are devoted to a technical development for practical applications of n -cluster GCM kernels. In §5, we first discuss a systematic evaluation of RGM kernels in the complex GCM. The transformation formula derived here plays an essential role in the evaluation of Gaussian matrix elements of the RGM kernels in §6. We can elaborate a new transformation formula for this purpose, by employing a simple reduction rule of Bargmann variables. Through this procedure, we can construct generating functions for the Gaussian matrix elements, from which those for angular-momentum coupled n -cluster states are easily obtained by the expansion

in terms of $SU_2 \times SU_{n-1}$ double Gel'fand polynomials. The 2- and 3-cluster formulae for the Gaussian matrix elements of the RGM kernels with respect to the central, LS , tensor, Coulomb, and the kinetic-energy terms are explicitly given to be readily used.

§2. Coupled-Channel Formulation of 3-Cluster Systems

In the multiconfiguration and multichannel RGM calculations by the present authors [50], the 6-, 7-, 8- and 10-nucleon systems are considered to be 3-cluster systems $C_1 + C_2 + C_3$, with all three clusters described by translationally-invariant shell-model functions of $(0s)$ -configurations with a common harmonic-oscillator (h.o.) width parameter ν . By using the mathematical techniques developed in ref. [51] or in the following sections, one can derive the 3-cluster kernel functions for these systems. To be more specific, let us express the 3-cluster basis functions in the RGM formalism as

$$\Psi = \mathcal{A} \{ \phi(C_1)\phi(C_2)\phi(C_3) \chi(\xi_1, \xi_2) Z(\mathbf{X}_G) \} , \quad (2.1)$$

where $\phi(C_\alpha)$ ($\alpha = 1, 2, 3$) denotes the cluster internal wave function for C_α and $Z(\mathbf{X}_G)$ is any normalizable function describing the total center-of-mass (c.m.) motion. For clarity in presentation, we shall conduct the following discussion by assuming that the clusters have no spin-isospin quantum numbers and by omitting angular-momentum couplings; in actual calculations these must of course be explicitly taken into consideration. Furthermore, we assume that the three clusters, C_1 , C_2 , and C_3 , are all different from each other. In Eq. (2.1), \mathcal{A} is the antisymmetrization operator among three clusters and $\chi(\xi_1, \xi_2)$ represents an intercluster relative-motion function with ξ_1 and ξ_2 being an appropriate set of the Jacobi coordinates. (See Eq. (3.8), for example.) The relative-motion function $\chi(\xi_1, \xi_2)$ is determined from the variational RGM projection equation

$$\langle \delta\Psi | H - E | \Psi \rangle = 0 , \quad (2.2)$$

where H is a Galilean-invariant Hamiltonian composed of the kinetic-energy term and the two-nucleon interaction ;

$$H = \sum_{s=1}^A t_s - T_G + \sum_{s<t}^A v_{st} . \quad (2.3)$$

Here, A is the total mass number $A = A_1 + A_2 + A_3$ with A_α ($\alpha = 1 \sim 3$) being that of the cluster C_α . The integro-differential equation for $\chi(\xi_1, \xi_2)$ is schematically written as

$$(\mathcal{H} - E\mathcal{N})\chi = 0 , \quad (2.4)$$

where \mathcal{H} and \mathcal{N} are integral kernels defined through

$$\left\{ \begin{array}{c} \mathcal{N} \\ \mathcal{H} \end{array} \right\} = \langle \phi(C_1)\phi(C_2)\phi(C_3) | \left\{ \begin{array}{c} 1 \\ H \end{array} \right\} \mathcal{A} | \phi(C_1)\phi(C_2)\phi(C_3) \rangle , \quad (2.5)$$

and their explicit derivation is the main subject of the following sections. Here we assume that they are already derived and outline how we should proceed further to derive coupled-channel equations.

FIGURES

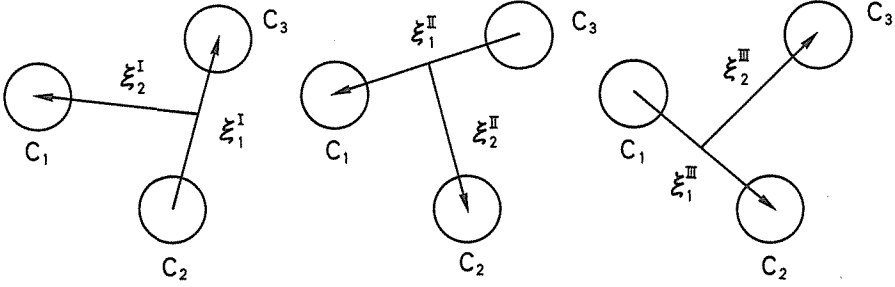


FIG. 1. Three independent sets of Jacobi coordinates for 3-cluster systems; $\xi^J = (\xi_1^J, \xi_2^J)$ with $J = \text{I, II, III}$, or $J = (\gamma)$ with $\gamma = 1, 2$, and 3.

An advantage of having explicit expressions of 3-cluster GCM kernels is that one can analyse their structure term by term, and hence investigate the roles of exchange modes and interaction types in detail. In particular, as we know in 2-cluster systems, the separation into the direct and exchange terms by the nucleon-exchange number is very important, since these terms have different number of Dirac's δ -functions in the form of RGM kernels, and a special treatment is needed to formulate RGM equations as integro-differential equations. In 3-cluster systems, we find that another special class called semi-direct terms emerges, which is characterized by nucleon exchange between 2-cluster subsystems with the third cluster left free. Naturally, almost all of these kernels are expressed by 2-cluster kernels of the subsystems. An exception is the semi-direct part of the interaction kernel, which can not be reduced to any kind of 2-cluster kernels, in spite of the appearance of one δ -function for the relative coordinate between the subsystem and the third cluster. This situation is conveniently described by introducing three different types of Jacobi coordinates depicted in Fig. 1. Suppose $(\alpha\beta\gamma)$ is an even permutation of (123). The subsystem $C_{\alpha\beta} \equiv C_\alpha + C_\beta$ is specified by the third index γ . We refer to $C_{\alpha\beta}$ as a subsystem of γ -pair, and use the notation γ and $\bar{\gamma}$ to denote the relative degrees of freedom between C_α and C_β , and between $C_{\alpha\beta}$ and C_γ , respectively. By using these notations, the structure of 3-cluster kernel is schematically expressed as

$$\begin{aligned} \mathcal{N} &= 1 + \sum_{\gamma} \mathcal{N}_{\gamma}^{(2)} + \mathcal{N}^{(3)} \quad , \\ \mathcal{K} &= \mathcal{K}^D + \sum_{\gamma} \mathcal{K}_{\gamma}^{SD} + \mathcal{K}^{(3)} \quad , \\ \mathcal{K}^D &= \sum_{\alpha} E_K^{(int)}(C_{\alpha}) + T_{\gamma} + T_{\bar{\gamma}} \quad , \\ \mathcal{K}_{\gamma}^{SD} &= \mathcal{N}_{\gamma}^{(2)} (E_K^{(int)}(C_{\gamma}) + T_{\bar{\gamma}}) + \mathcal{K}_{\gamma}^{(2)} \quad , \\ \mathcal{I} &= \mathcal{I}^D + \sum_{\gamma} \mathcal{I}_{\gamma}^{SD} + \mathcal{I}^{(3)} \quad , \end{aligned}$$

$$\begin{aligned} \mathcal{I}^D &= \sum_{\alpha} E_V^{(int)}(C_{\alpha}) + \sum_{\alpha} V_{\alpha}^D , \\ \mathcal{I}_{\gamma}^{SD} &= \mathcal{N}_{\gamma}^{(2)} E_V^{(int)}(C_{\gamma}) + \mathcal{I}_{\gamma}^{(2)} + V_{\gamma}^{SD} , \end{aligned} \quad (2.6)$$

where \mathcal{K} and \mathcal{I} are kinetic-energy and interaction parts of \mathcal{H} , respectively; $\mathcal{H} = \mathcal{K} + \mathcal{I}$. In Eq. (2.6), T_{γ} and $T_{\bar{\gamma}}$ are the relative kinetic-energy operators between C_{α} and C_{β} , and between $C_{\alpha\beta}$ and C_{γ} , respectively, V_{γ}^D is the direct potential between C_{α} and C_{β} , and V_{γ}^{SD} is the semi-direct potential. Furthermore, $E^{(int)}(C_{\gamma}) \equiv E_K^{(int)}(C_{\gamma}) + E_V^{(int)}(C_{\gamma})$ is the internal-energy contribution of the cluster C_{γ} , and $\mathcal{N}_{\gamma}^{(2)}$, $\mathcal{K}_{\gamma}^{(2)}$, and $\mathcal{I}_{\gamma}^{(2)}$ are the exchange kernels for the subsystem $C_{\alpha\beta}$. The genuine 3-cluster exchange kernels are denoted by $\mathcal{N}^{(3)}$, $\mathcal{K}^{(3)}$, and $\mathcal{I}^{(3)}$, and they involve no δ -functions.

Let us first consider the 2-cluster RGM equation for the subsystem of the γ -pair. It is given by

$$(\mathcal{K} + \mathcal{I} - E_{\gamma}^{(int)} \mathcal{N}) \phi_{\gamma} = 0 , \quad (2.7)$$

where \mathcal{N} , \mathcal{K} , and \mathcal{I} are now 2-cluster kernels expressed as

$$\begin{aligned} \mathcal{N} &= 1 + \mathcal{N}_{\gamma}^{(2)} , \\ \mathcal{K} &= E_K^{(int)}(C_{\alpha}) + E_K^{(int)}(C_{\beta}) + T_{\gamma} + \mathcal{K}_{\gamma}^{(2)} , \\ \mathcal{I} &= E_V^{(int)}(C_{\alpha}) + E_V^{(int)}(C_{\beta}) + V_{\gamma}^D + \mathcal{I}_{\gamma}^{(2)} . \end{aligned} \quad (2.8)$$

We substitute Eq. (2.8) into Eq. (2.7) and introduce the relative energy ε_{γ} of the γ -pair through

$$E_{\gamma}^{(int)} = \varepsilon_{\gamma} + E^{(int)}(C_{\alpha}) + E^{(int)}(C_{\beta}) . \quad (2.9)$$

Then, we obtain

$$(T_{\gamma} + V_{\gamma} - \varepsilon_{\gamma}) \phi_{\gamma} = 0 \quad (2.10)$$

with

$$V_{\gamma} = V_{\gamma}^D + G_{\gamma}^E , \quad G_{\gamma}^E = \mathcal{K}_{\gamma}^{(2)} + \mathcal{I}_{\gamma}^{(2)} - E_{\gamma}^{(int)} \mathcal{N}_{\gamma}^{(2)} , \quad (2.11)$$

where G_{γ}^E represents the contribution from the exchange kernels for the γ -pair. The normalization of ϕ_{γ} is determined from the condition

$$\langle \phi_{\gamma} | (1 + \mathcal{N}_{\gamma}^{(2)}) | \phi_{\gamma} \rangle = 1 . \quad (2.12)$$

On the other hand, 3-cluster RGM equation in Eq. (2.4) is expressed as

$$(\mathcal{K} + \mathcal{I} - E \mathcal{N}) \chi = 0 , \quad (2.13)$$

where \mathcal{N} , \mathcal{K} , and \mathcal{I} are 3-cluster kernels given in Eq. (2.6). Let us introduce the relative energy $\varepsilon_{\bar{\gamma}}$ for the γ -channel through

$$E = \varepsilon_{\bar{\gamma}} + E_{\gamma}^{(int)} + E^{(int)}(C_{\gamma}) , \quad (2.14)$$

Then, by substituting Eq. (2.6) into Eq. (2.13) and by using Eqs. (2.11) and (2.14), we obtain

$$\begin{aligned} & \left[(T_\gamma + V_\gamma - \varepsilon_\gamma) + (T_{\bar{\gamma}} - \varepsilon_{\bar{\gamma}})(1 + \mathcal{N}_\gamma^{(2)}) + \sum_{\alpha \neq \gamma} V_\alpha^D + V_\gamma^{SD} \right] \chi \\ & = - \left[\sum_{\alpha \neq \gamma} (\mathcal{K}_\alpha^{SD} + \mathcal{I}_\alpha^{SD} - EN_\alpha^{(2)}) + (\mathcal{K}^{(3)} + \mathcal{I}^{(3)} - EN^{(3)}) \right] \chi . \end{aligned} \quad (2.15)$$

Here we examine two types of approximations for the relative wave function χ of the 3-cluster system. In the first type, we set in Eq. (2.15) $\chi = \phi_\gamma \psi_{\bar{\gamma}}$ consisting of a relative wave function $\psi_{\bar{\gamma}}$ between $C_{\alpha\beta}$ and C_γ , and perform the integration for the inner product with ϕ_γ . Then, by using Eqs. (2.10) and (2.12), we obtain

$$(T_{\bar{\gamma}} + V_{\bar{\gamma}} - \varepsilon_{\bar{\gamma}}) \psi_{\bar{\gamma}} = 0 , \quad (2.16)$$

where we have defined

$$\begin{aligned} V_{\bar{\gamma}} &= V_{\bar{\gamma}}^D + G_{\bar{\gamma}}^E , \\ V_{\bar{\gamma}}^D &= \langle \phi_\gamma | \sum_{\alpha \neq \gamma} V_\alpha^D + V_\gamma^{SD} | \phi_\gamma \rangle , \\ G_{\bar{\gamma}}^E &= \langle \phi_\gamma | \sum_{\alpha \neq \gamma} (\mathcal{K}_\alpha^{SD} + \mathcal{I}_\alpha^{SD} - EN_\alpha^{(2)}) + (\mathcal{K}^{(3)} + \mathcal{I}^{(3)} - EN^{(3)}) | \phi_\gamma \rangle . \end{aligned} \quad (2.17)$$

This approximation corresponds to a single channel RGM equation for the relative-motion function $\psi_{\bar{\gamma}}$ of the γ -channel, and $V_{\bar{\gamma}}^D$ in Eq. (2.17) is the corresponding direct potential. The second type of approximation to obtain a coupled-channel RGM equation is achieved by assuming

$$\chi = \phi_\gamma \psi_{\bar{\gamma}} + \sum_{\alpha \neq \gamma} \phi_\alpha \psi_{\bar{\alpha}} . \quad (2.18)$$

With this assumption, we obtain

$$(T_{\bar{\gamma}} + V_{\bar{\gamma}} - \varepsilon_{\bar{\gamma}}) \psi_{\bar{\gamma}} + \sum_{\alpha \neq \gamma} (H_{\gamma\alpha} - EN_{\gamma\alpha}) \psi_{\bar{\alpha}} = 0 , \quad (2.19)$$

where we have defined, for $\alpha \neq \gamma$,

$$H_{\gamma\alpha} = \langle \phi_\gamma | \mathcal{K} + \mathcal{I} | \phi_\alpha \rangle = \langle \phi_\gamma | \mathcal{H} | \phi_\alpha \rangle , \quad N_{\gamma\alpha} = \langle \phi_\gamma | \mathcal{N} | \phi_\alpha \rangle . \quad (2.20)$$

§3. Structure of n -Cluster GCM Kernels for Systems Composed of $(0s)$ -Shell Clusters

3.1 General Procedure to Evaluate the GCM Kernels

Let C be one of the $(0s)$ -shell cluster systems with mass number $A \leq 4$. The shell-model wave function $\psi(C)$ with a common h.o. constant ν is composed of a totally symmetric product of $(0s)$ h.o. wave functions and a spin-isospin wave function

$\xi(1, 2, \dots, A)$ which is antisymmetric with respect to arbitrary interchanges of spin-isospin variables:

$$\psi(C) = \prod_{i=1}^A \phi_{(0s)}(\mathbf{x}_i; \nu) \xi(1, 2, \dots, A) . \quad (3.1)$$

Here, we have used a common notation

$$\phi_{(0s)}(\mathbf{x}; \nu) = \left(\frac{2\nu}{\pi} \right)^{\frac{3}{4}} e^{-\nu \mathbf{x}^2} \quad (3.2)$$

for the $(0s)$ h.o. wave function with ν , and the spin-isospin quantum numbers for the SU_4 irreducible representation $[\tilde{f}] = [1^A]$ of $\xi(1, 2, \dots, A)$ are suppressed for simplicity.

Owing to the complete quadratic nature of the Gaussian exponential factors, we can separate the c.m. motion described by $\phi_{(0s)}(\mathbf{X}; A\nu)$ with $\mathbf{X} = \sum_{i=1}^A \mathbf{x}_i/A$ in Eq. (3.1):

$$\psi(C) = \phi_{(0s)}(\mathbf{X}; A\nu) \phi(C) . \quad (3.3)$$

We call $\phi(C)$ in Eq. (3.3) an internal cluster wave function for the $(0s)$ -shell cluster C . The separation in Eq. (3.3) of the c.m. motion is of basic importance in the present treatment. For example, the translation of the coordinate system, $\mathbf{x}_i \rightarrow \mathbf{x}_i - \mathbf{S}$ ($i = 1 \sim A$), produces a simple relationship

$$\psi(C; \mathbf{S}) \equiv \prod_{i=1}^A \phi_{(0s)}^{\mathbf{S}}(\mathbf{x}_i; \nu) \xi(1, 2, \dots, A) = \phi_{(0s)}^{\mathbf{S}}(\mathbf{X}; A\nu) \phi(C) , \quad (3.4)$$

where $\phi_{(0s)}^{\mathbf{S}}(\mathbf{x}; \nu) \equiv \phi_{(0s)}(\mathbf{x} - \mathbf{S}; \nu)$.

Next, we consider an n -body system composed of such $(0s)$ -shell clusters C_i ($i = 1 \sim n$). For a c.m. coordinate \mathbf{X}_i of each cluster, it is sometimes more convenient to use a normalized one $\widehat{\mathbf{X}}_i = \sqrt{A_i} \mathbf{X}_i$ by the mass number A_i . In this paper, we use the notation $\widehat{}$ in order to specify the coordinate vectors normalized by the corresponding mass numbers [94]. The c.m. coordinate of a subsystem up to the i -th cluster thus becomes $\widehat{\widehat{\mathbf{X}}}_i = \sum_{j=1}^i \sqrt{A_j} \widehat{\mathbf{X}}_j / \sqrt{\overline{A}_i}$ ($i = 1 \sim n$), where $\overline{A}_i \equiv A_1 + A_2 + \dots + A_i$ is the mass number of the subsystem ($C_1 + C_2 + \dots + C_i$). The Jacobi coordinates $\widehat{\widehat{\boldsymbol{\xi}}}$ and the c.m. coordinate of the total system $\widehat{\widehat{\mathbf{X}}}_G$ are defined by using these notations as follows :

$$\begin{aligned} \widehat{\boldsymbol{\xi}}_i &\equiv \sqrt{\frac{\overline{A}_i}{A_{i+1}}} \widehat{\widehat{\mathbf{X}}}_{i+1} - \sqrt{\frac{A_{i+1}}{\overline{A}_{i+1}}} \widehat{\widehat{\mathbf{X}}}_i \quad (i = 1 \sim n-1) \\ \widehat{\widehat{\mathbf{X}}}_G &\equiv \sum_{i=1}^n \sqrt{A_i} \widehat{\widehat{\mathbf{X}}}_i / \sqrt{A} = \widehat{\widehat{\mathbf{X}}}_n , \end{aligned} \quad (3.5)$$

where $A = A_1 + \dots + A_n = \overline{A}_n$ and they satisfy

$$\sum_{i=1}^{n-1} \widehat{\boldsymbol{\xi}}_i^2 + \widehat{\widehat{\mathbf{X}}}_G^2 = \sum_{i=1}^n \widehat{\widehat{\mathbf{X}}}_i^2 . \quad (3.6)$$

The inverse transformation of Eq. (3.5) is found to be

$$\widehat{\mathbf{X}}_i \equiv \sqrt{\frac{A_i}{A}} \widehat{\mathbf{X}}_G + \sqrt{\frac{A_{i-1}}{A_i}} \widehat{\xi}_{i-1} - \sum_{j=i}^{n-1} \sqrt{\frac{A_i A_{j+1}}{A_j A_{j+1}}} \widehat{\xi}_j \quad (i = 1 \sim n) \quad (3.7)$$

under the convention $\xi_0 = 0$ and $\sum_{j=n}^{n-1} \dots = 0$. As an example, the unnormalized Jacobi coordinates in the case $n = 3$ are shown in Fig. 1. Furthermore, we use \mathbf{S}_i ($i = 1 \sim n$), \mathbf{S}_G and $\mathbf{z}_i/\sqrt{\nu}$ ($i = 1 \sim n - 1$) for the complex generator-coordinate vectors corresponding to \mathbf{X}_i ($i = 1 \sim n$), $\mathbf{X}_G = \widehat{\mathbf{X}}_G/\sqrt{A}$ and $\widehat{\xi}_i = \sqrt{\mu_i} \xi_i$ with $\mu_i = \bar{A}_i A_{i+1}/\bar{A}_{i+1}$, respectively. In Table I, we summarize various coordinate systems used in this paper.

TABLE I. Various coordinate systems used in this paper. In the second row, CGC denotes complex generator coordinates. In $\mathbf{z}_i/\sqrt{\gamma_i}$, γ_i is given by $\gamma_i = \sqrt{\mu_i} \nu$ with $\mu_i = \bar{A}_i A_{i+1}/\bar{A}_{i+1}$. Besides these, the notation $\widehat{}$ is used to specify the coordinate vectors normalized by the corresponding mass numbers.

| | usual coordinates | Jacobi coordinates | V-type coordinates |
|-----------------------|---------------------------------|---|---|
| dynamical coordinates | $\mathbf{X}_i \ (i = 1 \sim n)$ | $\xi_i \ (i = 1 \sim n - 1)$ \mathbf{X}_G | |
| CGC | $\mathbf{S}_i \ (i = 1 \sim n)$ | $\mathbf{z}_i/\sqrt{\gamma_i} \ (i = 1 \sim n - 1)$ \mathbf{S}_G | $\mathbf{T}_i \ (i = 1 \sim n - 1)$ \mathbf{S}_G |

For a fixed set of clusters C_1, C_2, \dots, C_n with $n \geq 3$, there are in general several different sets of Jacobi coordinates. The transformation among them is trivial, but important for practical applications of the present multicluster RGM formalism. We should be able to write down exchange kernels in any types of Jacobi coordinates, if we try to consider rearrangements of cluster groups. Since our main concern is on 3-cluster systems due to the present limitation of computer facilities, we will show transformations of Jacobi coordinates in detail only for 3-cluster systems. Three different sets of Jacobi coordinates $\xi^J = (\xi_1^J, \xi_2^J)$ ($J = I, II$ or III) are defined as is shown in Fig. 1. We reserve $J = III$ as a standard set of the Jacobi coordinates and usually omit the superscript III as is already assumed in Eq. (3.5) with $n=3$. This is convenient in §4.3 for the calculation of spin-isospin factors, since we assume C_3 as an α -core in the course of applying the valence orbital method. Now, suppose $(\alpha\beta\gamma)$ is an even permutation of (123) . If we introduce an alternative notation (γ) to specify the type of Jacobi coordinates J by $(1) = I, (2) = II, (3) = III$, we can compactly express $\xi_i^{(\gamma)}$ ($i = 1, 2$ and $\gamma = 1, 2, 3$) as

$$\xi_1^{(\gamma)} = \mathbf{X}_\beta - \mathbf{X}_\alpha \quad , \quad \xi_2^{(\gamma)} = \mathbf{X}_\gamma - \frac{A_\alpha \mathbf{X}_\alpha + A_\beta \mathbf{X}_\beta}{A_\alpha + A_\beta} \quad . \quad (3.8)$$

Let us define the reduced mass numbers $\mu_1^{(\gamma)}$ and $\mu_2^{(\gamma)}$ by

$$\mu_1^{(\gamma)} = \frac{A_\alpha A_\beta}{A_\alpha + A_\beta}, \quad \mu_2^{(\gamma)} = \frac{(A_\alpha + A_\beta)A_\gamma}{A}, \quad (3.9)$$

with $A_\alpha + A_\beta + A_\gamma = A_1 + A_2 + A_3 = A$. Then, the h.o. width parameters assigned to the two types of relative motion of the three clusters in the Jacobi coordinates of type-(γ) are given by $\gamma_i^{(\gamma)} = \mu_i^{(\gamma)}\nu$ ($i = 1, 2$). If we define a 3×2 matrix $\widehat{\xi}^{(\gamma)} = (\sqrt{\mu_1^{(\gamma)}}\boldsymbol{\xi}_1^{(\gamma)}, \sqrt{\mu_2^{(\gamma)}}\boldsymbol{\xi}_2^{(\gamma)})$, the orthogonal transformation of the Jacob-coordinates for an arbitrary set of α and β ($\alpha, \beta = 1 \sim 3$) is expressed as

$$\widehat{\xi}^{(\beta)} = \widehat{\xi}^{(\alpha)} \Xi^{(\alpha)(\beta)}, \quad (3.10)$$

where $\Xi^{(\alpha)(\beta)}$ is a 2×2 orthogonal matrix given by

$$\Xi^{(\alpha)(\beta)} = \frac{1}{\sqrt{A_\alpha^c A_\beta^c}} \begin{pmatrix} \delta_{\alpha\beta} A - \sqrt{A_\alpha A_\beta} & -\sum_\gamma e_{\alpha\beta\gamma} \sqrt{A_\gamma A} \\ \sum_\gamma e_{\alpha\beta\gamma} \sqrt{A_\gamma A} & \delta_{\alpha\beta} A - \sqrt{A_\alpha A_\beta} \end{pmatrix} \quad (3.11)$$

with $A_\alpha^c = A - A_\alpha$ etc. In Eq. (3.11), we have introduced 3-dimensional antisymmetric tensor defined through the usual rule; $e_{\alpha\beta\gamma} = 1$ if $(\alpha\beta\gamma)$ is an even permutation of (123), -1 if $(\alpha\beta\gamma)$ is an odd permutation, and zero otherwise.

The essential relationship which enables us to calculate the GCM kernels from the matrix elements of the Brink-type wave functions is based on Eqs. (3.4) and (3.6):

$$\prod_{i=1}^{n-1} A_{\gamma_i}(\boldsymbol{\xi}_i, \mathbf{z}_i) \phi_{(0s)}^{\mathbf{S}_G}(\mathbf{X}_G, A\nu) = \exp\left\{\frac{1}{2} \sum_{i=1}^{n-1} \mathbf{z}_i^2\right\} \prod_{i=1}^n \phi_{(0s)}^{\mathbf{S}_i}(\mathbf{X}_i, A_i\nu), \quad (3.12)$$

where $\gamma_i = \mu_i\nu$ and

$$A_\gamma(\boldsymbol{\xi}, \mathbf{z}) = \left(\frac{2\gamma}{\pi}\right)^{\frac{3}{4}} \exp\left\{-\gamma\left(\boldsymbol{\xi} - \frac{\mathbf{z}}{\sqrt{\gamma}}\right)^2 + \frac{\mathbf{z}^2}{2}\right\} \quad (3.13)$$

is the h.o. coherent state in the Bargmann space [92], [93]. The relationship between \mathbf{z}_i ($i = 1 \sim n-1$) and \mathbf{S}_i ($i = 1 \sim n$) are obtained from Eq. (3.5) or (3.7) by a trivial replacement $\widehat{\boldsymbol{\xi}}_i \rightarrow \mathbf{z}_i/\sqrt{\nu}$ and $\widehat{\mathbf{X}}_i \rightarrow \widehat{\mathbf{S}}_i = \sqrt{A_i} \mathbf{S}_i$. Here, we set $\mathbf{S}_G = 0$ in Eq. (3.12) and multiply it by all the internal cluster functions $\phi_0 \equiv \phi(C_1)\phi(C_2)\cdots\phi(C_n)$. Then, by using Eq. (3.4), one finds

$$\phi_G A(\boldsymbol{\xi}; z) \phi_0 = \exp\left\{\frac{1}{2} Tr(tzz)\right\} \prod_{i=1}^n \psi(C_i; \mathbf{S}_i), \quad (3.14)$$

where a simplifying notation

$$\phi_G = \phi_{(0s)}(\mathbf{X}_G, A\nu), \quad A(\boldsymbol{\xi}; z) = \prod_{i=1}^{n-1} A_{\gamma_i}(\boldsymbol{\xi}_i, \mathbf{z}_i) \quad (3.15)$$

is used. Furthermore, we use $3 \times (n-1)$ matrix notation like $\boldsymbol{\xi} = (\xi_{\gamma i}) = (\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_{n-1})$, $z = (z_{\gamma i}) = (\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_{n-1})$ and $Tr(tzz) = \sum_{\gamma i} z_{\gamma i}^2 = \sum_{i=1}^{n-1} \mathbf{z}_i^2$ with $\gamma = x, y$, and z . The explicit expressions for \mathbf{S}_i in terms of \mathbf{z}_i are given by¹

¹In Eq. (3.16a), the correct notation is not $P_\alpha \mathbf{z}$ but $\mathbf{z} P_\alpha$, if we use the matrix notation $P = (P_{i\alpha})$ with $P_{i\alpha} = (P_\alpha)_i$. (See Eq. (3.97).) We avoid this clumsy notation, unless it is inevitable.

$$\sqrt{\nu} \mathbf{S}_\alpha = P_\alpha \mathbf{z} = \sum_{i=1}^{n-1} (P_\alpha)_i \mathbf{z}_i \quad (3.16a)$$

with

$$(P_\alpha)_i = -\frac{1}{\sqrt{\mu_i}} (p_\alpha)_i \quad (3.16b)$$

and

$$(p_\alpha)_i = \begin{cases} 0 \\ -(\bar{A}_i/\bar{A}_{i+1}) \\ (A_{i+1}/\bar{A}_{i+1}) \end{cases} \quad \text{for } \begin{cases} i = 1 \sim \alpha - 2 \\ i = \alpha - 1 \\ i = \alpha \sim n - 1 \end{cases} \quad \text{or } \begin{cases} \alpha = i + 2 \sim n \\ \alpha = i + 1 \\ \alpha = 1 \sim i \end{cases} . \quad (3.16c)$$

(We have used a notation $\alpha = 1 \sim n$, instead of i , for the convenience of later applications to GCM kernels.) Note that we always have $\sum_{\alpha=1}^n A_\alpha \mathbf{S}_\alpha = 0$.

The relationship (3.12) is conveniently used for evaluating GCM kernels, which are now defined through

$$I^\Omega(z; z') = \langle A(\xi; z) \phi_0 | \mathcal{O}^\Omega \mathcal{A}' | A(\xi; z') \phi_0 \rangle \quad (3.17)$$

for any A -particle symmetric operator \mathcal{O}^Ω . The type of the GCM kernel is specified by Ω , which we assign to $\Omega = N$ for the normalization kernel, $\Omega = K$ for the kinetic-energy kernel, and any other types of the translationally and Galilean invariant two-body interactions for the others.²

$$\mathcal{O}^N = 1 \quad , \quad \mathcal{O}^K = \sum_{s=1}^A t_s - T_G \quad , \quad \mathcal{O}^\Omega = \sum_{s<t}^A v_{st}^{(\Omega)} . \quad (3.18)$$

In \mathcal{O}^K , $t_s = (-\hbar^2/2M) \nabla_{\mathbf{x}_s}^2$ and $T_G = (-\hbar^2/2AM) \nabla_{\mathbf{X}_G}^2$ with M being the averaged nucleon mass $M = (M_n + M_p)/2$. (We neglect the small mass difference of the proton and the neutron to utilize the isospin formalism.) The antisymmetrization operator \mathcal{A}' in Eq. (3.17) is only for permutations among different clusters with $A!/(A_1! \cdots A_n!)$ terms due to the antisymmetric property of the internal cluster wave functions. What we need to do is to evaluate the matrix elements³

$$G^\Omega(S; S') \equiv \langle \mathcal{A}' \prod_{i=1}^n \psi(C_i; \mathbf{S}_i) | \mathcal{O}^\Omega | \prod_{i=1}^n \psi(C_i; \mathbf{S}'_i) \rangle \quad (3.19)$$

by using the standard shell-model techniques. Then the necessary GCM kernels (3.17) are obtained through

$$I^\Omega(z; z') = \exp \left\{ \frac{1}{2} \left(Tr(t^* z^* z^*) + Tr(t z' z') \right) \right\} G^\Omega(S; S') . \quad (3.20)$$

²Of course, it is also possible to deal with a one-body operator $\mathcal{O}^\Omega = \sum_{s=1}^A \mathcal{O}_s^{(\Omega)}$.

³We move \mathcal{A}' to the bra side by using the totally symmetric nature of \mathcal{O}^Ω , which turns out to be convenient for later discussions.

As to the normalization kernels for the systems of ($0s$)-shell clusters, a quite general expression is already derived in refs. [95] and [96] by using the powerful techniques of double Gel'fand polynomials [86]. (See, for example, Eq.(3.20) of ref. [95].) The kinetic-energy kernels are simply obtained from the normalization kernel in the present case, as is shown in the next subsection. The main reason for this simplicity is because these operators do not involve any spin-isospin degrees of freedom. As a result, the SU_4 symmetry [\tilde{f}] and its internal quantum numbers, i.e., the total spin and isospin values, are all conserved. On the other hand, the two-body interactions $v_{st}^{(\Omega)}$ usually involve the spin-isospin dependence and general treatment of their matrix elements with respect to intricately coupled many-cluster spin-isospin wave functions is rather difficult. Therefore, we will develop in the next subsections rather standard techniques [79] to separately evaluate the spatial and spin-isospin matrix elements by the use of the double-coset generator expansion of the antisymmetrization operator \mathcal{A}' and the *cfp* expansion of the antisymmetric spin-isospin wave functions. A simpler treatment of three cluster systems involving at least one α -cluster is discussed in §4.3.

3.2 Double-Coset Generator Expansion and Particle-Exchange Tables

Since a quite extensive description of the double-coset generator expansion is already presented in the literature [79]~[82], only the essential result needed in our application is recapitulated here. Let us consider permutations of A particles,

$$p = \begin{pmatrix} 1 & 2 & \cdots & A \\ p_1 & p_2 & \cdots & p_A \end{pmatrix} \in S_A \quad , \quad (3.21)$$

where S_A is the symmetric group of the ordered set $\mathbf{A} \equiv \{1, 2, \dots, A\}$. Since this system is composed of n clusters, C_1, C_2, \dots, C_n , we can naturally introduce a subgroup of S_A , $H \subset S_A$, the elements of which transform particles only inside of their own clusters :

$$H = S_{A_1} \otimes S_{A_2} \otimes \cdots \otimes S_{A_n} \quad , \quad (3.22)$$

where S_{A_i} is composed of permutations of $\mathbf{A}_i \equiv \{\bar{A}_{i-1} + 1, \bar{A}_{i-1} + 2, \dots, \bar{A}_i\}$ with $\bar{A}_i = \bar{A}_{i-1} + A_i$ and $\bar{A}_0 = 0$. In terms of this subgroup H , S_A can be decomposed into a direct sum of the double cosets, $S_A = \cup_k H z_k H$;⁴ namely,

$$p = g z_k f \quad (g, f \in H) \quad (3.23)$$

with z_k being a generator of the double coset characterized by an index k . The central issue here is to find the index k which uniquely and completely characterizes the double coset and to find the explicit form of the generator z_k . It can be shown that these are achieved by simply partitioning the $A \times A$ matrix representation of $p = (p_{st})$ with $p_{st} = \delta_{p_s, t}$ ($s, t = 1 \sim A$) into n^2 blocks as is shown below :

⁴It is also possible to use two different subgroups $H = S_{A_1} \otimes S_{A_2} \otimes \cdots \otimes S_{A_n}$ and $K = S_{A'_1} \otimes S_{A'_2} \otimes \cdots \otimes S_{A'_n}$ ($A_1 + \cdots + A_n = A'_1 + \cdots + A'_n = A$) to achieve a double-coset expansion $S_A = \cup_k H z_k K$. Through this procedure, we can extend the present formalism to the case when two different cluster-decompositions are assumed for the bra and the ket states. (See, for example, Eq.(3.20) of ref. [95].) We will not dare to complicate equations by this rather trivial generalization.

$$p = \begin{pmatrix} D_{11} & \cdots & D_{1n} \\ \vdots & & \vdots \\ D_{n1} & \cdots & D_{nn} \end{pmatrix} . \tag{3.24}$$

The blocks D_{ij} are $A_i \times A_j$ matrices with elements 1 or 0. The number of one in each block, k_{ij} , depends on the permutation p , but is apparently the same for any permutations belonging to the same double coset. This is because D_{ij} for p in Eq. (3.23) is expressed as $D_{ij}(p) = g_i D_{ij}(z_k) f_j$ with $g_i \in S_{A_i}$ and $f_j \in S_{A_j}$. If we arrange the non-negative integers k_{ij} in the $n \times n$ matrix form just like the decomposition of p in Eq. (3.24), we can use this $[k] \equiv (k_{ij})$ as an index to specify the double coset in a unique way. In order to enumerate all possible types of double cosets for H , we only need to find solutions for the weight conditions

$$\sum_{i=1}^n k_{ij} = A_j \quad , \quad \sum_{j=1}^n k_{ij} = A_i \quad , \quad k_{ij} = \text{non-negative integers} . \tag{3.25}$$

Since we can show that the number of the elements for the double cosets $[k]$ is given by $(A_1! \cdots A_n!)^2 / k!$ with the convention $k! \equiv \prod_{i=1}^n \prod_{j=1}^n k_{ij}!$, the sum formula⁵

$$\sum_{[k]} \frac{(A_1! \cdots A_n!)^2}{k!} = A! \tag{3.26}$$

guarantees that all the permutations of S_A are reproduced through Eq. (3.23). These $n \times n$ matrices $[k]$ are called double-coset symbols or partition matrices.⁶ It is also legitimate to call these symbols particle-exchange tables, since among the A_j particles in $\mathbf{A}_j = \{\bar{A}_{j-1} + 1, \bar{A}_{j-1} + 2, \cdots, \bar{A}_{j-1} + A_j\}$, k_{1j} particles are transformed to C_1 , k_{2j} particles to C_2 , \cdots , and k_{nj} particles to C_n . If we define ordered sets $\mathbf{k}_{1j}, \mathbf{k}_{2j}, \cdots, \mathbf{k}_{nj}$ through the correspondence $\mathbf{A}_j = \{\mathbf{k}_{1j}, \mathbf{k}_{2j}, \cdots, \mathbf{k}_{nj}\}$, the $A_i \times A_j$ submatrix $D_{ij}(z_k)$ for z_k can be taken to be

⁵This formula is easily proved by combining several multi-nomial expansions.

⁶It is stated at a footnote of ref. [79] that these symbols have been introduced by H. H. Hackenbroich.

$$\begin{array}{c}
 \longleftarrow k_{1j} \longrightarrow \cdots \longleftarrow k_{ij} \longrightarrow \cdots \longleftarrow k_{nj} \longrightarrow \\
 \\
 D_{ij}(z_k) = \left(\begin{array}{c|c|c}
 & & \\
 \hline
 & 1 & \\
 & \ddots & \\
 & & 1 \\
 \hline
 & &
 \end{array} \right) \begin{array}{c}
 \uparrow \\
 k_{i1} \\
 \downarrow \\
 \vdots \\
 \uparrow \\
 k_{ij} \\
 \downarrow \\
 \vdots \\
 \uparrow \\
 k_{in} \\
 \downarrow
 \end{array} \quad (3.27)
 \end{array}$$

namely, $k_{ij} \times k_{ij}$ subblock is the unit matrix and the others are zero. Then, since we have $\sum_{j=1}^n D_{ij}(z_k) \mathbf{A}_j = \{\mathbf{k}_{i1}, \mathbf{k}_{i2}, \dots, \mathbf{k}_{in}\} \equiv \mathbf{A}'_i$, we get the correspondence $z_k \mathbf{A}_i = \mathbf{A}'_i$ or

$$z_k = \begin{pmatrix} 1 & 2 & \cdots & A \\ (z_k)_1 & (z_k)_2 & \cdots & (z_k)_A \end{pmatrix} = \begin{array}{c} \longleftarrow A_1 \longrightarrow \cdots \longleftarrow A_n \longrightarrow \\ \left(\begin{array}{cccc} \mathbf{k}_{11} & \mathbf{k}_{21} & \cdots & \mathbf{k}_{n1} \\ \mathbf{k}_{12} & \mathbf{k}_{22} & \cdots & \mathbf{k}_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{k}_{1n} & \mathbf{k}_{2n} & \cdots & \mathbf{k}_{nn} \end{array} \right) \end{array} \quad (3.28)$$

By using these results, we can easily derive that the antisymmetrization operator \mathcal{A}' in Eq. (3.19) is reduced to

$$\mathcal{A}' = \frac{1}{A_1! \cdots A_n!} \sum_{p \in S_A} \delta_p p \longrightarrow \sum_{[k]} \frac{A_1! \cdots A_n!}{k!} \delta_{z_k} z_k \equiv \sum_{[k]} C_k z_k \quad , \quad (3.29)$$

where δ_p or δ_{z_k} is the signature of the permutation.

The next step is to separate the spatial and spin-isospin parts in Eq. (3.19). We define $\prod_{i=1}^n \psi(C_i; \mathbf{S}_i) = \varphi \xi$ with

$$\varphi = \prod_{j=1}^n \prod_{s \in \mathbf{A}_j} \phi_{(0s)}^{\mathbf{S}_j}(\mathbf{x}_s; \nu) \quad , \quad \xi = \prod_{j=1}^n \xi(\bar{A}_{j-1} + 1, \dots, \bar{A}_j) \quad (3.30)$$

for the bra state and $\varphi' \xi'$ for the ket state. Then, the normalization kernel $G^N(S; S')$ is obtained from

$$G^N(S; S') = \sum_{[k]} X_k^N J_k^N \quad (3.31)$$

with

$$X_k^N = C_k \langle z_k \xi | \xi' \rangle, \quad J_k^N = \langle z_k \varphi | \varphi' \rangle. \quad (3.32)$$

In order to evaluate the spatial matrix elements J_k^N , it is convenient to express φ' as

$$\varphi' = \prod_{j=1}^n \prod_{i=1}^n \prod_{s \in \mathbf{k}_{ij}} \phi_{(0s)}^{\mathbf{S}'_j}(\mathbf{x}_s; \nu). \quad (3.33)$$

Then, the effect of $z_k \varphi$ is, from $z_k \mathbf{A}_j = \mathbf{A}'_j = \{\mathbf{k}_{j1}, \mathbf{k}_{j2}, \dots, \mathbf{k}_{jn}\}$ in Eq. (3.28),

$$\begin{aligned} z_k \varphi &= \prod_{j=1}^n \prod_{s \in \mathbf{A}'_j} \phi_{(0s)}^{\mathbf{S}_j}(\mathbf{x}_s; \nu) = \prod_{j=1}^n \prod_{i=1}^n \prod_{s \in \mathbf{k}_{ji}} \phi_{(0s)}^{\mathbf{S}_j}(\mathbf{x}_s; \nu) \\ &= \prod_{j=1}^n \prod_{i=1}^n \prod_{s \in \mathbf{k}_{ij}} \phi_{(0s)}^{\mathbf{S}_i}(\mathbf{x}_s; \nu). \end{aligned} \quad (3.34)$$

The spatial overlap integral J_k^N is calculated to be

$$\begin{aligned} J_k^N &= \prod_{j=1}^n \prod_{i=1}^n \prod_{s \in \mathbf{k}_{ij}} \langle \phi_{(0s)}^{\mathbf{S}_i}(\mathbf{x}_s; \nu) | \phi_{(0s)}^{\mathbf{S}'_j}(\mathbf{x}_s; \nu) \rangle \\ &= \prod_{j=1}^n \prod_{i=1}^n \exp \left\{ -\frac{\nu}{2} k_{ij} (\mathbf{S}_i^* - \mathbf{S}'_j)^2 \right\} = \exp \left\{ -\frac{\nu}{2} \sum_{j=1}^n \sum_{i=1}^n k_{ij} (\mathbf{S}_i^* - \mathbf{S}'_j)^2 \right\}, \end{aligned} \quad (3.35)$$

where we have used the single-particle overlap given by

$$\langle \phi_{(0s)}^{\mathbf{S}}(\mathbf{x}; \nu) | \phi_{(0s)}^{\mathbf{S}'}(\mathbf{x}; \nu) \rangle = \langle (0s)_{\mathbf{S}} | (0s)_{\mathbf{S}'} \rangle = \exp \left\{ -\frac{\nu}{2} (\mathbf{S}^* - \mathbf{S}')^2 \right\}. \quad (3.36)$$

From here on, we use a simplifying notation $|(0s)_{\mathbf{S}}\rangle$ defined through $\langle \mathbf{x} | (0s)_{\mathbf{S}} \rangle = \phi_{(0s)}^{\mathbf{S}}(\mathbf{x}; \nu) = \phi_{(0s)}(\mathbf{x} - \mathbf{S}; \nu)$. Thus we find, for $G^N(S; S')$ in Eq. (3.31),

$$G^N(S; S') = \exp \left\{ -\frac{\nu}{2} \sum_{i=1}^n A_i (\mathbf{S}_i^{*2} + \mathbf{S}_i'^2) \right\} \sum_{[k]} X_k^N \exp \left\{ \nu \sum_{i,j=1}^n k_{ij} (\mathbf{S}_i^* \cdot \mathbf{S}'_j) \right\}. \quad (3.37)$$

The front exponential factor in Eq. (3.37) is cancelled with that in Eq. (3.20) due to Eq. (3.6) for the generator coordinates. Further use of the coordinate transformation (3.16) yields⁷

$$I^N(z; z') = \sum_{[k]} X_k^N \exp \{ \text{Tr}(z^* Q[k]^t z') \}, \quad (3.38)$$

⁷The simple result that $I^N(z; z')$ is a function of only $(\mathbf{z}_i^* \cdot \mathbf{z}'_j)$ ($i, j = 1 \sim n-1$) is due to the SU_3 -scalar property of the antisymmetrization operator \mathcal{A}' with respect to the Elliott SU_3 algebra of h.o. wave functions [92], [97].

where $(n-1) \times (n-1)$ matrix $Q[k]$ represents the coefficients of the particle exchange for $[k]$ and the matrix elements are explicitly given by $(Q[k])_{ij} = \sum_{\alpha,\beta=1}^n k_{\alpha\beta} (P_\alpha)_i (P_\beta)_j$ or

$$(Q[k])_{ij} = \sqrt{\mu_i \mu_j} \left\{ \frac{1}{\bar{A}_i \bar{A}_j} \sum_{\alpha=1}^i \sum_{\beta=1}^j k_{\alpha\beta} - \frac{1}{\bar{A}_i \bar{A}_{j+1}} \sum_{\alpha=1}^i k_{\alpha,j+1} - \frac{1}{\bar{A}_{i+1} \bar{A}_j} \sum_{\beta=1}^j k_{i+1,\beta} + \frac{1}{\bar{A}_{i+1} \bar{A}_{j+1}} k_{i+1,j+1} \right\} \quad (i, j = 1 \sim n-1) . \quad (3.39)$$

In particular, $[k]$ for 2-cluster kernels is parametrized as

$$[k] = \begin{bmatrix} A_1 - x & x \\ x & A_2 - x \end{bmatrix} \quad \text{with} \quad x = 0 \sim \min\{A_1, A_2\} , \quad (3.40)$$

and the normalization kernel is given by

$$I^N(\mathbf{z}; \mathbf{z}') = \sum_{x=0}^{\min\{A_1, A_2\}} X_x^N \exp \left\{ \left(1 - \frac{x}{\mu}\right) (\mathbf{z}^* \cdot \mathbf{z}') \right\} . \quad (3.41)$$

In 3-cluster systems with $n=3$, $[k]$ is parametrized in ref. [51] as

$$[k] = \begin{bmatrix} A_1 - x & u & x - u \\ v & A_2 - y & y - v \\ x - v & y - u & A_3 - x - y + u + v \end{bmatrix} \quad \text{with} \quad \begin{cases} x = 0 \sim A_1, y = 0 \sim A_2 \\ u, v = 0 \sim \min\{x, y\} \\ x + y - u - v \leq A_3 \end{cases} . \quad (3.42)$$

The set of non-negative integers $\{x, y, u, v\}$ are extensively used in ref. [51] to specify the exchange types. In terms of these, the 2×2 matrix $Q_{xyuv} = (Q_{ij})$ is given by

$$\begin{aligned} Q_{11} &= 1 - \left(\frac{x}{A_1^2} + \frac{y}{A_2^2} + \frac{u+v}{A_1 A_2} \right) \mu_1 , & Q_{12} &= \left(-\frac{x-u}{A_1} + \frac{y-v}{A_2} \right) \sqrt{\frac{\mu_1}{\mu_2}} \\ Q_{21} &= \left(-\frac{x-v}{A_1} + \frac{y-u}{A_2} \right) \sqrt{\frac{\mu_1}{\mu_2}} , & Q_{22} &= 1 - \frac{x+y-u-v}{\mu_2} . \end{aligned} \quad (3.43)$$

Next, let us consider in general a single-particle operator $\mathcal{O} = \sum_{s=1}^A u_s w_s$, where we keep in mind applications to the kinetic-energy operator, as well as the two-body interaction in the next subsection. (The index Ω in \mathcal{O}^Ω is omitted for simplicity.) Here, we have separated the operator into the spatial part u_s and the spin-isospin part w_s . The GCM kernel in this particular case is calculated from

$$G(S; S') = \sum_{[k]} C_k \sum_{s=1}^A \langle z_k \varphi | u_s | \varphi' \rangle \langle z_k \xi | w_s | \xi' \rangle . \quad (3.44)$$

The spatial integrals⁸

⁸The assumption $u_s = u(\mathbf{x}_s)$ does not mean that the translational invariance is not kept in the present formalism. It is already incorporated into the whole GCM kernel at the time of supplementing an appropriate c.m. integral. See the next example for the charge form factors.

$$\langle z_k \varphi | u_s | \varphi' \rangle = \langle \prod_{j=1}^n \prod_{i=1}^n \prod_{t \in \mathbf{k}_{ij}} \phi_{(0s)}^{\mathbf{S}_i}(\mathbf{x}_t; \nu) | u(\mathbf{x}_s) | \prod_{j=1}^n \prod_{i=1}^n \prod_{t \in \mathbf{k}_{ij}} \phi_{(0s)}^{\mathbf{S}'_j}(\mathbf{x}_t; \nu) \rangle \quad (3.45)$$

are composed of only n^2 independent types, depending on which partition $\mathbf{k}_{\alpha\beta}$ ($\alpha, \beta = 1 \sim n$) of \mathbf{A} the particle index s belongs to. Thus, we can subdivide the summation over $s = 1 \sim A$ in Eq. (3.44) into $\sum_{\alpha, \beta=1}^n \sum_{s \in \mathbf{k}_{\alpha\beta}}$, and use the ordered pair $\{\alpha, \beta\}$ for the purpose of specifying different “interaction” types. (We use the word “interaction”, since this type classification is nothing but the one-body operator version of that used for the interaction kernels in the next subsection.) The basic one-body matrix element for the type $\{\alpha, \beta\}$ is conveniently defined through

$$\mathcal{T}_{\{\alpha, \beta\}} = \langle (0s)_{\mathbf{S}_\alpha} | (0s)_{\mathbf{S}'_\beta} \rangle^{-1} \langle (0s)_{\mathbf{S}_\alpha} | u | (0s)_{\mathbf{S}'_\beta} \rangle . \quad (3.46)$$

Since the spatial integrals are given by $J_k^N \mathcal{T}_{\{\alpha, \beta\}}$, the GCM kernel in Eq. (3.44) is given by

$$G(S; S') = \sum_{[k]} J_k^N \sum_{\alpha, \beta=1}^n X_{k\{\alpha, \beta\}} \mathcal{T}_{\{\alpha, \beta\}} , \quad (3.47)$$

where the spin-isospin factors are defined by

$$X_{k\{\alpha, \beta\}} = C_k \langle z_k \xi | \sum_{s \in \mathbf{k}_{\alpha\beta}} w_s | \xi' \rangle . \quad (3.48)$$

The transformation to $I(z; z')$ through Eq. (3.20) yields

$$I(z; z') = \sum_{[k]} \exp \{ \text{Tr}(z^* Q[k]^t z') \} \sum_{\alpha, \beta=1}^n X_{k\{\alpha, \beta\}} \mathcal{T}_{\{\alpha, \beta\}} . \quad (3.49)$$

Let us now specialize our discussion to the kinetic-energy kernels. In this case, we have $u_s = t_s$, $w_s = 1$, and the spin-isospin factor $X_{k\{\alpha, \beta\}}$ in Eq. (3.48) is simply given by $X_{k\{\alpha, \beta\}}^K = k_{\alpha\beta} X_k^N$. The spatial factor $\mathcal{T}_{\{\alpha, \beta\}}$ for t_s is obtained from

$$\langle (0s)_{\mathbf{S}} | t | (0s)_{\mathbf{S}'} \rangle = \frac{3\hbar^2\nu}{2M} \left\{ 1 - \frac{\nu}{3} (\mathbf{S}^* - \mathbf{S}')^2 \right\} \langle (0s)_{\mathbf{S}} | (0s)_{\mathbf{S}'} \rangle \quad (3.50a)$$

$$= \frac{3\hbar^2\nu}{2M} \left(1 + \frac{2}{3} \nu \frac{\partial}{\partial \nu} \right) \langle (0s)_{\mathbf{S}} | (0s)_{\mathbf{S}'} \rangle . \quad (3.50b)$$

It is now straightforward to use these results to obtain

$$I^K(z; z') = \frac{3\hbar^2\nu}{2M} \sum_{[k]} X_k^N \exp \{ \text{Tr}(z^* Q[k]^t z') \} \\ \times \left\{ A - 1 - \frac{1}{3} \left(\text{Tr}(t^* z^* z^*) + \text{Tr}(t^* z' z') \right) + \frac{2}{3} \text{Tr}(z^* Q[k]^t z') \right\} . \quad (3.51)$$

For $(0s)$ -shell cluster systems, however, the above procedure is not actually necessary. The second equation in Eq. (3.50b) shows that the effect of the single-particle kinetic-energy operator is simply generated through the differentiation of the h.o. width parameter ν ; i.e., $t \rightarrow 1 + (2/3)\nu(\partial/\partial\nu)$ except for a simple factor. By using this simple relationship, we can immediately write down

$$G^K(S; S') = \langle z_k \varphi \xi | \left(\sum_{s=1}^A t_s - T_G \right) | \varphi' \xi' \rangle = \frac{3\hbar^2\nu}{2M} \left(A - 1 + \frac{2}{3}\nu \frac{\partial}{\partial\nu} \right) G^N(S; S') , \quad (3.52)$$

from which the result in Eq. (3.51) is easily obtained by using the explicit expression of $G^N(S; S')$ in Eq. (3.37).

As another example of the one-body operator, let us discuss the charge-form-factor operator

$$\mathcal{O}^{cff}(\mathbf{q}) = \sum_{s=1}^A e^{i\mathbf{q}(\mathbf{x}_s - \mathbf{X}_G)} \frac{1 + \tau_{sz}}{2} . \quad (3.53)$$

For the spatial integral, we only need to consider $u(\mathbf{x}) = e^{i\mathbf{q}\mathbf{x}}$, since the \mathbf{X}_G -dependence in Eq. (3.53) can be eliminated, if the c.m. integral

$$\exp \left\{ \frac{\mathbf{q}^2}{8A\nu} \right\} \langle \phi_G | e^{i\mathbf{q}\mathbf{X}_G} | \phi_G \rangle = 1 \quad (3.54)$$

is imposed. Then, Eq. (3.46) becomes

$$T_{\{\alpha,\beta\}}^{cff} = \langle (0s)_{\mathbf{S}_\alpha} | (0s)_{\mathbf{S}'_\beta} \rangle^{-1} \langle (0s)_{\mathbf{S}_\alpha} | e^{i\mathbf{q}\mathbf{x}} | (0s)_{\mathbf{S}'_\beta} \rangle = \exp \left\{ -\frac{\mathbf{q}^2}{8\nu} + i\frac{1}{2}(\mathbf{S}_\alpha^* + \mathbf{S}'_\beta) \cdot \mathbf{q} \right\} . \quad (3.55)$$

If we further define the spin-isospin factors by

$$X_{k\{\alpha,\beta\}}^{cff} = C_k \langle z_k \xi | \sum_{s \in \mathbf{k}_{\alpha\beta}} \frac{1 + \tau_{sz}}{2} | \xi' \rangle , \quad (3.56)$$

the GCM kernel is given by

$$I^{cff}(z; z'; \mathbf{q}) = \exp \left\{ -\frac{\mathbf{q}^2}{8\nu} \left(1 - \frac{1}{A} \right) \right\} \sum_{[k]} \exp \{ Tr(z^* Q[k]^t z') \} \\ \times \sum_{\alpha,\beta=1}^n X_{k\{\alpha,\beta\}}^{cff} \exp \left\{ i \frac{1}{2\sqrt{\nu}} (P_\alpha \mathbf{z}^* + P_\beta \mathbf{z}') \cdot \mathbf{q} \right\} , \quad (3.57)$$

where $P_\alpha \mathbf{z} = \sum_{i=1}^{n-1} (P_\alpha)_i \mathbf{z}_i$ etc. with $(P_\alpha)_i$ given in Eq. (3.16).

3.3 Interaction Kernels

It is almost straightforward to extend the discussion for the one-body operator in the preceding subsection to any kind of two-body interactions $\mathcal{O}^\Omega = \sum_{s<t}^A v_{st}^{(\Omega)}$ with the space and spin-isospin decomposition $v_{st}^{(\Omega)} = u_{st}^{(\Omega)} w_{st}^{(\Omega)}$, and to obtain the general form of the GCM interaction kernels. Namely, we only need to consider the subdivision of two summations for s and t ($= 1 \sim A$) in $v_{st}^{(\Omega)}$ as

$$\sum_{s<t}^A \longrightarrow \sum_{\alpha,\beta=1}^n \sum_{\gamma,\delta=1}^n \sum_{s \in \mathbf{k}_{\alpha,\beta}} \sum_{t \in \mathbf{k}_{\gamma,\delta}} \quad \text{with} \quad s < t . \quad (3.58)$$

We denote this pairwise summation of $\{\alpha, \beta\}$ and $\{\gamma, \delta\}$ by $\sum_{\{\alpha\beta;\gamma\delta\}}$, and introduce the spatial interaction factors and the spin-isospin factors through

$$T_{\{\alpha\beta;\gamma\delta\}}^\Omega = \langle (0s)\mathbf{s}_\alpha | (0s)\mathbf{s}'_\beta \rangle^{-1} \langle (0s)\mathbf{s}_\gamma | (0s)\mathbf{s}'_\delta \rangle^{-1} \langle (0s)\mathbf{s}_\alpha (0s)\mathbf{s}_\gamma | u^{(\Omega)} | (0s)\mathbf{s}'_\beta (0s)\mathbf{s}'_\delta \rangle \quad (3.59a)$$

and

$$X_{k\{\alpha\beta;\gamma\delta\}}^\Omega = C_k \langle z_k \xi | \sum_{s \in \mathbf{k}_{\alpha\beta}, t \in \mathbf{k}_{\gamma\delta}, s < t} w_{st}^{(\Omega)} | \xi' \rangle , \quad (3.59b)$$

respectively. (See the similar definitions for one-body operators in Eqs. (3.46) and (3.48).) Then, as a natural extension of Eq. (3.49), we obtain

$$I^\Omega(z; z') = \sum_{[k]} \exp \{ Tr(z^* Q[k]^t z') \} \sum_{\{\alpha\beta;\gamma\delta\}} X_{k\{\alpha\beta;\gamma\delta\}}^\Omega T_{\{\alpha\beta;\gamma\delta\}}^\Omega , \quad (3.60a)$$

or more simply

$$I^\Omega(z; z') = \sum_{[k]} \exp \{ Tr(z^* Q[k]^t z') \} \sum_{\mathcal{T}} X_{k\mathcal{T}}^\Omega T^\Omega , \quad (3.60b)$$

if we identify the combination $\{\alpha\beta; \gamma\delta\}$ with \mathcal{T} itself; $T_{\{\alpha\beta;\gamma\delta\}} \equiv \mathcal{T}$. It is a trivial exercise to extend this discussion to a general m -body interaction. However, this only means that the calculation of the GCM interaction kernels is reduced to that of m -body spatial matrix elements T^Ω like Eq. (3.59a) and to that of more difficult spin-isospin factors $X_{k\mathcal{T}}^\Omega$. In this subsection, we restrict our discussion to rather standard two-body interactions of the central, Coulomb, LS and tensor types, and derive explicit expressions for spatial interaction factors with respect to n -cluster systems. It will be found that a more efficient and physical type-classification scheme is available for 2- and 3-cluster systems.

3.3.1 Two-Body Interactions and Spatial Interaction Factors

For the two-body interaction, we assume [98], [99]

$$\begin{aligned} \text{central} : \quad & v^{(C)} = v_0 e^{-\kappa r^2} (W + BP_\sigma - HP_\tau - MP_\sigma P_\tau) \\ \text{Coulomb} : \quad & v^{(CL)} = \frac{e^2}{r} \frac{1 + \tau_{1z}}{2} \frac{1 + \tau_{2z}}{2} \\ \text{LS} : \quad & v^{(LS)} = v_0 e^{-\kappa r^2} (W - HP_\tau) (\ell \cdot \mathbf{s}) \\ \text{tensor} : \quad & v^{(T)} = v_0 r^2 e^{-\kappa r^2} (W - HP_\tau) S_{12} , \end{aligned} \quad (3.61)$$

where $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$, $r = |\mathbf{r}|$, $\boldsymbol{\ell} = (-i)\mathbf{r} \times (\partial/\partial\mathbf{r})$, $\mathbf{s} = (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)/2$ and

$$S_{12} = 3 \frac{(\boldsymbol{\sigma}_1 \cdot \mathbf{r})(\boldsymbol{\sigma}_2 \cdot \mathbf{r})}{r^2} - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) = \sqrt{24\pi} [Y_2(\hat{\mathbf{r}}) [\sigma_1 \sigma_2]^{(2)}]^{(0)} . \quad (3.62)$$

We have also used a standard notation $P_\sigma = (1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)/2$ ($P_\tau = (1 + \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)/2$) for the spin (isospin) exchange operator. The full antisymmetrization in the present formalism allows us to use the generalized Pauli principle, $P_x P_\sigma P_\tau = -1$, through which we can eliminate the isospin dependence in Eq. (3.61) except for the Coulomb force.⁹ We will discuss this procedure in §4. Here we simply assume that the spin-isospin factors for $w = (W + BP_\sigma - HP_\tau - MP_\sigma P_\tau)$, $w^{(CL)} = (1 + \tau_{1z})(1 + \tau_{2z})/4$, $w^{(LS)} = (W - HP_\tau)(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)/2$, and $w^{(T)} = (W - HP_\tau) [\sigma_1 \sigma_2]_\mu^{(2)}$ are obtained as X_{kT} , X_{kT}^{CL} , $X_{kT}^{LS} \mathbf{S}$, and $X_{kT}^T S_\mu^{(2)}$, respectively, through the defining relationship in Eq. (3.59b).¹⁰ For LS and tensor factors, it is convenient to introduce a spin vector \mathbf{S} and the second-rank spin-tensor $S_\mu^{(2)}$ which are an abstract extension of $\mathbf{s} = (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)/2$ and $[\sigma_1 \sigma_2]_\mu^{(2)}$ for two-nucleon systems, respectively. By using the spherical harmonic polynomials

$$\mathcal{Y}_{\ell m}(\mathbf{r}) = \sqrt{\frac{4\pi}{(2\ell + 1)!!}} r^\ell Y_{\ell m}(\hat{\mathbf{r}}) , \quad (3.63)$$

the tensor factor $r^2 S_{12}$ in Eq. (3.62) is expressed as

$$r^2 S_{12} = 3\sqrt{10} [\mathcal{Y}_2(\mathbf{r}) [\sigma_1 \sigma_2]^{(2)}]^{(0)} . \quad (3.64)$$

For more detailed definition of X_{kT}^{LS} and X_{kT}^T and their evaluations, §4 should again be referred to. The explicit expressions of the spatial interaction factors \mathcal{T}^Ω in Eq. (3.59a) for the basic spatial functions $u = \exp\{-\kappa r^2\}$, $u^{(CL)} = (1/r)$, $u^{(LS)} = \exp\{-\kappa r^2\} \boldsymbol{\ell}$ and $u^{(T)} = \exp\{-\kappa r^2\} \mathcal{Y}_{2\mu}(\mathbf{r})$ are given by

$$\begin{aligned} \mathcal{T} &= \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} \rho^2 \right\} \quad \text{with} \quad \lambda = \frac{\kappa}{2(\nu + \kappa)} , \\ \mathcal{T}^{CL} &= \frac{2\sqrt{\nu}}{|\rho|} \operatorname{erf} \left(\frac{|\rho|}{2} \right) \quad \text{with} \quad \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x dt e^{-t^2} , \\ \mathcal{T}^{LS} &= \mathcal{T} \left(\frac{\nu}{\nu + \kappa} \right) \left(-\frac{\nu}{2} \right) i [\mathbf{S}'_\alpha - \mathbf{S}'_\gamma, \mathbf{S}'_\beta - \mathbf{S}'_\delta] , \\ \mathcal{T}^T &= \mathcal{T} \left(\frac{\nu}{\nu + \kappa} \right)^2 \left(\frac{1}{4\nu} \right) \mathcal{Y}_{2\mu}(\rho) , \end{aligned} \quad (3.65)$$

where the Coulomb factor is obtained from the Gaussian factor by using a simple formula

⁹Note that we can set $P_\sigma = 1$ for $\Omega = LS$ and tensor, since these are non-zero only for pairs with the spin-value $S=1$.

¹⁰We omit the type index C for the central Gaussian potential for simplicity, as long as no confusion takes place.

$$\frac{1}{r} = \frac{2}{\sqrt{\pi}} \int_0^\infty d\chi e^{-\chi^2 r^2} . \quad (3.66)$$

In Eq. (3.65), $\rho = \sqrt{\nu} (\mathbf{S}_\alpha^* - \mathbf{S}_\gamma^* + \mathbf{S}'_\beta - \mathbf{S}'_\delta)$ and the transformation from \mathbf{S}_α to \mathbf{z}_i etc. is achieved through Eq. (3.16). We find that ρ for the type $\{\alpha\beta; \gamma\delta\}$ is expressed as

$$\rho = P^{\{\alpha\gamma\}} \mathbf{z}^* + P^{\{\beta\delta\}} \mathbf{z}' = - \sum_{i=1}^{n-1} \frac{1}{\sqrt{\mu_i}} \left(p_i^{\{\alpha\gamma\}} \mathbf{z}_i^* + p_i^{\{\beta\delta\}} \mathbf{z}'_i \right) , \quad (3.67)$$

where $P^{\{\alpha\gamma\}} \equiv P_\alpha - P_\gamma$ or $p_i^{\{\alpha\gamma\}} = (p_\alpha)_i - (p_\gamma)_i$ etc. are antisymmetric with respect to the interchange of α and γ , and are explicitly given by

$$p_i^{\{\alpha\gamma\}} = \begin{cases} 0 & \left\{ \begin{array}{l} 1 \leq \alpha < \gamma \leq i \\ 1 \leq \alpha \leq i, \gamma = i+1 \\ 1 \leq \alpha \leq i, i+2 \leq \gamma \leq n \\ \alpha = i+1, i+2 \leq \gamma \leq n \\ i+2 \leq \alpha < \gamma \leq n \end{array} \right. \\ 1 & \\ A_{i+1}/\bar{A}_{i+1} & \\ -\bar{A}_i/\bar{A}_{i+1} & \\ 0 & \end{cases} \quad \text{for} \quad \begin{cases} 1 \leq \alpha < \gamma \leq i \\ 1 \leq \alpha \leq i, \gamma = i+1 \\ 1 \leq \alpha \leq i, i+2 \leq \gamma \leq n \\ \alpha = i+1, i+2 \leq \gamma \leq n \\ i+2 \leq \alpha < \gamma \leq n \end{cases} \quad (3.68)$$

for a particular order $1 \leq \alpha < \gamma \leq n$. If we use a simplified notation $P = P^{\{\alpha\gamma\}}$ and $P' = P^{\{\beta\delta\}}$ and express ρ as $\rho = P\mathbf{z}^* + P'\mathbf{z}'$, the full GCM kernel is given by

$$\begin{aligned} I(z; z') &= v_0 \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \sum_{[k]} \exp \{ \text{Tr}(z^* Q[k]^t z') \} \sum_T X_{kT} \exp \left\{ -\frac{\lambda}{2} (P\mathbf{z}^* + P'\mathbf{z}')^2 \right\} , \\ I^{CL}(z; z') &= e^2 \sum_{[k]} \exp \{ \text{Tr}(z^* Q[k]^t z') \} \sum_T X_{kT}^{CL} \frac{2\sqrt{\nu}}{|P\mathbf{z}^* + P'\mathbf{z}'|} \text{erf} \left(\frac{1}{2} |P\mathbf{z}^* + P'\mathbf{z}'| \right) , \\ I^{LS}(z; z') &= v_0 \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{5}{2}} \sum_{[k]} \exp \{ \text{Tr}(z^* Q[k]^t z') \} \sum_T X_{kT}^{LS} \exp \left\{ -\frac{\lambda}{2} (P\mathbf{z}^* + P'\mathbf{z}')^2 \right\} \\ &\quad \times \left(-\frac{1}{2} \right) i [P\mathbf{z}^*, P'\mathbf{z}'] \cdot \mathbf{S} , \\ I^T(z; z') &= v_0 \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{7}{2}} \sum_{[k]} \exp \{ \text{Tr}(z^* Q[k]^t z') \} \sum_T X_{kT}^T \exp \left\{ -\frac{\lambda}{2} (P\mathbf{z}^* + P'\mathbf{z}')^2 \right\} \\ &\quad \times \left(\frac{1}{4\nu} \right) 3\sqrt{10} [\mathcal{Y}_2(P\mathbf{z}^* + P'\mathbf{z}') S^{(2)}]^{(0)} . \end{aligned} \quad (3.69)$$

An important property of the spatial interaction factors T^Ω derived in Eqs. (3.65) and (3.67) is that the type index $\{\alpha\beta; \gamma\delta\}$ is further simplified by enumerating independent quadratic polynomials of the Jacobi generator-coordinate vectors $\mathbf{z}^* = (\mathbf{z}_1^*, \dots, \mathbf{z}_{n-1}^*)$ and $\mathbf{z}' = (\mathbf{z}'_1, \dots, \mathbf{z}'_{n-1})$;

$$f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}') \equiv (P^{\{\alpha\gamma\}} \mathbf{z}^* + P^{\{\beta\delta\}} \mathbf{z}')^2 . \quad (3.70)$$

First of all we should note that these polynomials satisfy many symmetry properties:

$$f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}') = f^{(\gamma\alpha)(\delta\beta)}(\mathbf{z}^*, \mathbf{z}') \quad , \quad (3.71a)$$

$$f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}') = f^{(\beta\delta)(\alpha\gamma)}(\mathbf{z}', \mathbf{z}^*) \quad , \quad (3.71b)$$

$$f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}') = f^{(\alpha\gamma)(\delta\beta)}(\mathbf{z}^*, -\mathbf{z}') \quad . \quad (3.71c)$$

The first symmetry is a simple result of the quadratic nature of the polynomials, and corresponds to the symmetry $\{\alpha\beta; \gamma\delta\} = \{\gamma\delta; \alpha\beta\}$ for the interaction types.¹¹ Thus we have all together $\binom{n^2+2-1}{2} = n^2(n^2+1)/2$ independent combinations of $\{\alpha\beta; \gamma\delta\}$, which we divide into several groups with different polynomial forms of \mathbf{z}^* and \mathbf{z}' . Owing to this symmetry, we can assume $\alpha \leq \gamma$ in the following discussions without loss of generality. The second symmetry (3.71b) is related to the hermiticity of the two-body interaction. This means that we can also assume $(\alpha\gamma) \leq (\beta\delta)$ with some appropriate definition of ordering. The interaction factor with $(\alpha\gamma) > (\beta\delta)$ is obtained from that of $(\alpha\gamma) < (\beta\delta)$ through the hermitian conjugation. If $(\alpha\gamma) = (\beta\delta)$, it is self-conjugate. The third symmetry (3.71c) is related to the relative phase of the coefficients for \mathbf{z}^* and \mathbf{z}' and the case for $\beta > \delta$ is obtained from $\beta < \delta$ by the simple replacement $\mathbf{z}' \rightarrow -\mathbf{z}'$. After all, we only need to consider the situations with $\alpha \leq \gamma$, $\beta \leq \delta$, $(\alpha\gamma) \leq (\beta\delta)$ for the complete type specification.

We first consider the following four cases.

- (1) $\alpha = \gamma$ and $\beta = \delta$: E -type
 - (2) $\alpha \neq \gamma$ and $\beta = \delta$: S -type
 - (3) $\alpha = \gamma$ and $\beta \neq \delta$: S' -type
 - (4) $\alpha \neq \gamma$ and $\beta \neq \delta$: D -type or V -type .
- (3.72)

For example, $f^{(\alpha\alpha)(\beta\beta)} = 0$ for E -type and this term of the GCM kernel is simply proportional to that of the normalization kernel. In accordance with the type identification $T = T_{\{\alpha\beta; \gamma\delta\}}$, we set

$$E_{\alpha\beta} = T_{\{\alpha\beta; \alpha\beta\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \quad (3.73)$$

for n^2 such combinations of α and β . This type contributes to the internal energies of clusters and LS and tensor contributions in Eq. (3.69) are zero, since we are dealing with only s -shell clusters. Similarly, we have $n^2(n-1)/2$ S -type and S' -type factors, which we denote

$$\begin{aligned} S_{\beta}^{(\alpha\gamma)} &= T_{\{\alpha\beta; \gamma\beta\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} (P^{\{\alpha\gamma\}} \mathbf{z}^*)^2 \right\} \quad , \\ S_{\alpha}^{\prime(\beta\delta)} &= S_{\alpha}^{(\beta\delta)} \quad \text{with} \quad \mathbf{z}^* \leftrightarrow \mathbf{z}' \quad . \end{aligned} \quad (3.74)$$

¹¹The same is applied to the spin-isospin factors in Eq. (3.59b), which is nothing but the exchange symmetry $w_{st}^{(\Omega)} = w_{ts}^{(\Omega)}$.

The type (3) is related to (2) by the hermitian conjugation in Eq. (3.71b). In general, we use the notation T' for the type which is obtained from T by the interchange $\mathbf{z}^* \leftrightarrow \mathbf{z}'$. It is also clear from Eq. (3.69) that these types do not contribute to the LS kernels. Note that the subscripts like β in $S_\beta^{(\alpha\gamma)}$ and α, β in $E_{\alpha\beta}$ are dummy indices which do not affect the spatial interaction factors. Namely, we have $n(n-1)/2$ independent S -type spatial factors corresponding to the unordered pairs $(\alpha\gamma)$ and their multiplicity is n for each. Finally, let us consider $2\binom{n}{2}^2 = n^2(n-1)^2/2$ $\{\alpha\beta; \gamma\delta\}$ factors belonging to the type (4) in (3.72). These are specified by the combination of two unordered pairs $(\alpha\gamma)$ and $(\beta\delta)$ with the relative exchange of β and δ . (Note that we have assumed $\alpha < \gamma$.) If $(\alpha\gamma)$ coincides with $(\beta\delta)$ as a set, we call such $\{\alpha\beta; \gamma\delta\}$ D -type and, if not, V -type:

$$\begin{aligned} (4a) \quad (\alpha\gamma) = (\beta\delta) &: D\text{-type} \\ (4b) \quad (\alpha\gamma) < (\beta\delta) &: V\text{-type} \\ (4c) \quad (\alpha\gamma) > (\beta\delta) &: V'\text{-type} \end{aligned} \quad (3.75)$$

These types are further subdivided according to the relative sign of the coefficients for \mathbf{z}^* and \mathbf{z}' . For example, factors for D -type are composed of

$$\begin{aligned} (4a)_+ \quad \alpha = \beta \quad \text{and} \quad \gamma = \delta &: D_+\text{-type} \\ (4a)_- \quad \alpha = \delta \quad \text{and} \quad \gamma = \beta &: D_-\text{-type} \end{aligned} \quad (3.76)$$

For these types, we assign

$$\begin{aligned} D_+^{(\alpha\gamma)} &= T_{\{\alpha\alpha; \gamma\gamma\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} \left(P^{\{\alpha\gamma\}}(\mathbf{z}^* + \mathbf{z}') \right)^2 \right\}, \\ D_-^{(\alpha\gamma)} &= T_{\{\alpha\gamma; \gamma\alpha\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} \left(P^{\{\alpha\gamma\}}(\mathbf{z}^* - \mathbf{z}') \right)^2 \right\}, \end{aligned} \quad (3.77)$$

and they yield $n(n-1)/2$ different D_\pm -types, respectively. Note that these are self-conjugate and related to each other through the sign change of \mathbf{z}' due to the symmetries (3.71a)~(3.71c). The fact that V -type and V' -type always appear as a pair is also confirmed by counting the total number of these factors $n^2(n-1)^2/2 - n(n-1) = (n-2)(n-1)n(n+1)/2$, which is even. For (4b) the relative sign of \mathbf{z}^* and \mathbf{z}' terms is fixed by setting the order of $\alpha < \gamma$ and $\beta < \delta$. Thus we get

$$\begin{aligned} (4b)_+ \quad (\alpha\gamma) < (\beta\delta) \quad \text{and} \quad \alpha < \gamma, \beta < \delta &: V_+\text{-type} \\ (4b)_- \quad (\alpha\gamma) < (\beta\delta) \quad \text{and} \quad \alpha < \gamma, \beta > \delta &: V_-\text{-type} \\ (4c)_+ \quad (\alpha\gamma) > (\beta\delta) \quad \text{and} \quad \alpha < \gamma, \beta < \delta &: V'_+\text{-type} \\ (4c)_- \quad (\alpha\gamma) > (\beta\delta) \quad \text{and} \quad \alpha < \gamma, \beta > \delta &: V'_-\text{-type} \end{aligned} \quad (3.78)$$

each of which consists of $(n-2)(n-1)n(n+1)/8$ different types. We specifically define the V_+ -type interaction factors through

$$V_+^{(\alpha\gamma)(\beta\delta)} = T_{\{\alpha\beta; \gamma\delta\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} \left(P^{\{\alpha\gamma\}}\mathbf{z}^* + P^{\{\beta\delta\}}\mathbf{z}' \right)^2 \right\}, \quad (3.79)$$

for $(\alpha\gamma) < (\beta\delta)$ and $\alpha < \gamma$, $\beta < \delta$. The other types V_- , V'_+ , and V'_- are obtained through the general rule

$$\begin{aligned} \mathcal{T}' &= \mathcal{T} \quad \text{with } \mathbf{z}^* \leftrightarrow \mathbf{z}' \quad , \\ \mathcal{T}_- &= \mathcal{T}_+ \quad \text{with } \mathbf{z}' \rightarrow -\mathbf{z}' \quad . \end{aligned} \quad (3.80)$$

The structure of the spatial interaction factors discussed above may be more transparently understood by geometrical consideration of two boxes in the double-coset symbol $[k]$. We recall that the indices α and β in $\{\alpha\beta; \gamma\delta\}$ are related to the assignment of the particle index s to some particular ordered set $\mathbf{k}_{\alpha\beta}; s \in \mathbf{k}_{\alpha\beta}$. This means that the present type classification in terms of $\{\alpha\beta; \gamma\delta\}$ is nothing but counting two boxes of the double-coset symbol connected by the interaction. These two boxes are degenerate for E -type, and located vertically or horizontally for S -type or S' -type. In D_+ -type, two different boxes are selected from the diagonal part, and these are exchanged for D_- -type. The others are the irregular off-diagonal selection of two boxes for V -type. The relationship between \mathcal{T} and \mathcal{T}' corresponds to the transposition of the double-coset symbol.

3.3.2 2-Cluster Interaction Types

The type classification of interaction factors \mathcal{T}^Ω for 2-cluster systems is very simple, since the factor $P_1^{\{12\}} = -(1/\sqrt{\mu})$ with $\mu = A_1 A_2 / (A_1 + A_2)$ is only needed. Since the overall sign of P is irrelevant, the full 2-cluster GCM kernel is obtained by setting $P = (1/\sqrt{\mu})p$ and $P' = (1/\sqrt{\mu})q$ in Eq. (3.69), where p and q are 0 or ± 1 given in Table II. These values depend on the type indices $E_{\alpha\beta}$, S'_α , S_β , D_+ and D_- , which has the multiplicity 4, 2, 2, 1 and 1, respectively. The summation over the dummy indices α and β may be carried out for spin-isospin factors. Thus, these 10 terms can be reduced to only 5 interaction types; $\mathcal{T} = E, S', S, D_+$ and D_- .¹²

TABLE II. Two-cluster interaction types and their factors $\mathcal{T}_{\{\alpha\beta; \gamma\delta\}} = (\nu/(\nu + \kappa))^{3/2} \times \exp\{-(\lambda/2) f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}')\}$ in terms of the coefficients p and q through $P = p/\sqrt{\mu}$ and $P' = q/\sqrt{\mu}$ with $\mu = A_1 A_2 / (A_1 + A_2)$.

| \mathcal{T} | $\{\alpha\beta; \gamma\delta\}$ | multiplicity | p | q | $f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}')$ |
|-------------------|---------------------------------|--------------|-----|-----|--|
| $E_{\alpha\beta}$ | $\{\alpha\beta; \alpha\beta\}$ | 4 | 0 | 0 | 0 |
| S_β | $\{1\beta; 2\beta\}$ | 2 | 1 | 0 | $(\mathbf{z}^*)^2/\sqrt{\mu}$ |
| S'_α | $\{\alpha 1; \alpha 2\}$ | 2 | 0 | 1 | $(\mathbf{z}')^2/\sqrt{\mu}$ |
| D_+ | $\{11; 22\}$ | 1 | 1 | 1 | $(\mathbf{z}^* + \mathbf{z}')^2/\sqrt{\mu}$ |
| D_- | $\{12; 21\}$ | 1 | 1 | -1 | $(\mathbf{z}^* - \mathbf{z}')^2/\sqrt{\mu}$ |

From the geometrical interpretation of the interaction types discussed in the preced-

¹²The origin of these names is almost obvious from Table II. These are related to the structure of the GCM interaction factors; namely, E for a unit factor, S and S' for a single vector \mathbf{z}^* or \mathbf{z}' involved in \mathcal{T} , and D_\pm for double vectors or for the direct term to which D_+ type contributes.

ing section, it is obvious that, for the direct term with no nucleon exchanged, $E_{\alpha\alpha}$ and D_+ types are only possible. The internal energies for clusters C_1 and C_2 get contributions only from E type, and the direct potential between C_1 and C_2 are described by the D_+ -type interaction factor. If the two clusters C_1 and C_2 are identical, a complete interchange between C_1 and C_2 gives the same contribution as that of the direct term except for a possible sign change, but the types called here are $E_{\alpha\beta}$ ($\alpha \neq \beta$) and D_- . To LS terms only D_+ and D_- types contribute, while to tensor terms all but E contribute. The S and S' types are hermitian conjugate to each other, while the others are all self-conjugate in 2-cluster systems.

These five interaction types are, of course, well known in any formulations of 2-cluster RGM. Different authors use different notations. For example, LeMere, Stubeda, Horiuchi and Tang [100] have introduced the notation a, b, c and (d, e) for E, D_+, D_- and (S, S') types, respectively. This paper was followed by many detailed studies on the different roles of the interaction types combined with the nucleon exchange classification. (See, for example, refs. [101]~ [103].) It is well known that the D_- -type or c -type interaction term with a single nucleon exchange usually gives the most important contribution among many complicated terms of exchange kernels. [104], [103] This term is called a knock-on term in the study of light-ion optical potentials. The importance of the so-called core-exchange terms for the systems with small mass-number difference is also found through detailed studies of interaction types in terms of various localization techniques of the nonlocal exchange kernels. [105], [106], [102] Thus, the type classification of the interaction types is not just a matter of nomenclature, but has benefited a great deal the microscopic understanding of interactions between composite particles. [14], [50]

3.3.3 3-Cluster Interaction Types

The interaction types for 3-cluster systems are more conveniently expressed in terms of the cyclic definition of the unordered pairs $(\alpha\beta) \equiv \gamma$, where $(\alpha\beta\gamma)$ is one of the permutations of (123). This is related to the three different sets of Jacobi coordinates $\xi_i^{(\gamma)}$ introduced in Eq. (3.8). For the generator-coordinate vectors, the first equation in Eq. (3.8) yields

$$\sqrt{\nu} (\mathbf{S}_\alpha - \mathbf{S}_\gamma) = \sum_\varepsilon e_{\gamma\alpha\varepsilon} \frac{\mathbf{z}_1^{(\varepsilon)}}{\sqrt{\mu_1^{(\varepsilon)}}}, \tag{3.81}$$

where ε is uniquely specified for $\alpha \neq \gamma$ through $\varepsilon = (\alpha\gamma)$. We can also prove Eq. (3.81) directly from Eq. (3.68) by using the coordinate transformation in Eqs. (3.10) and (3.11). Namely, we can easily show

$$\Xi^{(\varepsilon)(3)} P\{\alpha\gamma\} = \begin{pmatrix} 1/\sqrt{\mu_1^{(\varepsilon)}} \\ 0 \end{pmatrix} \tag{3.82}$$

for $(\gamma\alpha\varepsilon)$ = an even permutation of (123). Then, if we note that $\mathbf{z} = (\mathbf{z}_1, \mathbf{z}_2)$ is the standard set $\mathbf{z}^{(3)}$, the matrix multiplication

$$\sqrt{\nu}(\mathbf{S}_\alpha - \mathbf{S}_\gamma) = \mathbf{z}^{(3)} P^{\{\alpha\gamma\}} = \mathbf{z}^{(\varepsilon)} \Xi^{(\varepsilon)(3)} P^{\{\alpha\gamma\}} \quad (3.83)$$

with Eq. (3.82) yields Eq. (3.81). Therefore, the quadratic polynomials in Eq. (3.70) for 3-cluster systems are most easily expressed as

$$f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}') = \left(\sum_{\varepsilon} e_{\gamma\alpha\varepsilon} \frac{\mathbf{z}_1^{(\varepsilon)*}}{\sqrt{\mu_1^{(\varepsilon)}}} + \sum_{\lambda} e_{\delta\beta\lambda} \frac{\mathbf{z}_1^{(\lambda)'}}{\sqrt{\mu_1^{(\lambda)}}} \right)^2, \quad (3.84)$$

by using appropriate types of Jacobi coordinates for the interaction type $\{\alpha\beta; \gamma\delta\}$. If either of the pairs $(\alpha\gamma)$ or $(\beta\delta)$ is collapsed, one can adopt a natural definition

$$S(\gamma) = T_{\{\alpha\delta; \beta\delta\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} \frac{1}{\mu_1^{(\gamma)}} \left(\mathbf{z}_1^{(\gamma)*} \right)^2 \right\}, \quad (3.85)$$

which corresponds to $S^{(\alpha\beta)}$ in Eq. (3.74). Also, $(\alpha\gamma) = (\beta\delta)$ case is given by

$$D_+(\gamma) = T_{\{\alpha\alpha; \beta\beta\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} \frac{1}{\mu_1^{(\gamma)}} \left(\mathbf{z}_1^{(\gamma)*} + \mathbf{z}_1^{(\gamma)'} \right)^2 \right\}, \quad (3.86a)$$

$$D_-(\gamma) = T_{\{\alpha\beta; \beta\alpha\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} \frac{1}{\mu_1^{(\gamma)}} \left(\mathbf{z}_1^{(\gamma)*} - \mathbf{z}_1^{(\gamma)'} \right)^2 \right\}, \quad (3.86b)$$

where $(\alpha\beta\gamma)$ is again assumed to be a permutation of (123). These are just a 3-dimensional generalization of the 2-cluster interaction types $T = S, S'$ and D_{\pm} for the three different 2-cluster subsystems formed by C_α and C_β . Thus we use the notation $T = TJ$, where $T = S, S', D_{\pm}$ and J specifies one of the three different Jacobi coordinates $J = I, II$ or III (or $J = (\gamma)$ with $\gamma = 1, 2$ or 3).

A similar classification scheme is also applied to the V -type interaction types. In this case, ε and λ in Eq. (3.84) are uniquely specified by assuming that $(\gamma\alpha\varepsilon)$ and $(\delta\beta\lambda)$ are permutations of (123). Thus we get

$$f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}') = \left(\frac{\mathbf{z}_1^{(\varepsilon)*}}{\sqrt{\mu_1^{(\varepsilon)}}} + e_{\gamma\alpha\varepsilon} e_{\delta\beta\lambda} \frac{\mathbf{z}_1^{(\lambda)'}}{\sqrt{\mu_1^{(\lambda)}}} \right)^2. \quad (3.87)$$

Since we have $\alpha \neq \gamma, \beta \neq \delta$ and $\varepsilon \neq \lambda$, the ν determined from $\nu = (\varepsilon\lambda)$ should again be equal to α or γ in $(\alpha\gamma)$, and β or δ in $(\beta\delta)$; namely, we have $(\alpha\gamma) = (\lambda\nu)$ and $(\beta\delta) = (\varepsilon\nu)$ as identical sets. This involves the following four different cases ;

- i) $\alpha = \lambda, \beta = \varepsilon, \gamma = \delta = \nu$
 - ii) $\alpha = \lambda, \beta = \gamma = \nu, \delta = \varepsilon$
 - iii) $\alpha = \delta = \nu, \gamma = \lambda, \beta = \varepsilon$
 - iv) $\alpha = \beta = \nu, \gamma = \lambda, \delta = \varepsilon$.
- (3.88)

Due to the symmetry (3.71a), we only need to consider the case i) or ii). In order to fix the phase $e_{\gamma\alpha\varepsilon} e_{\delta\beta\lambda}$ in Eq. (3.87), we now assume that $(\lambda\varepsilon\nu)$ is an even permutation of (123). Then it is easy to see that $e_{\gamma\alpha\varepsilon} e_{\delta\beta\lambda} = -1$ for i) and 1 for ii). Thus we are naturally led to the definition¹³

$$V_+(\nu) = \mathcal{T}_{\{\lambda\varepsilon; \nu\nu\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} \left(\frac{\mathbf{z}_1^{(\varepsilon)*}}{\sqrt{\mu_1^{(\varepsilon)}}} - \frac{\mathbf{z}_1^{(\lambda)'}}{\sqrt{\mu_1^{(\lambda)}}} \right)^2 \right\}, \quad (3.89a)$$

$$V_-(\nu) = \mathcal{T}_{\{\lambda\nu; \nu\varepsilon\}} = \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \exp \left\{ -\frac{\lambda}{2} \left(\frac{\mathbf{z}_1^{(\varepsilon)*}}{\sqrt{\mu_1^{(\varepsilon)}}} + \frac{\mathbf{z}_1^{(\lambda)'}}{\sqrt{\mu_1^{(\lambda)}}} \right)^2 \right\}, \quad (3.89b)$$

where $(\lambda\varepsilon\nu)$ is an even permutation of (123).¹⁴ The explicit expressions for the 3-cluster interaction types thus defined are summarized in Table III.

From this table, we can see that the symmetries in Eq. (3.80) are satisfied for TJ , irrespective of J . In particular, we have

$$T'J = (TJ)^\dagger, \quad (3.90)$$

where the dagger symbol in the right-hand side means the operation of hermitian conjugation. Furthermore, it is easy to verify the following symmetries for V -type terms :

$$\begin{aligned} V_\pm(\gamma) (\alpha \leftrightarrow \beta) &= V'_\pm(\gamma), \\ V_\pm(\alpha) (\alpha \leftrightarrow \beta) &= V'_\pm(\beta), \\ V_\pm(\beta) (\alpha \leftrightarrow \beta) &= V'_\pm(\alpha), \end{aligned} \quad (3.91)$$

where $(\alpha\beta\gamma) =$ an even permutation of (123), and $TJ (\alpha \leftrightarrow \beta)$ denotes the expression obtained by the interchange of the clusters C_α and C_β in TJ .

In summary, we have obtained a simple conclusion that 3-cluster interaction types \mathcal{T} are specified by the combination of the 2-cluster interaction types T with a slight extension to V_\pm and V'_\pm types, together with the type of Jacobi coordinates J specifying the 2-cluster subsystems ; $\mathcal{T} = TJ$. This type-specification scheme is extremely useful for practical applications of the present 3-cluster formalism to coupled channel problems

¹³The origin of the name V for the members of this group is clear from $V_+(3) = \mathcal{T}_{\{12;33\}}$ in Eq. (3.89a). Namely, the quadratic form in Eq. (3.84) is expressed as $\nu(\mathbf{T}_1^* + \mathbf{T}_2')^2$ in terms of the V -type coordinates $\mathbf{T}_\alpha = \mathbf{S}_\alpha - \mathbf{S}_3$ ($\alpha=1, 2$), which resembles the D_+ type in the 2-cluster classification scheme.

¹⁴It seems to be natural to introduce the ordering $(\alpha\gamma) < (\beta\delta)$ in Eq. (3.75) by $\varepsilon < \lambda$ for $\varepsilon = (\alpha\gamma)$ and $\lambda = (\beta\delta)$, and to identify $V_+^{(\alpha\gamma)(\beta\delta)} = V_+^{\varepsilon\lambda}$ with V_+^ν by $\nu = (\varepsilon\lambda)$. However, this procedure gives a little different definition of V_+ -type interaction types from $V_+(\nu)$ due to the cyclic permutation phase. The correct correspondence between $V_+(\nu)$ and $V_+^{\varepsilon\lambda}$ is given by $V_+(\nu) = V_+^{\nu\lambda\varepsilon}$ for $\nu = 1, 3$ and $V_+^{\nu\lambda}$ for $\nu = 2$, when $(\lambda\varepsilon\nu)$ is an even permutation of (123).

with many cluster configurations.

TABLE III. Three-cluster interaction types, $\mathcal{T} = TJ$, and their factors in terms of $f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}')$ in Eq. (3.87). The type of Jacobi coordinates J is specified by $J = (\gamma)$ etc., with $(\alpha\beta\gamma)$ being an even permutation of (123). In $S(\gamma)$ or $S'(\gamma)$, δ can be either of 1, 2 or 3. For E -type, no specification of γ is needed.

| $\mathcal{T} = TJ$ | $\{\alpha\beta; \gamma\delta\}$ | multiplicity | $f^{(\alpha\gamma)(\beta\delta)}(\mathbf{z}^*, \mathbf{z}')$ |
|--------------------|---------------------------------|--------------|---|
| E | $\{\alpha\beta; \alpha\beta\}$ | 9 | 0 |
| $S(\gamma)$ | $\{\alpha\delta; \beta\delta\}$ | 9 | $(\mathbf{z}_1^{(\gamma)*})^2 / \mu_1^{(\gamma)}$ |
| $S'(\gamma)$ | $\{\delta\alpha; \delta\beta\}$ | 9 | $(\mathbf{z}_1^{(\gamma)'})^2 / \mu_1^{(\gamma)}$ |
| $D_+(\gamma)$ | $\{\alpha\alpha; \beta\beta\}$ | 3 | $(\mathbf{z}_1^{(\gamma)*} + \mathbf{z}_1^{(\gamma)'})^2 / \mu_1^{(\gamma)}$ |
| $D_-(\gamma)$ | $\{\alpha\beta; \beta\alpha\}$ | 3 | $(\mathbf{z}_1^{(\gamma)*} - \mathbf{z}_1^{(\gamma)'})^2 / \mu_1^{(\gamma)}$ |
| $V_+(\gamma)$ | $\{\alpha\beta; \gamma\gamma\}$ | 3 | $(\mathbf{z}_1^{(\beta)*} / \sqrt{\mu_1^{(\beta)}} - \mathbf{z}_1^{(\alpha)' / \sqrt{\mu_1^{(\alpha)}}})^2$ |
| $V_-(\gamma)$ | $\{\alpha\gamma; \gamma\beta\}$ | 3 | $(\mathbf{z}_1^{(\beta)*} / \sqrt{\mu_1^{(\beta)}} + \mathbf{z}_1^{(\alpha)' / \sqrt{\mu_1^{(\alpha)}}})^2$ |
| $V'_+(\gamma)$ | $\{\beta\alpha; \gamma\gamma\}$ | 3 | $(\mathbf{z}_1^{(\alpha)*} / \sqrt{\mu_1^{(\alpha)}} - \mathbf{z}_1^{(\beta)' / \sqrt{\mu_1^{(\beta)}}})^2$ |
| $V'_-(\gamma)$ | $\{\beta\gamma; \gamma\alpha\}$ | 3 | $(\mathbf{z}_1^{(\alpha)*} / \sqrt{\mu_1^{(\alpha)}} + \mathbf{z}_1^{(\beta)' / \sqrt{\mu_1^{(\beta)}}})^2$ |

3.4 Transformation Properties of the Coefficients $Q[k]$ and $P^{\{\alpha\gamma\}}$ for Rearrangements of Jacobi Coordinates.

One of the prominent properties of the GCM kernels derived in the preceding subsections is their invariance with respect to a different choice of the Jacobi coordinates. This particular property is a direct consequence from that the generating functions $A(\xi; z)$ in Eq. (3.15) is invariant with respect to simultaneous orthogonal transformations of the real coordinates $\hat{\xi}$ and the corresponding generator-coordinate vectors $z/\sqrt{\nu}$. To be more specific, let us consider the coordinate transformation

$$\hat{\xi} = \hat{\xi}^{(a)} \Xi^{(a)} \quad (3.92)$$

with some appropriate indices a for the bra side and b for the ket side. The invariance of the GCM kernel defined by¹⁵

$$I^{(a)(b)\Omega}(z^{(a)}; z^{(b)'}) = \langle A(\xi^{(a)}; z^{(a)}) \phi_0 | \mathcal{O}^\Omega \mathcal{A}' | A(\xi^{(b)}; z^{(b)'}) \phi_0 \rangle \quad (3.93)$$

is expressed as

¹⁵For systems of three non-alpha clusters or more, we also need to make spin-isospin recouplings to achieve this rearrangement. We assume here that such a procedure is implicitly carried out in the spin-isospin factors discussed in §4.

$$I^{(a)(b)\Omega}(z^{(a)}; z^{(b)'}) = I^\Omega(z; z') = I^\Omega(z^{(a)} \Xi^{(a)}; z^{(b)'} \Xi^{(b)}) , \quad (3.94)$$

where $A(\xi^{(a)}, z^{(a)}) = A(\xi, z)$ etc. is used. Thus, in order to derive the GCM kernel $I^{(a)(b)\Omega}(z; z')$ in the different sets of the Jacobi coordinates a and b , we only need to apply the orthogonal transformation Ξ in the explicit expressions obtained before. For example, the normalization kernel $I^{(a)(b)}(z; z')$ are obtained from Eq. (3.38) by the replacement

$$Q[k] \rightarrow \Xi^{(a)} Q[k] {}^t \Xi^{(b)} \equiv Q^{(a)(b)}[k] . \quad (3.95)$$

Similarly, for the interaction kernels, we modify

$$P^{\{\alpha\gamma\}} \rightarrow \Xi^{(a)} P^{\{\alpha\gamma\}} \equiv \tilde{P}^{(a)\{\alpha\gamma\}} , \quad (3.96a)$$

$$P^{\{\beta\delta\}} \rightarrow \Xi^{(b)} P^{\{\beta\delta\}} \equiv \tilde{P}^{(b)\{\beta\delta\}} . \quad (3.96b)$$

We can include the original case with respect to the standard Jacobi coordinates, by assuming $a = b = e$ and $\Xi^{(e)} = \Xi^{(e)(e)} = 1$. Therefore, this transformation is simply considered to be a result of different representations for the coefficients $Q[k]$ and $P^{\{\alpha\gamma\}}$.

In order to find the explicit expressions of the transformed coefficients $Q^{(a)(b)}[k]$ etc. in Eqs. (3.95) and (3.96), we return to the coordinate transformation in Eq. (3.16). We express this in the matrix notation as

$$\sqrt{\nu} S = z P , \quad (3.97)$$

where P is the $(n-1) \times n$ matrix with the matrix elements $P_{i\alpha} = (P_\alpha)_i$ given in Eq. (3.16). A simple example of the present transformation is the case in which the representation a is reproduced by a permutation of n -clusters; i.e., $a = \begin{pmatrix} 1 & 2 & \cdots & n \\ a_1 & a_2 & \cdots & a_n \end{pmatrix}$.¹⁶ The matrix representation of a is denoted by M_a in the following; $(M_a)_{\alpha\beta} = \delta_{\alpha\beta} = \delta_{\alpha, a^{-1}(\beta)}$. We modify A_1, \dots, A_n to A_{a_1}, \dots, A_{a_n} in Eq. (3.97) and define $z^{(a)}$ instead of z . Since we have $(S_{a_1}, \dots, S_{a_n}) = S^t M_a = S M_a^{-1}$, this definition of $z^{(a)}$ is expressed as

$$\sqrt{\nu} S M_a^{-1} = z^{(a)} P^{(a)} , \quad (3.98)$$

where $P^{(a)}$ denotes the matrix P with A_1, \dots, A_n being replaced with A_{a_1}, \dots, A_{a_n} . From Eqs. (3.97), (3.98) and $z = z^{(a)} \Xi^{(a)}$, we can easily find

$$\Xi^{(a)} P = P^{(a)} M_a . \quad (3.99)$$

This equation relates the orthogonal transformation of the Jacobi coordinates with the permutation matrix of n -cluster c.m. vectors. By using this relationship, $Q[k] = P k {}^t P$ in the standard Jacobi coordinate is transformed into

¹⁶In four-cluster systems or more, we also have such types of relative coordinate systems as can not be realized by the permutations of clusters from the standard set of Jacobi coordinates. For example, we need H-type coordinates to describe a system of two ${}^8\text{Be}$ -clusters for ${}^{16}\text{O}$. In this case, we simply use Eqs. (3.95) and (3.96) to find the necessary coefficients for the GCM kernels.

$$Q^{(a)(b)}[k] = P^{(a)} k^{(a)(b)} {}^t P^{(b)} \quad \text{with} \quad k^{(a)(b)} = M_a k {}^t M_b . \quad (3.100)$$

Similarly, the interaction factors in Eq. (3.96) are given by

$$\tilde{P}^{(a)\{\alpha\gamma\}} = P^{(a)\{a^{-1}(\alpha) \ a^{-1}(\gamma)\}} \quad \text{etc.} \quad (3.101)$$

Besides a trivial renaming of A_1, \dots, A_n to A_{a_1}, \dots, A_{a_n} , we need a rearrangement of rows and columns in $k^{(a)(b)}$ and a transformation of the indices α and γ for the interaction types $\{\alpha\beta; \gamma\delta\}$.

In 3-cluster systems, it is convenient to use a permutation of (123) for three independent Jacobi coordinate systems shown in Fig. 1. Namely, we identify $(a) \equiv (123)^a$ with $a = 1 \sim 3$. In particular, $(3) \equiv (123)^3 = e$ specifies the standard Jacobi coordinate. Furthermore, we use the $(xyuv)$ parametrization of the 3×3 double-coset symbol in Eq. (3.42), and also a notation $Q_{xyuv}(A_1, A_2, A_3)$ for the 2×2 matrix given in Eq. (3.43). In the following, we find compact expressions for

$$Q_{xyuv}^{(a)(b)} = \Xi^{(a)(3)} Q_{xyuv}(A_1, A_2, A_3) \Xi^{(3)(b)} , \quad (3.102)$$

and for necessary interaction factors.

Let us first consider the diagonal case $a = b = c$ in Eq. (3.102). We can perform a simultaneous transformation of rows and columns in $k^{(c)(c)} = M_c k {}^t M_c$ and choose a new set of $(x^{(c)} y^{(c)} u^{(c)} v^{(c)})$ such that the resultant matrix has the same form as the original one with respect to the renamed particle numbers $(A_\alpha, A_\beta, A_\gamma)$ for (A_1, A_2, A_3) . Here we assume that $(\alpha\beta\gamma)$ is an even permutation of (123). From this procedure, we easily find

$$\begin{pmatrix} x^{(1)} \\ y^{(1)} \\ u^{(1)} \\ v^{(1)} \end{pmatrix} = \begin{pmatrix} y \\ x + y - u - v \\ y - v \\ y - u \end{pmatrix} , \quad \begin{pmatrix} x^{(2)} \\ y^{(2)} \\ u^{(2)} \\ v^{(2)} \end{pmatrix} = \begin{pmatrix} x + y - u - v \\ x \\ x - v \\ x - u \end{pmatrix} , \quad (3.103)$$

where $x^{(3)} = x$, $y^{(3)} = y$, $u^{(3)} = u$ and $v^{(3)} = v$. The matrix thus obtained can be denoted by $k^{(\gamma)}$ in conformity with the notation rule adopted for $P^{(a)}$. Then, the relationship (3.100) is expressed as

$$Q^{(\gamma)(\gamma)}[k] = P^{(\gamma)} k^{(\gamma)} {}^t P^{(\gamma)} . \quad (3.104)$$

If we compare this with $Q[k] = P k {}^t P$, we obtain

$$Q_{xyuv}^{(\gamma)(\gamma)} = Q_{x^{(\gamma)}y^{(\gamma)}u^{(\gamma)}v^{(\gamma)}}(A_\alpha, A_\beta, A_\gamma) , \quad (3.105)$$

where $(\alpha\beta\gamma)$ is an even permutation of (123).

In order to obtain $Q_{xyuv}^{(a)(b)}$ for $a \neq b$, we first calculate $Q_{xyuv}^{(1)(2)}$ by using Eq. (3.105) and

$$\begin{aligned} Q_{xyuv}^{(1)(2)} &= \Xi^{(1)(2)} Q_{xyuv}^{(2)(2)} = \Xi^{(1)(2)} Q_{x^{(2)}y^{(2)}u^{(2)}v^{(2)}}(A_3, A_1, A_2) \\ &\equiv \tilde{Q}_{xyuv}(A_1, A_2, A_3) . \end{aligned} \quad (3.106)$$

The straightforward calculation in terms of Eqs. (3.43) and (3.11) yields $\tilde{Q}_{xyuv}(A_1, A_2, A_3) = (\tilde{Q}_{ij})$ with

$$\begin{aligned}\tilde{Q}_{11} &= -\sqrt{\frac{A_1 A_2}{A_1^c A_2^c}} \left(1 - \frac{x}{\mu_1^{(2)}} - \frac{y}{\mu_1^{(1)}} + \frac{u}{A_3} + \frac{A_3}{\mu_1^{(1)} \mu_1^{(2)}} v \right), \\ \tilde{Q}_{12} &= -\sqrt{\frac{A_3 A}{A_1^c A_2^c}} \left(1 - \frac{y}{\mu_1^{(1)}} + \frac{u}{A_3} \right), \\ \tilde{Q}_{21} &= \sqrt{\frac{A_3 A}{A_1^c A_2^c}} \left(1 - \frac{x}{\mu_1^{(2)}} + \frac{u}{A_3} \right), \\ \tilde{Q}_{22} &= -\sqrt{\frac{A_1 A_2}{A_1^c A_2^c}} \left(1 - \frac{A}{A_1 A_2} u \right).\end{aligned}\quad (3.107)$$

Note that this expression gives

$$\tilde{Q}_{xyuv}(A_1, A_2, A_3) = P^{(1)}(M_1 k^t M_2)^t P^{(2)}, \quad (3.108)$$

a special case of Eq. (3.100). The same equation for $a \rightarrow \alpha$ and $b \rightarrow \beta$ gives

$$\begin{aligned}Q_{xyuv}^{(\alpha)(\beta)} &= P^{(\alpha)}(M_\alpha k^t M_\beta)^t P^{(\beta)} \\ &= P^{(\alpha)} M_1 (M_1^{\alpha-1} k^t M_1^{\beta-2})^t M_2^t P^{(\beta)},\end{aligned}\quad (3.109)$$

where we have used $M_\alpha = M_1^\alpha$ with M_1 being a matrix representation of the permutation (123). This notation is particularly convenient, since we can easily show that $\alpha - 1 = \beta - 2 = \gamma$ (mode 3) if $(\alpha\beta\gamma)$ is an even permutation of (123), so that $k^{(\gamma)} = M_1^\gamma k^t M_1^\gamma$ in Eq. (3.104) yields

$$Q_{xyuv}^{(\alpha)(\beta)} = P^{(\alpha)}(M_1 k^{(\gamma)} M_2)^t P^{(\beta)}. \quad (3.110)$$

This is nothing but the renaming of A_1, A_2, A_3 and $(x^{(3)}y^{(3)}u^{(3)}v^{(3)}) = (xyuv)$ in Eq. (3.108) by the permutation $(\gamma) = (123)^\gamma$. Thus we find

$$Q_{xyuv}^{(\alpha)(\beta)} = \tilde{Q}_{x^{(\gamma)}y^{(\gamma)}u^{(\gamma)}v^{(\gamma)}}(A_\alpha, A_\beta, A_\gamma), \quad (3.111)$$

where $(\alpha\beta\gamma)$ is an even permutation of (123). If $(\alpha\beta\gamma)$ is an odd permutation of (123), we can use ${}^t Q_{xyuv}^{(\alpha)(\beta)} = Q_{xyvu}^{(\beta)(\alpha)}$ and Eq. (3.111) to obtain

$$Q_{xyuv}^{(\alpha)(\beta)} = {}^t \tilde{Q}_{x^{(\gamma)}y^{(\gamma)}v^{(\gamma)}u^{(\gamma)}}(A_\beta, A_\alpha, A_\gamma) \quad (3.112)$$

with $(\alpha\beta\gamma)$ being an odd permutation of (123). Note that the interchange of u and v corresponds to that of $u^{(\gamma)}$ and $v^{(\gamma)}$ in Eq. (3.103).

Let us finally proceed to the transformation of the interaction factors $P^{(\alpha\gamma)}$ in Eq. (3.101). In 3-cluster systems, it is simpler to deal with vectors $\mathbf{z}_1^{(\gamma)}/\sqrt{\mu_1^{(\gamma)}}$ in Eq. (3.81) directly. We express these vectors in $\mathbf{z}_1^{(\alpha)}$ and $\mathbf{z}_2^{(\alpha)}$:

$$\frac{\mathbf{z}_1^{(\gamma)}}{\sqrt{\mu_1^{(\gamma)}}} = p_\alpha^\gamma \mathbf{z}_1^{(\alpha)} + q_\alpha^\gamma \mathbf{z}_2^{(\alpha)}, \quad (3.113)$$

where p_α^γ and q_α^γ are functions of A_1 , A_2 and A_3 defined through

$$\begin{pmatrix} p_\alpha^\gamma \\ q_\alpha^\gamma \end{pmatrix} = \begin{pmatrix} P_1^{(\alpha)} \{ \alpha^{-1}\gamma(2), \alpha^{-1}\gamma(1) \} \\ P_2^{(\alpha)} \{ \alpha^{-1}\gamma(2), \alpha^{-1}\gamma(1) \} \end{pmatrix}. \quad (3.114)$$

In the right-hand side of Eq. (3.114), α and γ should be understood as permutations; $\alpha \equiv (123)^\alpha$ etc. Although these factors are obtained from $P_i^{\{\alpha\gamma\}} = -(1/\sqrt{\mu_i})p_i^{\{\alpha\gamma\}}$ in Eq. (3.68) through appropriate permutations of the mass-number indices, it is much easier to use Eq. (3.11) directly; namely, they are explicitly given by

$$\begin{aligned} p_\alpha^\gamma &= \frac{1}{\sqrt{\mu_1^{(\gamma)}}} \Xi_{11}^{(\alpha)(\gamma)} = \frac{1}{\sqrt{\mu_1^{(\alpha)}}} \frac{1}{A_\alpha^c} (\delta_{\alpha\gamma} A - A_\gamma) \quad , \\ q_\alpha^\gamma &= \frac{1}{\sqrt{\mu_1^{(\gamma)}}} \Xi_{21}^{(\alpha)(\gamma)} = \frac{1}{\sqrt{\mu_2^{(\alpha)}}} \sum_\beta e_{\alpha\gamma\beta} \quad . \end{aligned} \quad (3.115)$$

Then the quadratic polynomials in Eq. (3.84) represented in the coordinate systems (α) and (β) are given by

$$f_{TJ}^{(\alpha)(\beta)}(\mathbf{z}^*; \mathbf{z}') = \left(P_1 \mathbf{z}_1^{(\alpha)*} + P_2 \mathbf{z}_2^{(\alpha)*} + P'_1 \mathbf{z}_1^{(\beta)'} + P'_2 \mathbf{z}_2^{(\beta)'} \right)^2, \quad (3.116)$$

where the coefficients P_1 , P_2 , P'_1 and P'_2 for each interaction types $T = TJ$ can be expressed in terms of p_α^γ and q_α^γ as shown in Table IV.

TABLE IV. The coefficients P_1 , P_2 , P'_1 , and P'_2 in Eq. (3.116) for the 3-cluster interaction types $T = TJ$ with the sets of Jacobi coordinates $J = (\alpha)$ in the bra state and $J = (\beta)$ in the ket state. The quantities p_α^γ and q_α^γ are defined in Eq. (3.115). The superscripts ε and λ in this table are determined such that $(\varepsilon\lambda\gamma)$ becomes an even permutation of (123) .

| $T = TJ$ | P_1 | P_2 | P'_1 | P'_2 |
|----------------|------------------------|------------------------|------------------------|------------------------|
| E | 0 | 0 | 0 | 0 |
| $S(\gamma)$ | p_α^γ | q_α^γ | 0 | 0 |
| $S'(\gamma)$ | 0 | 0 | p_β^γ | q_β^γ |
| $D_+(\gamma)$ | p_α^γ | q_α^γ | p_β^γ | q_β^γ |
| $D_-(\gamma)$ | p_α^γ | q_α^γ | $-p_\beta^\gamma$ | $-q_\beta^\gamma$ |
| $V_+(\gamma)$ | p_α^λ | q_α^λ | $-p_\beta^\varepsilon$ | $-q_\beta^\varepsilon$ |
| $V_-(\gamma)$ | p_α^λ | q_α^λ | p_β^ε | q_β^ε |
| $V'_+(\gamma)$ | p_α^ε | q_α^ε | $-p_\beta^\lambda$ | $-q_\beta^\lambda$ |
| $V'_-(\gamma)$ | p_α^ε | q_α^ε | p_β^λ | q_β^λ |

§4. Evaluation of Spin-Isospin Factors

4.1 General Procedure

In the preceding section, we have shown that, as long as the spatial part of GCM kernels is concerned, a quite general formulation is possible even in n -cluster systems if they are composed of only s -shell clusters. Therefore, the main effort to set up the GCM kernels is reduced to the evaluation of spin-isospin factors. There already exist numbers of shell model calculations in which such spin-isospin factors are evaluated by using the *cfp* expansions of the antisymmetrized wave functions and also by using recoupling techniques in the angular momentum algebra. We can employ these techniques even in cluster systems, although the nature of the procedure is a little different from the shell-model one. This is because in cluster systems we need to deal with a number of non-standard coupling schemes due to many different types of cluster decompositions and to their rearrangements. In this section, we first try to clarify what are really needed to construct whole set of the spin-isospin factors, and outline the general procedure to obtain them. A good example of this procedure is given for general 2-cluster systems in the next subsection. The result is then extended to the spin-isospin factors of 3-cluster systems composed of an alpha cluster plus two s -shell clusters, in which a much simpler technique called the valence orbital method can be employed.

The spin-isospin factors defined through Eq. (3.59b) are with respect to the spin-isospin operators w involved in the two-body interactions in Eq. (3.61). These are given by $w = (W + BP_\sigma - HP_\tau - MP_\sigma P_\tau)$, $w^{(CL)} = (1 + \tau_{1z})(1 + \tau_{2z})/4$, $w^{(LS)} = (W - HP_\tau)(\sigma_1 + \sigma_2)/2$, and $w^{(T)} = (W - HP_\tau)[\sigma_1 \sigma_2]_\mu^{(2)}$ for the central, Coulomb, LS and tensor forces, respectively. Let us first consider the central, LS and tensor operators. As is already discussed in the §3.3.1, the isospin part of these interactions can be eliminated by using the generalized Pauli principle $(-P_\sigma P_\tau) = P_x$, where P_x is the exchange operator of two particles in the spatial coordinates. Suppose $T_{\{\alpha\beta;\gamma\delta\}}$ is the spatial interaction factor for a two-body interaction u defined through Eq. (3.59a). In a shorthand notation $A_{\alpha\beta} \equiv \langle (0s)_{\mathbf{s}_\alpha} | (0s)_{\mathbf{s}'_\beta} \rangle$, the interaction factor for $u^r \equiv u P_x$ is given by

$$T_{\{\alpha\beta;\gamma\delta\}}^r = A_{\alpha\beta}^{-1} A_{\gamma\delta}^{-1} A_{\alpha\delta} A_{\gamma\beta} T_{\{\alpha\delta;\gamma\beta\}} \quad (4.1)$$

We should use this in Eq. (3.60b) to obtain the GCM kernel $I^r(z; z')$ for u^r . The readjustment of the powers of $A_{\alpha\beta}$ etc. leads to the modification of the double-coset symbol $[k]$ in $Q[k]$ as follows ;

$$k \rightarrow k^{\{\alpha\beta;\gamma\delta\}} \equiv k - e^{(\alpha\beta)} - e^{(\gamma\delta)} + e^{(\alpha\delta)} + e^{(\gamma\beta)} \quad , \quad (4.2)$$

where $e^{(\alpha\beta)} = (e_{\mu\nu}^{(\alpha\beta)})$ denotes an $n \times n$ matrix with the matrix element given by $e_{\mu\nu}^{(\alpha\beta)} = \delta_{\mu\alpha} \delta_{\nu\beta}$. We can rearrange the summation over $[k]$ such that the norm exponential factor $Tr(zQ[k]^t z')$ is restored to the original form. If we further interchange β and δ in the summation of the interaction types $\{\alpha\beta;\gamma\delta\}$, we find that $I^r(z; z')$ is given by Eq. (3.60a) with the following simple modification ;

$$X_{k^{\{\alpha\beta;\gamma\delta\}}} \rightarrow X_{k^{\{\alpha\beta;\gamma\delta\}}\{\alpha\delta;\gamma\beta\}} \quad . \quad (4.3)$$

In terms of the type specification \mathcal{T} introduced in the §3.3.1, this change can be expressed as follows. In E , S and S' types which involve no \pm indices, their spin-isospin factors are invariant, while in $\mathcal{T} = D$, V and V' types in Eq. (3.72), \mathcal{T}_+ and \mathcal{T}_- types are interchanged with an appropriate modification of the double-coset symbols. For example, in 2-cluster systems, we have

$$\begin{aligned} X_{x\mathcal{T}} &\rightarrow X_{x\mathcal{T}} & \text{for } \mathcal{T} = E_{\alpha\beta}, S'_\alpha, S_\beta, \\ X_{xD_+} &\rightarrow X_{x+1D_-}, & X_{xD_-} \rightarrow X_{x-1D_+}. \end{aligned} \quad (4.4)$$

From this consideration, we essentially need to deal with the operators

$$w^{(d)} = 1, \quad w^{(e)} = P_\sigma = \frac{1 + \sigma_1 \cdot \sigma_2}{2}, \quad (4.5a)$$

$$w^{(LS)} = \frac{\sigma_1 + \sigma_2}{2}, \quad w^{(T)} = [\sigma_1 \sigma_2]_\mu^{(2)}, \quad (4.5b)$$

and their spin-isospin factors defined through Eq. (3.59b).¹⁷ Then the full spin-isospin factors for the central, LS and tensor forces are given by

$$X_{k\{\alpha\beta;\gamma\delta\}}^C = X_{k\{\alpha\beta;\gamma\delta\}}^d W + X_{k\{\alpha\beta;\gamma\delta\}}^e B + X_{k\{\alpha\beta;\gamma\delta\}\{\alpha\delta;\gamma\beta\}}^e H + X_{k\{\alpha\beta;\gamma\delta\}\{\alpha\delta;\gamma\beta\}}^d M, \quad (4.6a)$$

$$\left(X_{k\{\alpha\beta;\gamma\delta\}}^\Omega \right)^{total} = X_{k\{\alpha\beta;\gamma\delta\}}^\Omega W + X_{k\{\alpha\beta;\gamma\delta\}\{\alpha\delta;\gamma\beta\}}^\Omega H \quad \text{for } \Omega = LS \text{ and tensor}. \quad (4.6b)$$

The simplest spin-isospin factors $X_{k\{\alpha\beta;\gamma\delta\}}^d$ are obtained by counting the numbers of pairs :

$$\begin{aligned} X_{k\{\alpha\beta;\alpha\beta\}}^d &= \binom{k_{\alpha\beta}}{2} X_k^N & \text{for } E_{\alpha\beta}, \\ X_{k\{\alpha\beta;\gamma\delta\}}^d &= k_{\alpha\beta} k_{\gamma\delta} X_k^N & \text{otherwise}, \end{aligned} \quad (4.7)$$

where X_k^N is the spin-isospin factor for the normalization kernel defined in Eq. (3.32). Similarly, the LS factors are reduced to one-body spin-isospin factors. This is a common feature of the two-body interaction that can be expressed as a simple sum of a one-body operator; $w_{st} = w_s + w_t$. In this case, all the two-body spin-isospin factors are reduced to one-body spin-isospin factors through a similar relationship to Eq. (4.7) :

¹⁷As is discussed in the §3.3.1, the LS and tensor spin-isospin factors can be conveniently defined through the reduced matrix elements. If we set the LS and tensor matrix elements in Eq. (3.59b) equal to $X_{kT}^{LS} \mathbf{S}$ and $X_{kT}^T S_\mu^{(2)}$ in terms of formal operators \mathbf{S} and $S_\mu^{(2)}$ for the total system, these reduced matrix elements should be divided by those of \mathbf{S} and $S_\mu^{(2)}$, respectively. The choice of $\langle S \parallel \mathbf{S} \parallel S' \rangle$ and $\langle S \parallel S^{(2)} \parallel S' \rangle$ is arbitrary (as long as they are non-zero) and they are assumed to be unity in the following discussions. For the Coulomb factors, this procedure is not taken in Eq. (3.69), since T_z is a conserved quantity related to the total charge.

$$\begin{aligned} X_{k\{\alpha\beta;\alpha\beta\}}^{\Omega} &= (k_{\alpha\beta} - 1)X_{k\{\alpha\beta\}}^{\Omega} && \text{for } E_{\alpha\beta} \text{ ,} \\ X_{k\{\alpha\beta;\gamma\delta\}}^{\Omega} &= k_{\gamma\delta} X_{k\{\alpha\beta\}}^{\Omega} + k_{\alpha\beta} X_{k\{\gamma\delta\}}^{\Omega} && \text{otherwise ,} \end{aligned} \quad (4.8)$$

where $X_{k\{\alpha\beta\}}^{\Omega}$ is defined in Eq. (3.48). The LS operator in Eq. (4.5b) and $(N-1)T_z$ term in the Coulomb operator discussed below are of this type and these factors are obtained by calculating the reduced matrix elements

$$X_{k\{\alpha\beta\}}^{(\sigma)} = C_k \langle z_k \xi_{ST} \parallel \sum_{s \in \mathbf{k}_{\alpha\beta}} \left\{ \begin{array}{c} \sigma_s/2 \\ \tau_s/2 \end{array} \right\} \parallel \xi'_{S'T'} \rangle \text{ ,} \quad (4.9)$$

and by using the relationship in Eq. (4.8).

The standard procedure to calculate the spin-isospin factors X_k^N for the normalization kernel and those for the one-body operators like $X_{k\{\alpha\beta\}}^{\Omega}$ in Eq. (4.9) is to use the following decomposition of the antisymmetric spin-isospin wave functions $\xi_{ST}(1, \dots, A)$;

$$\begin{aligned} \xi_{ST}(1, \dots, A) &= \sum_{S_1 T_1 S_2 T_2} \langle [1^{A_1}]S_1 T_1 [1^{A_2}]S_2 T_2 \parallel [1^A]ST \rangle \\ &\times [\xi_{S_1 T_1}(1, \dots, A_1) \xi_{S_2 T_2}(A_1 + 1, \dots, A)]_{ST} \end{aligned} \quad (4.10)$$

with $A = A_1 + A_2 \leq 4$. Here, the stretched $SU_4 \supset SU_2 \times SU_2$ Clebsch-Gordan (C-G) coefficients have simple values 1 or $\pm 1/\sqrt{2}$, depending on the combinations of $[1^{A_1}]S_1 T_1$ and $[1^{A_2}]S_2 T_2$. [96], [107] For $A_1 \geq A_2$, these are given by

$$\begin{aligned} \langle [11] \left\{ \begin{array}{c} 10 \\ 01 \end{array} \right\} [1] \frac{1}{2} \frac{1}{2} \parallel [111] \frac{1}{2} \frac{1}{2} \rangle &= \left\{ \begin{array}{c} 1/\sqrt{2} \\ -1/\sqrt{2} \end{array} \right\} \text{ ,} \\ \langle [11] \left\{ \begin{array}{c} 10 \\ 01 \end{array} \right\} [11] \left\{ \begin{array}{c} 10 \\ 01 \end{array} \right\} \parallel [1111]00 \rangle &= \left\{ \begin{array}{c} 1/\sqrt{2} \\ -1/\sqrt{2} \end{array} \right\} \text{ ,} \end{aligned} \quad (4.11)$$

besides the trivial values $\langle [1] \frac{1}{2} \frac{1}{2} [1] \frac{1}{2} \frac{1}{2} \parallel [11]10 \rangle = \langle [111] \frac{1}{2} \frac{1}{2} [1] \frac{1}{2} \frac{1}{2} \parallel [1111]00 \rangle = 1$. For the interchange between $[1^{A_1}]S_1 T_1$ and $[1^{A_2}]S_2 T_2$, the above values should be multiplied by an extra phase factor $(-1)^{A_1 A_2} (-1)^{S_1 + S_2 - S} (-1)^{T_1 + T_2 - T}$. By employing Eq. (4.10), the spin-isospin coupled wave functions of n s -shell clusters are further decomposed into those of n^2 s -shell clusters. We write this decomposition symbolically as

$$\xi_{ST} = \sum_{\{S_{ij}\}\{T_{ij}\}r} \xi_{\{S_{ij}\}\{T_{ij}\}r;ST} \langle \{S_{ij}\}\{T_{ij}\}r \parallel \xi_{ST} \rangle \quad (4.12)$$

where $\xi_{\{S_{ij}\}\{T_{ij}\}r;ST}$ denotes that the k_{ij} -nucleon spin-isospin wave functions with S_{ij} and T_{ij} are coupled into the total S and T with extra spin-isospin quantum numbers r for intermediate couplings. The coefficient $\langle \{S_{ij}\}\{T_{ij}\}r \parallel \xi_{ST} \rangle$ is given as a product of the SU_4 C-G coefficients in Eq. (4.10). In order to facilitate the operation z_k in Eq. (3.28), we also introduce $\tilde{\xi}_{\{S_{ji}\}\{T_{ji}\}\tilde{r};ST}$ in which the clusters C_j with $\mathbf{A}_j = \{\mathbf{k}_{1j}, \dots, \mathbf{k}_{nj}\}$ are decomposed into C_{j1}, \dots, C_{jn} with the particle numbers k_{j1}, \dots, k_{jn} and the spin-isospin values $S_{j1}T_{j1}, \dots, S_{jn}T_{jn}$, respectively ;

$$\xi_{ST} = \sum_{\{S_{ji}\}\{T_{ji}\}\tilde{r}} \tilde{\xi}_{\{S_{ji}\}\{T_{ji}\}\tilde{r};ST} \langle \{S_{ji}\}\{T_{ji}\}\tilde{r} | \xi_{ST} \rangle . \quad (4.13)$$

Then the effect of z_k on ξ_{ST} restores it to the same form as in Eq. (4.12), but the ordering of the intermediate couplings is entirely different :

$$z_k \xi_{ST} = \sum_{\{S_{ji}\}\{T_{ji}\}\tilde{r}} \xi_{\{S_{ji}\}\{T_{ji}\}\tilde{r};ST} \langle \{S_{ji}\}\{T_{ji}\}\tilde{r} | \xi_{ST} \rangle . \quad (4.14)$$

Then by applying the decomposition in Eq. (4.10) to the ket side also, we obtain

$$\begin{aligned} X_k^N &= C_k \langle z_k \xi_{ST} | \xi'_{ST} \rangle \\ &= C_k \sum_{\{S_{ij}\}\{T_{ij}\}r} \langle \{S_{ji}\}\{T_{ji}\}\tilde{r} | \xi_{ST} \rangle \langle \{S_{ij}\}\{T_{ij}\}r | \xi'_{ST} \rangle \\ &\quad \times \langle \xi_{\{S_{ji}\}\{T_{ji}\}\tilde{r};ST} | \xi_{\{S_{ij}\}\{T_{ij}\}r;ST} \rangle . \end{aligned} \quad (4.15)$$

The last matrix elements in Eq. (4.15) are obtained by the angular-momentum recouplings of n^2 -cluster spin-isospin wave functions. In order to calculate the one-body spin-isospin factors $X_{k\{\alpha\beta\}}^{\sigma(1)}$ in Eq. (4.9), for example, we only need to assume $S \neq S'$ and augment the last matrix element in Eq. (4.15) with a multiplication of the one-body reduced matrix element $\langle \xi_{S_{\alpha\beta}T_{\alpha\beta}}(\mathbf{k}_{\alpha\beta}) | \sum_{s \in \mathbf{k}_{\alpha\beta}} \sigma_s / 2 | \xi_{S_{\alpha\beta}T_{\alpha\beta}}(\mathbf{k}_{\alpha\beta}) \rangle$, which is equal to $\sqrt{S_{\alpha\beta}(S_{\alpha\beta} + 1)}$.

Before proceeding to the evaluation of the other spin-isospin factors for the operators in Eq. (4.5) and also for the Coulomb operator $w^{(CL)} = (1 + \tau_{1z})(1 + \tau_{2z})/4$, let us consider the tensorial representation of the operators. In the definition of spin-isospin factors in Eq. (3.59b), we have summed up the two-body operators over the particle indices ($s < t$) of $w_{st}^{(\Omega)}$ with respect to all the nucleons which yield a common spatial integral for some particular exchange and interaction type $\mathcal{T} = \{\alpha\beta; \gamma\delta\}$. Therefore, it is useful to find simple expressions for

$$\mathcal{W}^\Omega = \sum_{s < t}^N w_{st}^{(\Omega)} \quad (4.16)$$

for an N -nucleon system. For P_σ in Eq. (4.5a), it is given by

$$\mathcal{W}^e = \sum_{s < t}^N \frac{1 + \sigma_s \cdot \sigma_t}{2} = \frac{1}{4} N(N - 4) + \mathbf{S}^2 , \quad (4.17)$$

where $\mathbf{S} = \sum_{s=1}^N \sigma_s / 2$ is the total spin operator of the N -nucleon system.¹⁸ Similarly, we find

¹⁸This notation should not be confused with the formal spin \mathbf{S} and the second-rank spin tensor $S_\mu^{(2)}$ in Eq. (3.69). These are not a sum of the total A -nucleon system and need not be represented as $S_\mu^{(2)} = 2[SS]_\mu^{(2)}$ either. In fact, they have in general off-diagonal matrix elements $\langle S || S || S' \rangle \neq 0$ etc., unlike the single particle operators of the N -nucleon system defined here.

$$\mathcal{W}^{(LS)} = \sum_{s < t}^N \frac{\sigma_s + \sigma_t}{2} = (N - 1)\mathbf{S} \quad , \quad (4.18)$$

$$\mathcal{W}^{(T)} = \sum_{s < t}^N [\sigma_s \sigma_t]_{\mu}^{(2)} = 2 [SS]_{\mu}^{(2)} \equiv S_{\mu}^{(2)} \quad . \quad (4.19)$$

In the tensor operator, we have used $[\sigma\sigma]_{\mu}^{(2)} = 0$ for the Pauli matrices σ . Furthermore, the second-rank tensor for the N -nucleon system is defined by $S_{\mu}^{(2)} = 2 [SS]_{\mu}^{(2)}$. For the two-nucleon system with $\mathbf{S} = (\sigma_1 + \sigma_2)/2$, this definition yields $S_{\mu}^{(2)} = [\sigma_1\sigma_2]_{\mu}^{(2)}$ as expected. The reduced matrix elements of $S = S^{(1)} = \mathbf{S}$ and $S_{\mu}^{(2)}$ are obtained from $S_0^{(2)} = \sqrt{6} (S_z^2 - S^2/3)$ and C-G coefficients

$$\begin{aligned} \langle SS_z 10 \mid SS_z \rangle &= \frac{S_z}{\sqrt{S(S+1)}} \quad , \\ \langle SS_z 20 \mid SS_z \rangle &= \frac{3S_z^2 - S(S+1)}{\sqrt{S(S+1)(2S-1)(2S+3)}} \quad , \end{aligned} \quad (4.20)$$

with the results given by¹⁹

$$\begin{aligned} \langle S \parallel \mathbf{S} \parallel S \rangle &= \sqrt{S(S+1)} \quad , \\ \langle S \parallel S^{(2)} \parallel S \rangle &= \sqrt{\frac{2}{3} S(S+1)(2S-1)(2S+3)} \quad . \end{aligned} \quad (4.21)$$

The Coulomb factor $\mathcal{W}^{(CL)}$ is also expressed by the tensor operators in the isospin space :

$$\begin{aligned} \mathcal{W}^{(CL)} &= \sum_{s < t}^N \frac{1 + \tau_{sz}}{2} \frac{1 + \tau_{tz}}{2} = \frac{N}{4} \left(\frac{N}{2} - 1 \right) + \frac{N-1}{2} T_z + \frac{1}{2} T_z^2 \\ &= \left[\frac{N}{4} \left(\frac{N}{2} - 1 \right) + \frac{1}{6} \mathbf{T}^2 \right] + \frac{N-1}{2} T_z + \frac{1}{2\sqrt{6}} T_0^{(2)} \quad . \end{aligned} \quad (4.22)$$

Here, \mathbf{T} and $T_{\mu}^{(2)} = 2 [TT]_{\mu}^{(2)}$ are defined similarly to the spin case and their reduced matrix elements are given by Eq. (4.21) with all the S being replaced by T . As an immediate application of \mathcal{W}^{Ω} derived here, we can calculate internal energies of *s*-shell clusters. These are explicitly given by

$$\begin{aligned} E^{(int)}(C) &= (N - 1) \frac{3\hbar^2 \nu}{2M} \\ &+ v_0 \left(\frac{\nu}{\nu + \kappa} \right)^{\frac{3}{2}} \left\{ \binom{N}{2} (W + M) + \left[\frac{1}{4} N(N - 4) + S(S + 1) \right] (B + H) \right\} \\ &+ 2e^2 \sqrt{\frac{\nu}{\pi}} \left[\frac{N}{4} \left(\frac{N}{2} - 1 \right) + \frac{N-1}{2} T_z + \frac{1}{2} T_z^2 \right] \end{aligned} \quad (4.23)$$

¹⁹The reduced matrix elements in this paper are defined by : (full matrix element) = (reduced matrix element) \times (Wigner coefficient), without dimensional factors such as $\hat{J}^{-1} = 1/\sqrt{2J+1}$. Also, 9-*j* symbols with square brackets are used for denoting their unitary form with $\hat{J}_{12}\hat{J}_{34}\hat{J}_{13}\hat{J}_{24}$ factors.

for $(0s)^N$ clusters with SS_zTT_z , interacting by the two-nucleon interaction in Eq. (3.61).

One of the merits of \mathcal{W}^Ω is that they are single particle operators of the N -nucleon clusters, so that they do not transfer the spin and isospin values of clusters. This property is conveniently used for evaluating the other spin-isospin factors just in the same way as we have done for the single particle operators in the preceding paragraph. Namely, for the non- E type interaction type $\{\alpha\beta; \gamma\delta\}$, we consider a merged system $\mathbf{k}_{\alpha\beta} \cup \mathbf{k}_{\gamma\delta}$ and extend the definition of the spin-isospin factors in Eq. (3.59b) to

$$X_{k\{\alpha\beta\} \cup \{\gamma\delta\}}^\Omega \equiv C_k \langle z_k \xi \mid \sum_{s, t \in \mathbf{k}_{\alpha\beta} \cup \mathbf{k}_{\gamma\delta}, s < t} w_{st}^{(\Omega)} \mid \xi' \rangle , \quad (4.24)$$

The operator involved in Eq. (4.24) is \mathcal{W}^Ω for the $(k_{\alpha\beta} + k_{\gamma\delta})$ -nucleon subsystem. Then if we further recouple $\xi_{\{S_{ij}\}\{T_{ij}\}r;ST}$ in Eq. (4.15) in such a way that a coupled combination $[\xi_{S_{\alpha\beta}T_{\alpha\beta}}(\mathbf{k}_{\alpha\beta}) \xi_{S_{\gamma\delta}T_{\gamma\delta}}(\mathbf{k}_{\gamma\delta})]_{S_{\alpha\beta\gamma\delta}T_{\alpha\beta\gamma\delta}}$ is explicitly involved, we can replace the operator with a possible c-number term and the reduced matrix elements of single particle operators. Once $X_{k\{\alpha\beta\} \cup \{\gamma\delta\}}^\Omega$ are obtained, we can easily find $X_{k\{\alpha\beta; \gamma\delta\}}^\Omega$ through²⁰

$$X_{k\{\alpha\beta; \gamma\delta\}}^\Omega = X_{k\{\alpha\beta\} \cup \{\gamma\delta\}}^\Omega - X_{k\{\alpha\beta; \alpha\beta\}}^\Omega - X_{k\{\gamma\delta; \gamma\delta\}}^\Omega . \quad (4.25)$$

In the following, we deem Eq. (4.24) an extension of E -type spin-isospin factors $X_{k\mathcal{T}}^\Omega$ with $\mathcal{T} = \{\alpha\beta; \alpha\beta\}$ to $\mathcal{T} = \{\alpha\beta\} \cup \{\gamma\delta\}$, and use a shorthand notation

$$X_{k\mathcal{T}}^\Omega = C_k \langle z_k \xi \mid \mathcal{W}_{\mathcal{T}}^\Omega \mid \xi' \rangle . \quad (4.26)$$

From these discussions, a general procedure to evaluate the spin-isospin factors by the use of the *cfp* expansions and angular-momentum recoupling techniques is formulated as follows. For the extended E -type interaction types \mathcal{T} described above, we first calculate

$$\left. \begin{array}{l} X_k^N \\ X_{k\mathcal{T}}^{\sigma(\lambda)} \\ X_{k\mathcal{T}}^{\tau(\lambda)} \end{array} \right\} = C_k \langle z_k \xi_{ST} \parallel \left\{ \begin{array}{l} 1 \\ S_{\mathcal{T}}^{(\lambda)} \\ T_{\mathcal{T}}^{(\lambda)} \end{array} \right\} \parallel \xi'_{S'T'} \rangle . \quad (4.27)$$

Here, $S_{\mathcal{T}}^{(\lambda)}$ and $T_{\mathcal{T}}^{(\lambda)}$ are single-particle spin and isospin operators of rank λ defined for the nucleon ensemble specified by \mathcal{T} . To be more specific, we assume

$$S^{(0)} = \mathbf{S}^2 , \quad S_\mu^{(1)} = S_\mu , \quad S_\mu^{(2)} = 2[S_\mu S_\mu]_\mu^{(2)} \quad (4.28)$$

for the spin operators and $S \rightarrow T$ for the isospin operators. The reduced matrix elements of these operators are given in Eq. (4.21), together with $\mathbf{S}^2 = S(S+1)$. After these factors are converted to two-body spin-isospin factors $X_{k\mathcal{T}}^\Omega$ for \mathcal{W}^Ω , those for general interaction types \mathcal{T} are obtained by using Eq. (4.25). The exchange central factors $X_{k\{\alpha\beta; \gamma\delta\}}^e$ in Eq. (4.6a) are given by

²⁰The results in Eqs. (4.7) and (4.8) are also obtained from this procedure.

$$\begin{aligned}
 X_{k\{\alpha\beta;\alpha\beta\}}^e &= \frac{1}{4}k_{\alpha\beta}(k_{\alpha\beta} - 4) X_k^N + X_{k\{\alpha\beta;\alpha\beta\}}^{\sigma(0)} \quad \text{for } E_{\alpha\beta} , \\
 X_{k\{\alpha\beta;\gamma\delta\}}^e &= \frac{1}{2}k_{\alpha\beta} k_{\gamma\delta} X_k^N + X_{k\{\alpha\beta;\gamma\delta\}}^{\sigma(0)} \quad \text{otherwise} , \quad (4.29)
 \end{aligned}$$

where $X_{k\{\alpha\beta;\gamma\delta\}}^{\sigma(0)}$ are defined through Eq. (4.25) with $\Omega = \sigma(0)$. For the LS factors (and also for a part of Coulomb factors), the definition of $X_{kT}^{\sigma(1)}$ or $X_{kT}^{\tau(1)}$ in Eq. (4.27) is equivalent to that in Eq. (4.9), if we identify the type classification $\{\alpha\beta\}$ of the one-body operators with $E_{\alpha\beta}$ for the two-body interaction types. Due to the additivity of these first-rank tensors, we only need to calculate these $E_{\alpha\beta}$ -type factors. The others are obtained through Eq. (4.8); namely,²¹

$$\begin{aligned}
 X_{k\{\alpha\beta;\alpha\beta\}}^{LS} &= (k_{\alpha\beta} - 1) X_{k\{\alpha\beta;\alpha\beta\}}^{\sigma(1)} \quad \text{for } E_{\alpha\beta} , \\
 X_{k\{\alpha\beta;\gamma\delta\}}^{LS} &= k_{\gamma\delta} X_{k\{\alpha\beta;\alpha\beta\}}^{\sigma(1)} + k_{\alpha\beta} X_{k\{\gamma\delta;\gamma\delta\}}^{\sigma(1)} \quad \text{otherwise} . \quad (4.30)
 \end{aligned}$$

The tensor factors in Eq. (4.6b) are directly given by

$$X_{k\{\alpha\beta;\gamma\delta\}}^T = X_{k\{\alpha\beta;\gamma\delta\}}^{\sigma(2)} . \quad (4.31)$$

(We have assumed unity for the reduced matrix elements of the formal spin and tensor operators in Eq. (3.69).) Finally, the Coulomb factors are given by

$$\begin{aligned}
 X_{k\{\alpha\beta;\alpha\beta\}}^{CL} &= \delta_{T,T'} \left[\frac{k_{\alpha\beta}}{4} \left(\frac{k_{\alpha\beta}}{2} - 1 \right) + \frac{1}{6} X_{k\{\alpha\beta;\alpha\beta\}}^{\tau(0)} \right] + \langle T' T_z 10 | T T_z \rangle \frac{k_{\alpha\beta} - 1}{2} \\
 &\quad \times X_{k\{\alpha\beta;\alpha\beta\}}^{\tau(1)} + \langle T' T_z 20 | T T_z \rangle \frac{1}{2\sqrt{6}} X_{k\{\alpha\beta;\alpha\beta\}}^{\tau(2)} \quad \text{for } E_{\alpha\beta} , \\
 X_{k\{\alpha\beta;\gamma\delta\}}^{CL} &= \delta_{T,T'} \left[\frac{1}{4} k_{\alpha\beta} k_{\gamma\delta} + \frac{1}{6} X_{k\{\alpha\beta;\gamma\delta\}}^{\tau(0)} \right] \\
 &\quad + \langle T' T_z 10 | T T_z \rangle \frac{1}{2} \left[k_{\gamma\delta} X_{k\{\alpha\beta;\alpha\beta\}}^{\tau(1)} + k_{\alpha\beta} X_{k\{\gamma\delta;\gamma\delta\}}^{\tau(1)} \right] \\
 &\quad + \langle T' T_z 20 | T T_z \rangle \frac{1}{2\sqrt{6}} X_{k\{\alpha\beta;\gamma\delta\}}^{\tau(2)} \quad \text{otherwise} . \quad (4.32)
 \end{aligned}$$

Before closing this subsection, it is useful to show some kind of sum formulae for spin-isospin factors, which can be easily obtained as a further extension of the relationship in Eq. (4.25). These formulae are also useful for a check of spin-isospin factors in numerical calculations. These are given by

$$\sum_{\alpha} X_{kE_{\alpha\beta}}^{\Omega} + \sum_{(\alpha\gamma)} X_{kS_{\beta}^{(\alpha\gamma)}}^{\Omega} = (X_k^N)_{ST} H_{\beta}^{\prime\Omega} , \quad (4.33a)$$

$$\sum_{\beta} X_{kE_{\alpha\beta}}^{\Omega} + \sum_{(\beta\delta)} X_{kS_{\alpha}^{(\beta\delta)}}^{\Omega} = H_{\alpha}^{\Omega} (X_k^N)_{S'T'} , \quad (4.33b)$$

²¹Note that the relationship in Eq. (4.25) is not directly applicable to $X_{kT}^{\sigma(1)}$ and $X_{kT}^{\tau(1)}$ in Eq. (4.27). For example, we need to use $\mathcal{W}^{LS} = (N - 1) \mathbf{S}$, instead of \mathbf{S} itself.

where different spin-isospin values ST and $S'T'$ for the bra and the ket sides, respectively, are possible in general. Furthermore, H_α^Ω etc. are factors of subunit clusters defined through

$$H'_\beta{}^\Omega = \langle \xi'_{ST} | \sum_{s, t \in \mathbf{A}_\beta, s < t} w_{st}^{(\Omega)} | \xi'_{S'T'} \rangle , \quad (4.34a)$$

$$H_\alpha^\Omega = \langle \xi_{ST} | \sum_{s, t \in \mathbf{A}_\alpha, s < t} w_{st}^{(\Omega)} | \xi_{S'T'} \rangle . \quad (4.34b)$$

In particular, the central factors are explicitly given by

$$H_\alpha^C = \binom{A_\alpha}{2} (W + M) + \left[\frac{1}{4} A_\alpha (A_\alpha - 4) + S_\alpha (S_\alpha + 1) \right] (B + H) , \quad (4.35)$$

where S_α is the spin-value of the cluster C_α . Another relationship is obtained if we add up all the spin-isospin factors :

$$\sum_{\{\alpha\beta; \gamma\delta\}} X_{k\{\alpha\beta; \gamma\delta\}}^\Omega = \delta_{S, S'} \delta_{T, T'} X_k^N H_0^\Omega , \quad (4.36)$$

where H_0^Ω is given by

$$H_0^\Omega = \langle \xi_{ST} | \sum_{s < t}^A w_{st}^{(\Omega)} | \xi_{ST} \rangle = \langle \xi'_{ST} | \sum_{s < t}^A w_{st}^{(\Omega)} | \xi'_{ST} \rangle . \quad (4.37)$$

4.2 2-Cluster Systems

In order to carry out the procedure discussed in the preceding subsection for general 2-cluster systems composed of $A = A_1 + A_2$ ($1 \leq A_2 \leq A_1 \leq 4$) nucleons, we assume a particular spin-isospin wave function

$$\xi_{S_1 T_1 S_2 T_2; S S_z T T_z} = [\xi_{S_1 T_1}(1, \dots, A_1) \xi_{S_2 T_2}(A_1 + 1, \dots, A)]_{S S_z T T_z} \quad (4.38)$$

for the bra state and $\xi_{S'_1 T'_1 S'_2 T'_2; S'_z S'_z T'_z}$ for the ket state with $S'_z = S_z$ and $T'_z = T_z$.

First of all, as to the coefficients with $\lambda = 1$ in Eq. (4.27), we only need to calculate them for four $\mathcal{T} = E_{\alpha\beta}$ types. When $\lambda = 0$ and 2, the sum formulae in Eqs. (4.33) and (4.36) reduce the number of independent coefficients to a great extent. One can easily show that,

$$H_1^{\sigma(\lambda)} = \begin{bmatrix} S_1 & S_2 & S' \\ \lambda & 0 & \lambda \\ S_1 & S_2 & S \end{bmatrix} \langle S_1 \parallel S^{(\lambda)} \parallel S_1 \rangle , \quad (4.39a)$$

$$H_2^{\sigma(\lambda)} = \begin{bmatrix} S_1 & S_2 & S' \\ 0 & \lambda & \lambda \\ S_1 & S_2 & S \end{bmatrix} \langle S_2 \parallel S^{(\lambda)} \parallel S_2 \rangle , \quad (4.39b)$$

$$H_1^{\prime\sigma(\lambda)} = \begin{bmatrix} S'_1 & S'_2 & S' \\ \lambda & 0 & \lambda \\ S'_1 & S'_2 & S \end{bmatrix} \langle S'_1 \parallel S^{(\lambda)} \parallel S'_1 \rangle , \quad (4.39c)$$

$$H_2^{\prime\sigma(\lambda)} = \begin{bmatrix} S'_1 & S'_2 & S' \\ 0 & \lambda & \lambda \\ S'_1 & S'_2 & S \end{bmatrix} \langle S'_2 \parallel S^{(\lambda)} \parallel S'_2 \rangle , \quad (4.39d)$$

for the operators $S^{(\lambda)}$ in Eq. (4.28). The factors for $H_\alpha^{\tau(\lambda)}$ and $H_\beta^{\prime\tau(\lambda)}$ are obtained by $S \rightarrow T$. Then, $X_{xS'_\alpha}^{\sigma(0)}$ and $X_{xS_\beta}^{\sigma(0)}$ in Eq. (4.29), for example, are obtained from²²

$$X_{xS'_\alpha}^{\sigma(0)} = H_\alpha^{\sigma(0)} X_x^N - \sum_\beta X_{xE_{\alpha\beta}}^{\sigma(0)} , \quad (4.40a)$$

$$X_{xS_\beta}^{\sigma(0)} = X_x^N H_\beta^{\prime\sigma(0)} - \sum_\alpha X_{xE_{\alpha\beta}}^{\sigma(0)} , \quad (4.40b)$$

with $S = S'$ and $T = T'$. We can also add up these spin-isospin factors with respect to the dummy indices α and β for the spatial integrals. Namely, in general Ω , we define

$$X_{xE}^\Omega = \sum_{\alpha\beta} X_{xE_{\alpha\beta}}^\Omega , \quad (4.41a)$$

$$X_{xS'}^\Omega = \sum_\alpha X_{xS'_\alpha}^\Omega , \quad X_{xS}^\Omega = \sum_\beta X_{xS_\beta}^\Omega , \quad (4.41b)$$

$$H^\Omega = \sum_\alpha H_\alpha^\Omega , \quad H'^\Omega = \sum_\beta H_\beta'^\Omega . \quad (4.41c)$$

Then, we find

$$X_{xS'}^\Omega = H^\Omega X_x^N - X_{xE}^\Omega , \quad (4.42a)$$

$$X_{xS}^\Omega = X_x^N H'^\Omega - X_{xE}^\Omega . \quad (4.42b)$$

On the other hand, $X_{xD_+}^\Omega$ and $X_{xD_-}^\Omega$ are also related to each other through the sum formula in Eq. (4.36). Thus we only need to introduce just one extra E -type factor $X_{x\{12\}\cup\{21\}}^\Omega$ in Eq. (4.24). We call $T = \{12\} \cup \{21\}$ E_- type. Then we find

$$X_{xD_-}^\Omega = X_{xE_-}^\Omega - X_{xE_{12}}^\Omega - X_{xE_{21}}^\Omega , \quad (4.43a)$$

²²The interaction-type indices S'_α and S_β should not be confused with the spin values of clusters. They always come up with the nucleon exchange number x .

$$X_{x D_+}^\Omega = \delta_{S,S'} \delta_{T,T'} X_x^N H_0^\Omega + X_{x E}^\Omega - X_x^N H'^\Omega - H^\Omega X_x^N - X_{x D_-}^\Omega . \quad (4.43b)$$

After all, we only need to calculate the spin-isospin factors in Eq. (4.27) for $T = E_{\alpha\beta}$ and E_- , if $\lambda = 0$ or 2.

After a straightforward calculation, we obtain

$$\left. \begin{array}{l} X_x^N \\ X_x^{\sigma(\lambda)} \\ X_x^{\tau(\lambda)} \end{array} \right\} = (-1)^x \binom{A_1}{x} \binom{A_2}{x} \sum_{\{S_{\alpha\beta}\}\{T_{\alpha\beta}\}} \langle [1^{A_1-x}] S_{11} T_{11} [1^x] S_{12} T_{12} \parallel [1^{A_1}] S_1 T_1 \rangle \\ \times \langle [1^x] S_{21} T_{21} [1^{A_2-x}] S_{22} T_{22} \parallel [1^{A_2}] S_2 T_2 \rangle \langle [1^{A_1-x}] S_{11} T_{11} [1^x] S_{21} T_{21} \parallel [1^{A_1}] S'_1 T'_1 \rangle \\ \times \langle [1^x] S_{12} T_{12} [1^{A_2-x}] S_{22} T_{22} \parallel [1^{A_2}] S'_2 T'_2 \rangle \left\{ \begin{array}{l} X_{x N}^\sigma X_{x N}^\tau \\ X_x^{\sigma(\lambda)} X_x^{\tau(\lambda)} \\ X_{x N}^\sigma X_x^{\tau(\lambda)} \end{array} \right. , \quad (4.44)$$

with

$$X_{x N}^\sigma = \delta_{S,S'} \begin{bmatrix} S_{11} & S_{12} & S_1 \\ S_{21} & S_{22} & S_2 \\ S'_1 & S'_2 & S \end{bmatrix} ,$$

$$\left. \begin{array}{l} X_{x E_{11}}^{\sigma(\lambda)} \\ X_{x E_{12}}^{\sigma(\lambda)} \end{array} \right\} = \sum_{S'_1} \begin{bmatrix} S_{11} & S_{12} & S''_1 \\ S_{21} & S_{22} & S_2 \\ S'_1 & S'_2 & S' \end{bmatrix} \begin{bmatrix} S''_1 & S_2 & S' \\ \lambda & 0 & \lambda \\ S_1 & S_2 & S \end{bmatrix} \left\{ \begin{array}{l} \begin{bmatrix} S_{11} & S_{12} & S''_1 \\ \lambda & 0 & \lambda \\ S_{11} & S_{12} & S_1 \end{bmatrix} \langle S_{11} \parallel S^{(\lambda)} \parallel S_{11} \rangle \\ \begin{bmatrix} S_{11} & S_{12} & S''_1 \\ 0 & \lambda & \lambda \\ S_{11} & S_{12} & S_1 \end{bmatrix} \langle S_{12} \parallel S^{(\lambda)} \parallel S_{12} \rangle \end{array} \right. ,$$

$$\left. \begin{array}{l} X_{x E_{21}}^{\sigma(\lambda)} \\ X_{x E_{22}}^{\sigma(\lambda)} \end{array} \right\} = \sum_{S''_2} \begin{bmatrix} S_{11} & S_{12} & S_1 \\ S_{21} & S_{22} & S''_2 \\ S'_1 & S'_2 & S' \end{bmatrix} \begin{bmatrix} S_1 & S''_2 & S' \\ 0 & \lambda & \lambda \\ S_1 & S_2 & S \end{bmatrix} \left\{ \begin{array}{l} \begin{bmatrix} S_{21} & S_{22} & S''_2 \\ \lambda & 0 & \lambda \\ S_{21} & S_{22} & S_2 \end{bmatrix} \langle S_{21} \parallel S^{(\lambda)} \parallel S_{21} \rangle \\ \begin{bmatrix} S_{21} & S_{22} & S''_2 \\ 0 & \lambda & \lambda \\ S_{21} & S_{22} & S_2 \end{bmatrix} \langle S_{22} \parallel S^{(\lambda)} \parallel S_{22} \rangle \end{array} \right. ,$$

$$\begin{aligned}
 X_{x E_-}^{\sigma(\lambda)} = & \sum_{S'_1, S'_2} (-1)^{2S_{22}-S_2-S'_2+S'_2} \begin{bmatrix} S_{11} & S_{12} & S_1 \\ S_{22} & S_{21} & S_2 \\ S'_1 & S'_2 & S \end{bmatrix} \begin{bmatrix} S_{11} & S_{21} & S'_1 \\ S_{22} & S_{12} & S'_2 \\ S'_1 & S'_2 & S' \end{bmatrix} \begin{bmatrix} S'_1 & S'_2 & S' \\ 0 & \lambda & \lambda \\ S'_1 & S'_2 & S \end{bmatrix} \\
 & \times \langle S'_2 \parallel S^{(\lambda)} \parallel S'_2 \rangle \quad (\lambda = 0 \text{ or } 2) .
 \end{aligned} \tag{4.45}$$

In Eq. (4.44), the summation $\{S_{\alpha\beta}\}$ means that over S_{11}, S_{12}, S_{21} and S_{22} etc. The reduced matrix elements of the spin operators are given in Eq. (4.21) and $\langle S \parallel S^{(0)} \parallel S \rangle = S(S+1)$ for $S^{(0)} = \mathbf{S}^2$. For $X_{xT}^{\tau(\lambda)}$, all the S should be converted into T in Eq. (4.45).

Although Eqs. (4.44) and (4.45) are not too much complicated, we can efficiently compute them with a computer machine. However, if one of the two *s*-shell clusters is an alpha cluster ($A_1 = 4$, for example), we can obtain simple analytic expressions for the spin-isospin factors, if we use the valence orbital method [83]. Since this technique is discussed in the next subsection in some detail, we show here only the final result of the calculations for the diagonal ($ST = S'T'$) configurations :

$$X_x^N = (-1)^x \binom{A_2}{x} , \quad X_{xT} = X_x^N F_{xT} , \tag{4.46}$$

with

$$\begin{aligned}
 F_{x E_{11}} &= X_{0 E_{11}} - \frac{x}{A_2} (X_{0 D_+} + X_{1 D_-}) + \frac{x(x-1)}{A_2(A_2-1)} X_{0 E_{22}} , \\
 F_{x E_{12}} &= F_{x E_{21}} = \frac{x(x-1)}{A_2(A_2-1)} X_{0 E_{22}} , \\
 F_{x E_{22}} &= \frac{(A_2-x)(A_2-x-1)}{A_2(A_2-1)} X_{0 E_{22}} , \\
 F_{x S_1} &= F_{x S'_1} = \frac{x}{A_2} \left(X_{0 D_+} + X_{1 D_-} - 2 \frac{x-1}{A_2-1} X_{0 E_{22}} \right) , \\
 F_{x S_2} &= F_{x S'_2} = 2 \frac{x(A_2-x)}{A_2(A_2-1)} X_{0 E_{22}} , \\
 F_{x D_+} &= \left(1 - \frac{x}{A_2} \right) \left(X_{0 D_+} - 2 \frac{x}{A_2-1} X_{0 E_{22}} \right) , \\
 F_{x D_-} &= -\frac{x}{A_2} \left(X_{1 D_-} - 2 \frac{x-1}{A_2-1} X_{0 E_{22}} \right) .
 \end{aligned} \tag{4.47}$$

The basic spin-isospin factors, $X_{0 E_{11}}, X_{0 E_{22}}, X_{0 D_+}$ and $X_{1 D_-}$ are easily derived for each type of interactions. They are explicitly given by

[*central*]

$$\begin{aligned}
X_{0E_{11}} &= X_d + X_e , \\
X_{0E_{22}} &= H^C = \binom{A_2}{2} (W + M) + \left[\frac{1}{4} A_2 (A_2 - 4) + S(S + 1) \right] (B + H) , \\
X_{0D_+} &= \frac{A_2}{2} X_d , \quad X_{1D_-} = \frac{A_2}{2} X_e ,
\end{aligned} \tag{4.48a}$$

where $X_d = 8W + 4B - 4H - 2M$ and $X_e = 8M + 4H - 4B - 2W$ as usual,

[*LS*]

$$X_{0E_{11}} = 0 , \quad \left\{ \begin{array}{c} X_{0E_{22}} \\ X_{0D_+} \\ X_{1D_-} \end{array} \right\} = \left\{ \begin{array}{c} A_2 - 1 \\ 4 \\ -4 \end{array} \right\} \sqrt{S(S + 1)} , \tag{4.48b}$$

[*tensor*]

$$X_{0E_{11}} = X_{0D_+} = X_{1D_-} = 0 , \quad X_{0E_{22}} = \sqrt{\frac{2}{3} S(S + 1)(2S - 1)(2S + 3)} , \tag{4.48c}$$

[*Coulomb*]

$$X_{0E_{11}} = 1 , \quad X_{0E_{22}} = \frac{1}{2} A_p (A_p - 1) , \quad X_{0D_+} = 2A_p , \quad X_{1D_-} = -A_p , \tag{4.48d}$$

where $A_p = A_2/2 + T_z$ is the number of the protons in C_2 , and $S = S_2$ is the spin value of C_2 or the total system. It should be noted that D_{\pm} -types and S^- , S'^- , D_{\pm} -types only contribute to LS and tensor kernels, respectively, due to the spatial factors. (See §3.3.2.)

4.3 *Alpha Plus Two s-Shell-Cluster Systems*

If we employ the valence orbital method, we can extend the spin-isospin factors, obtained in the preceding section for general 2-cluster systems, to 3-cluster systems which involve an extra α -cluster. Suppose that C_1 , C_2 and C_3 are two s -shell clusters with mass numbers, A_1 , A_2 ($1 \leq A_2 \leq A_1 \leq 4$) and an α -cluster with $A_3 = 4$, respectively, and that the spin-isospin wave functions for the total $A = A_1 + A_2 + 4$ nucleon system are described by $\xi_{S_1 T_1 S_2 T_2; ST}$ in Eq. (4.38), augmented with the α -cluster wave function $\xi(\alpha)$. By using the property that $\xi(\alpha)$ is spin-isospin saturated and also the effect of antisymmetrization, the single particle wave functions $\varphi_{\alpha} \equiv |(0s)_{S_{\alpha}}\rangle$ and $\psi_{\beta} \equiv |(0s)_{S'_{\beta}}\rangle$ in the GCM kernel in Eq. (3.19) can be modified into

$$\begin{aligned}
\varphi_{\alpha} &\rightarrow \tilde{\varphi}_{\alpha} \equiv \varphi_{\alpha} - |\varphi_3\rangle \langle \psi_3 | \varphi_{\alpha} \rangle \langle \psi_3 | \varphi_3 \rangle^{-1} , \\
\psi_{\beta} &\rightarrow \tilde{\psi}_{\beta} \equiv \psi_{\beta} - |\psi_3\rangle \langle \varphi_3 | \psi_{\beta} \rangle \langle \varphi_3 | \psi_3 \rangle^{-1} ,
\end{aligned} \tag{4.49}$$

for $\alpha, \beta = 1$ or 2 . For the normalization kernel, this replacement simplifies the effect of antisymmetrization \mathcal{A} such that the permutation between $C_1 \cup C_2$ and α gives zero contribution due to $\langle \tilde{\varphi}_\alpha | \psi_3 \rangle = \langle \varphi_3 | \tilde{\psi}_\beta \rangle = 0$ for $\alpha, \beta = 1$ or 2 . As the result, we only need to consider a 2-cluster normalization kernel with respect to the single particle wave functions $\tilde{\varphi}_\alpha$ and $\tilde{\psi}_\beta$. The overlap between $\tilde{\varphi}_\alpha$ and $\tilde{\psi}_\beta$ is

$$\tilde{A}_{\alpha\beta} \equiv \langle \tilde{\varphi}_\alpha | \tilde{\psi}_\beta \rangle = A_{\alpha\beta} - \frac{A_{\alpha 3} A_{3\beta}}{A_{33}} \quad , \quad (4.50)$$

where $A_{\alpha\beta} = \langle (0s)_{S_\alpha} | (0s)_{S'_\beta} \rangle$ ($\alpha, \beta = 1, 2, 3$) is used. We assume that the 2-cluster double-coset symbol $Q[k]$ is specified by $x \rightarrow a$ in Eq. (3.40). Then the full spatial overlap, which corresponds to J_k^N in Eq. (3.35), is given by

$$\begin{aligned} \tilde{J}_k^N &= \left(\prod_{\alpha, \beta=1}^2 \tilde{A}_{\alpha\beta}^{k_{\alpha\beta}} \right) A_{33}^4 \\ &= \sum_{n_{11}=0}^{k_{11}} \sum_{n_{12}=0}^{k_{12}} \sum_{n_{21}=0}^{k_{21}} \sum_{n_{22}=0}^{k_{22}} (-1)^{\sum_{\alpha, \beta=1}^2 (k_{\alpha\beta} - n_{\alpha\beta})} \prod_{\alpha, \beta=1}^2 \binom{k_{\alpha\beta}}{n_{\alpha\beta}} \prod_{\alpha, \beta=1}^2 A_{\alpha\beta}^{n_{\alpha\beta}} \\ &\quad \times \prod_{\alpha=1}^2 A_{\alpha 3}^{\sum_{\beta=1}^2 (k_{\alpha\beta} - n_{\alpha\beta})} \prod_{\beta=1}^2 A_{3\beta}^{\sum_{\alpha=1}^2 (k_{\alpha\beta} - n_{\alpha\beta})} A_{33}^{4 - \sum_{\alpha, \beta=1}^2 (k_{\alpha\beta} - n_{\alpha\beta})} \quad , \quad (4.51) \end{aligned}$$

where the binomial expansions of $\tilde{A}_{\alpha\beta}$ in Eq. (4.50) are employed. For the powers of $A_{\alpha 3}$ etc., we can use the weight conservation $\sum_{\alpha=1}^2 k_{\alpha\beta} = A_\beta$ and $\sum_{\beta=1}^2 k_{\alpha\beta} = A_\alpha$. Then, if we extend $n_{\alpha\beta}$ to include $\alpha, \beta = 3$ by defining $n_{\alpha 3}$, $n_{3\beta}$ and n_{33} through

$$\begin{aligned} n_{\alpha 3} &= A_\alpha - \sum_{\beta=1}^2 n_{\alpha\beta} \quad , \quad n_{3\beta} = A_\beta - \sum_{\alpha=1}^2 n_{\alpha\beta} \quad , \\ n_{33} &= 4 - A_1 - A_2 + \sum_{\alpha, \beta=1}^2 n_{\alpha\beta} \quad , \end{aligned} \quad (4.52)$$

we find

$$\sum_{\beta=1}^3 n_{\alpha\beta} = A_\alpha \quad , \quad \sum_{\alpha=1}^3 n_{\alpha\beta} = A_\beta \quad . \quad (4.53)$$

Namely, the 3×3 matrix $[n]$ is nothing but the 3-cluster double-coset symbol given by Eq. (3.42). In terms of $[n]$, the full overlap in Eq. (4.51) is expressed as

$$\tilde{J}_k^N = \sum_{n_{11}=0}^{k_{11}} \cdots \sum_{n_{22}=0}^{k_{22}} (-1)^{n_{33}} \prod_{\alpha, \beta=1}^2 \binom{k_{\alpha\beta}}{n_{\alpha\beta}} \prod_{\alpha, \beta=1}^3 A_{\alpha\beta}^{n_{\alpha\beta}} \quad , \quad (4.54)$$

which is combined with the 2-cluster spin-isospin factors X_k^N as in Eq. (3.31) and yields

$$G^N(S; S') = \sum_{[n]} X_n^N \prod_{\alpha, \beta=1}^3 A_{\alpha\beta}^{n_{\alpha\beta}} \quad , \quad (4.55)$$

with

$$X_n^N = (-1)^{n_{33}} \sum_{[k]} \prod_{\alpha, \beta=1}^2 \binom{k_{\alpha\beta}}{n_{\alpha\beta}} X_k^N . \quad (4.56)$$

We can write this symbolically

$$X_n^N = (-1)^{n_{33}} \sum_{[k]} \binom{k}{n} X_k^N . \quad (4.57)$$

If we use the notation X_a^N and $X_{(xyuv)}^N$ for the 2-cluster and 3-cluster spin-isospin factors, respectively, the relationship in Eq. (4.56) or Eq. (4.57) is explicitly given by

$$X_{(xyuv)}^N = (-1)^{x+y-u-v} \sum_{a=\max\{u,v\}}^{\min\{x,y\}} \binom{A_1-a}{A_1-x} \binom{a}{u} \binom{a}{v} \binom{A_2-a}{A_2-y} X_a^N . \quad (4.58)$$

Namely, the 3-cluster spin-isospin factors are given by a simple superposition of the 2-cluster factors.

We can easily extend the above discussion to the spin-isospin factors for the interaction kernel. In this case, the sum of the two-body interaction $\sum_{s<t} w_{st}$ is divided into three groups; namely,

$$\sum_{s<t} v_{st} = \sum_{s,t \in \alpha, s<t} v_{st} + \sum_{s \in C_1 \cup C_2} \sum_{t \in \alpha} v_{st} + \sum_{s,t \in C_1 \cup C_2, s<t} v_{st} , \quad (4.59)$$

which we call α -core, Hartree-Fock, and valence contributions, respectively. For the α -core contribution, we can easily show

$$G^{core} = \sum_{[n]} X_n^{core} A^n \mathcal{T}_{\{33,33\}} , \quad (4.60)$$

where X_n^{core} is proportional to X_n^N ;

$$X_n^{core} = X_n^N \langle \xi(\alpha) | \sum_{s<t} w_{st} | \xi(\alpha) \rangle . \quad (4.61)$$

In Eq. (4.60), a shorthand notation $A^n = \prod_{\alpha, \beta=1}^3 A_{\alpha\beta}^{n_{\alpha\beta}}$ is employed. The Hartree-Fock contribution is composed of the direct term $G^{HF(d)}$ and the exchange term $G^{HF(e)}$. The direct term is given by

$$G^{HF(d)} = \sum_{[k]} \tilde{A}^k A_{33}^4 \sum_{\alpha, \beta=1}^2 X_{k E_{\alpha\beta}}^d \tilde{E}_{\alpha\beta} , \quad (4.62)$$

where the Hartree-Fock type spin-isospin factors are given by

$$\begin{aligned} X_{k E_{\alpha\beta}}^d &= X_{a E_{\alpha\beta}}^d = (-1)^a \binom{A_1}{a} \binom{A_2}{a} \\ &\times \langle z_a \xi_{ST}(C_1 \cup C_2) \xi(\alpha) | \sum_{s \in E_{\alpha\beta}} \sum_{t \in \alpha} w_{st} | \xi_{S'T'}(C_1 \cup C_2) \xi(\alpha) \rangle \end{aligned} \quad (4.63)$$

and

$$\begin{aligned} \tilde{E}_{\alpha\beta} &= \tilde{A}_{\alpha\beta}^{-1} A_{33}^{-1} \langle \tilde{\varphi}_\alpha \varphi_3 | u | \tilde{\psi}_\beta \psi_3 \rangle \\ &= \tilde{A}_{\alpha\beta}^{-1} \left\{ A_{\alpha\beta} \mathcal{T}_{\{\alpha\beta;33\}} - \frac{A_{\alpha 3} A_{3\beta}}{A_{33}} [\mathcal{T}_{\{\alpha 3;33\}} + \mathcal{T}_{\{3\beta;33\}} - \mathcal{T}_{\{33;33\}}] \right\} . \end{aligned} \quad (4.64)$$

We use this $\tilde{E}_{\alpha\beta}$ in Eq. (4.62) and expand \tilde{A}^k by using the notation

$$k^{\alpha\beta} \equiv k - e^{(\alpha\beta)} \quad \text{and} \quad n^{\alpha\beta} \equiv n - e^{(\alpha\beta)} \quad (4.65)$$

for $\alpha, \beta = 1, 2$ and $1, 2, 3$, respectively. Then we find

$$G^{HF(d)} = \sum_{[n]} A^n \sum_{\alpha, \beta=1}^2 \left\{ X_{n\{\alpha\beta\}}^{HF(1)} \mathcal{T}_{\{\alpha\beta;33\}} + X_{n\{\alpha\beta\}}^{HF(2)} [\mathcal{T}_{\{\alpha 3;33\}} + \mathcal{T}_{\{3\beta;33\}} - \mathcal{T}_{\{33;33\}}] \right\}, \quad (4.66)$$

with

$$\left. \begin{array}{l} X_{n\{\alpha\beta\}}^{HF(1)} \\ X_{n\{\alpha\beta\}}^{HF(2)} \end{array} \right\} = (-1)^{n_{33}} \sum_{[k]} \left\{ \begin{array}{l} (k^{\alpha\beta} \\ n^{\alpha\beta} \end{array} \right\} X_{k E_{\alpha\beta}}^d . \quad (4.67)$$

Similarly, we can obtain $G^{HF(e)}$ by the modification $v_{st} \rightarrow -P_{st} v_{st}$; namely,

$$G^{HF(e)} = - \sum_{[n]} A^n \sum_{\alpha, \beta=1}^2 X_{n\{\alpha\beta\}}^{HF(3)} [\mathcal{T}_{\{\alpha 3;3\beta\}} - \mathcal{T}_{\{\alpha 3;33\}} - \mathcal{T}_{\{3\beta;33\}} + \mathcal{T}_{\{33;33\}}] , \quad (4.68)$$

where

$$X_{n\{\alpha\beta\}}^{HF(3)} = (-1)^{n_{33}} \sum_{[k]} \binom{k^{\alpha\beta}}{n} X_{k E_{\alpha\beta}}^e , \quad (4.69)$$

with

$$\begin{aligned} X_{k E_{\alpha\beta}}^e &= X_{a E_{\alpha\beta}}^e = (-1)^a \binom{A_1}{a} \binom{A_2}{a} \\ &\times \langle z_a \xi_{ST}(C_1 \cup C_2) \xi(\alpha) | \sum_{s \in E_{\alpha\beta}} \sum_{t \in \alpha} (-P_{st}) w_{st} | \xi_{S'T'}(C_1 \cup C_2) \xi(\alpha) \rangle . \end{aligned} \quad (4.70)$$

Finally, the valence contribution is given through

$$G^{valence} = \sum_{[k]} \tilde{A}^k A_{33}^4 \sum_{\mathcal{T}} X_k \mathcal{T} \tilde{\mathcal{T}} , \quad (4.71)$$

with

$$\begin{aligned}
X_k \mathcal{T} &= X_a \{ \alpha \beta ; \gamma \delta \} \\
&= (-1)^a \binom{A_1}{a} \binom{A_2}{a} \langle z_a \xi_{ST} (C_1 \cup C_2) \mid \sum_{s < t}^{\mathcal{T}} w_{st} \mid \xi_{S'T'} (C_1 \cup C_2) \rangle \quad (4.72)
\end{aligned}$$

and

$$\begin{aligned}
\tilde{\mathcal{T}} &= \tilde{\mathcal{T}}_{\{ \alpha \beta ; \gamma \delta \}} \\
&= \tilde{A}_{\alpha \beta}^{-1} \tilde{A}_{\gamma \delta}^{-1} \left\{ A_{\alpha \beta} A_{\gamma \delta} \mathcal{T}_{\{ \alpha \beta ; \gamma \delta \}} - A_{\alpha \beta} \frac{A_{\gamma 3} A_{3 \delta}}{A_{33}} \left[\mathcal{T}_{\{ \alpha \beta ; 3 \delta \}} + \mathcal{T}_{\{ \alpha \beta ; \gamma 3 \}} - \mathcal{T}_{\{ \alpha \beta ; 33 \}} \right] \right. \\
&\quad - \frac{A_{\alpha 3} A_{3 \beta}}{A_{33}} A_{\gamma \delta} \left[\mathcal{T}_{\{ 3 \beta ; \gamma \delta \}} + \mathcal{T}_{\{ \alpha 3 ; \gamma \delta \}} - \mathcal{T}_{\{ 33 ; \gamma \delta \}} \right] \\
&\quad + \frac{A_{\alpha 3} A_{3 \beta}}{A_{33}} \frac{A_{\gamma 3} A_{3 \delta}}{A_{33}} \left[\left(\mathcal{T}_{\{ \alpha 3 ; \gamma 3 \}} + \mathcal{T}_{\{ 3 \beta ; 3 \delta \}} + \mathcal{T}_{\{ 33 ; 33 \}} \right) \right. \\
&\quad \left. \left. + \left(\mathcal{T}_{\{ \alpha 3 ; 3 \delta \}} - \mathcal{T}_{\{ \alpha 3 ; 33 \}} - \mathcal{T}_{\{ 3 \beta ; 33 \}} \right) + \left(\mathcal{T}_{\{ 3 \beta ; \gamma 3 \}} - \mathcal{T}_{\{ 33 ; \gamma 3 \}} - \mathcal{T}_{\{ 33 ; 3 \delta \}} \right) \right] \right\} . \quad (4.73)
\end{aligned}$$

The expansion of \tilde{A}^k in Eq. (4.71) yields

$$\begin{aligned}
G^{valence} &= \sum_{[n]} A^n \sum_{\{ \alpha \beta ; \gamma \delta \}}^2 \left\{ X_n^{V(1)} \{ \alpha \beta ; \gamma \delta \} \mathcal{T}_{\{ \alpha \beta ; \gamma \delta \}} \right. \\
&\quad + 2X_n^{V(2)} \{ \alpha \beta ; \gamma \delta \} \left[\mathcal{T}_{\{ \alpha \beta ; \gamma 3 \}} + \mathcal{T}_{\{ \alpha \beta ; 3 \delta \}} - \mathcal{T}_{\{ \alpha \beta ; 33 \}} \right] \\
&\quad \left. + X_n^{V(3)} \{ \alpha \beta ; \gamma \delta \} \left[\left(\mathcal{T}_{\{ \alpha 3 ; \gamma 3 \}} + \mathcal{T}_{\{ 3 \beta ; 3 \delta \}} + \mathcal{T}_{\{ 33 ; 33 \}} \right) + 2 \left(\mathcal{T}_{\{ \alpha 3 ; 3 \delta \}} - \mathcal{T}_{\{ \alpha 3 ; 33 \}} - \mathcal{T}_{\{ 3 \beta ; 33 \}} \right) \right] \right\}, \quad (4.74)
\end{aligned}$$

where the basic factors $X_n^{V(1)} \{ \alpha \beta ; \gamma \delta \}$ etc. are defined by

$$\left. \begin{array}{l} X_n^{V(1)} \{ \alpha \beta ; \gamma \delta \} \\ X_n^{V(2)} \{ \alpha \beta ; \gamma \delta \} \\ X_n^{V(3)} \{ \alpha \beta ; \gamma \delta \} \end{array} \right\} = (-1)^{n_{33}} \sum_{[k]} \left\{ \begin{array}{l} \binom{k^{\alpha \beta ; \gamma \delta}}{n^{\alpha \beta ; \gamma \delta}} \\ \binom{k^{\alpha \beta ; \gamma \delta}}{n^{\alpha \beta}} \\ \binom{k^{\alpha \beta ; \gamma \delta}}{n} \end{array} \right\} X_k \{ \alpha \beta ; \gamma \delta \} \quad (4.75)$$

with

$$k^{\alpha \beta ; \gamma \delta} = k - e^{(\alpha \beta)} - e^{(\gamma \delta)} \quad \text{and} \quad n^{\alpha \beta ; \gamma \delta} = n - e^{(\alpha \beta)} - e^{(\gamma \delta)} . \quad (4.76)$$

The full spin-isospin factors $X_n \{ \alpha \beta ; \gamma \delta \}$ for the interaction kernel is obtained through

$$\begin{aligned}
G &= G^{core} + G^{HF(d)} + G^{HF(e)} + G^{valence} \\
&= \sum_{[n]} A^n \sum_{\{ \alpha \beta ; \gamma \delta \}}^3 X_n \{ \alpha \beta ; \gamma \delta \} \mathcal{T}_{\{ \alpha \beta ; \gamma \delta \}} , \quad (4.77)
\end{aligned}$$

with the final result given by $(\alpha, \beta, \gamma, \delta = 1 \text{ or } 2)$

$$\begin{aligned}
X_n\{\alpha\beta;\gamma\delta\} &= X_n^{V(1)}\{\alpha\beta;\gamma\delta\} , \\
X_n\{\alpha\beta;\gamma3\} &= \sum_{\delta} X_n^{V(2)}\{\alpha\beta;\gamma\delta\} + \delta_{\gamma,\alpha} X_n^{V(2)}\{\alpha\beta;\alpha\beta\} , \\
X_n\{\alpha\beta;3\delta\} &= \sum_{\gamma} X_n^{V(2)}\{\alpha\beta;\gamma\delta\} + \delta_{\delta,\beta} X_n^{V(2)}\{\alpha\beta;\alpha\beta\} , \\
X_n\{\alpha\beta;33\} &= X_n^{HF(1)}\{\alpha\beta\} - \sum_{\gamma,\delta} X_n^{V(2)}\{\alpha\beta;\gamma\delta\} - X_n^{V(2)}\{\alpha\beta;\alpha\beta\} , \\
X_n\{\alpha3;\gamma3\} &= (1 - \frac{1}{2}\delta_{\alpha,\gamma}) \sum_{\beta,\delta} X_n^{V(3)}\{\alpha\beta;\gamma\delta\} + \delta_{\alpha,\gamma} \frac{1}{2} \sum_{\beta} X_n^{V(3)}\{\alpha\beta;\alpha\beta\} , \\
X_n\{3\beta;3\delta\} &= (1 - \frac{1}{2}\delta_{\beta,\delta}) \sum_{\alpha,\gamma} X_n^{V(3)}\{\alpha\beta;\gamma\delta\} + \delta_{\beta,\delta} \frac{1}{2} \sum_{\alpha} X_n^{V(3)}\{\alpha\beta;\alpha\beta\} , \\
X_n\{\alpha3;3\delta\} &= -X_n^{HF(3)}\{\alpha\delta\} + \sum_{\beta,\gamma} X_n^{V(3)}\{\alpha\beta;\gamma\delta\} + X_n^{V(3)}\{\alpha\delta;\alpha\delta\} , \\
X_n\{\alpha3;33\} &= \sum_{\beta} (X_n^{HF(2)}\{\alpha\beta\} + X_n^{HF(3)}\{\alpha\beta\}) - \sum_{\beta,\gamma,\delta} X_n^{V(3)}\{\alpha\beta;\gamma\delta\} - \sum_{\beta} X_n^{V(3)}\{\alpha\beta;\alpha\beta\} , \\
X_n\{3\beta;33\} &= \sum_{\alpha} (X_n^{HF(2)}\{\alpha\beta\} + X_n^{HF(3)}\{\alpha\beta\}) - \sum_{\alpha,\gamma,\delta} X_n^{V(3)}\{\alpha\beta;\gamma\delta\} - \sum_{\alpha} X_n^{V(3)}\{\alpha\beta;\alpha\beta\} , \\
X_n\{33;33\} &= X_n^{core} - \sum_{\alpha,\beta} (X_n^{HF(2)}\{\alpha\beta\} + X_n^{HF(3)}\{\alpha\beta\}) + \sum_{\{\alpha\beta;\gamma\delta\}} X_n^{V(3)} . \quad (4.78)
\end{aligned}$$

Here, the basic factors $X_n^{HF(1)}\{\alpha\beta\}$, $X_n^{HF(2)}\{\alpha\beta\}$, $X_n^{HF(3)}\{\alpha\beta\}$, $X_n^{V(1)}\{\alpha\beta;\gamma\delta\}$, $X_n^{V(2)}\{\alpha\beta;\gamma\delta\}$ and $X_n^{V(3)}\{\alpha\beta;\gamma\delta\}$ are obtained through Eqs. (4.67), (4.69) and (4.75), by using

$$X_n^{core} = X_n^N \begin{cases} (X_d + X_e) \\ 1 \\ 0 \end{cases} \text{ for } \begin{cases} \text{central} \\ \text{Coulomb} \\ \text{LS and tensor} \end{cases} , \quad (4.79a)$$

$$\left. \begin{matrix} X_{kE\alpha\beta}^d \\ X_{kE\alpha\beta}^e \end{matrix} \right\} = k_{\alpha\beta} X_k^N \frac{1}{2} \begin{cases} X_d \\ X_e \end{cases} \text{ for } \text{central} , \quad (4.79b)$$

$$X_{kE\alpha\beta}^d = (-2)X_{kE\alpha\beta}^e = k_{\alpha\beta} X_k^N + 2 \langle T^1 T_z 10 | T T_z \rangle X_{kE\alpha\beta}^{\tau(1)} \text{ for } \text{Coulomb} , \quad (4.79c)$$

$$\left. \begin{matrix} X_{kE\alpha\beta}^d \\ X_{kE\alpha\beta}^e \end{matrix} \right\} = X_{kE\alpha\beta}^{\sigma(1)} \begin{cases} (4W - 2H) \\ (4H - 2W) \end{cases} \text{ for } \text{LS} , \quad (4.79d)$$

$$X_{kE\alpha\beta}^d = X_{kE\alpha\beta}^e = 0 \text{ for } \text{tensor} . \quad (4.79e)$$

Furthermore, X_k^N and $X_k\{\alpha\beta;\gamma\delta\}$ are the 2-cluster spin-isospin factors derived in the preceding subsection, and X_d , X_e , $X_{kE\alpha\beta}^{\tau(1)}$ and $X_{kE\alpha\beta}^{\sigma(1)}$ are given by $X_d = 8W + 4B - 4H - 2M$, $X_e = 8M + 4H - 4B - 2W$ and Eqs. (4.44), (4.45).

§5. Systematic Evaluation of RGM Kernels in the Complex Generator-Coordinate Method

In §3, we have found that the GCM kernels for n -cluster systems of $(0s)$ -shell clusters have rather simple structure with respect to the $(n - 1)$ -dimensional set of complex generator-coordinate vectors, $z = (\mathbf{z}_1, \dots, \mathbf{z}_{n-1})$, whatsoever we choose for relative-coordinate systems between clusters. These kernels are usually referred to as complex GCM kernels. It is well known that the complex GCM kernels have a nice property of non-singular transformation between the GCM and RGM kernels. [108], [10] There exist a couple of different versions of complex GCM. [92], [7] However, these are essentially equivalent to each other and they share the property mentioned above; namely, the transformation from GCM to RGM kernels are easily carried out by simple Gaussian integration. Here, we use the Bargmann-integral [93] version of complex GCM, developed by Horiuchi [92] for particular applications to eigenvalue problems of normalization kernels in Elliott SU_3 scheme [97]. We find in the next section that this scheme is also convenient for evaluating Gaussian matrix elements of RGM kernels.

A basic relationship used for the present kernel transformation is the Bargmann's integral representation for the Dirac's δ -function, which is satisfied by the generating function $A_\gamma(\xi, \mathbf{z})$ in Eq. (3.13) ;

$$\int d\mu(\mathbf{z}) A_\gamma(\mathbf{r}, \mathbf{z})^* A_\gamma(\xi, \mathbf{z}) = \delta(\mathbf{r} - \xi) \quad , \quad (5.1)$$

where $d\mu(\mathbf{z})$ is the 3-dimensional Bargmann measure [93] defined by

$$d\mu(\mathbf{z}) = \pi^{-3} e^{-(\mathbf{z}^* \cdot \mathbf{z})} d^3(\Re \mathbf{z}) d^3(\Im \mathbf{z}) \quad . \quad (5.2)$$

By using $3(n - 1)$ -dimensional version of Eq. (5.1), we can find the RGM kernel for $I^\Omega(z; z')$ in Eq. (3.17) through

$$\begin{aligned} \mathcal{M}^\Omega(R; R') &= \langle \delta(\xi - R) \phi_0 \mid \mathcal{O}^\Omega \mathcal{A}' \mid \delta(\xi - R') \phi_0 \rangle \\ &= \int d\mu(z) d\mu(z') A(R; z) A(R'; z')^* I^\Omega(z; z') \quad , \end{aligned} \quad (5.3)$$

where $R = (\mathbf{R}_1, \dots, \mathbf{R}_{n-1})$, $\delta(\xi - R) = \prod_{i=1}^{n-1} \delta(\xi_i - \mathbf{R}_i)$, $d\mu(z) = \prod_{i=1}^{n-1} d\mu(\mathbf{z}_i)$ etc., and $A(R; z)$ is given in Eq. (3.15). Here again, we can get quite general expressions for the explicit result of Bargmann integrals, due to the Gaussian nature of GCM kernels for s -shell cluster systems. If we fix a particular type of nucleon-exchange [k] and also an interaction type \mathcal{T} for interaction kernels, each term of the GCM kernels in Eqs. (3.38), (3.51) and (3.69) is conveniently factorized into

$$\begin{aligned} I^N(z; z') &= \exp \{ \text{Tr}(z^* Q^t z') \} \quad , \\ I^{exp}(z; z') &= I^N(z; z') \exp \left\{ -\frac{\lambda}{2} (P\mathbf{z}^* + P'\mathbf{z}')^2 \right\} \quad , \\ I^\Omega(z; z') &= I^{exp}(z; z') \mathcal{P}_{GCM}^\Omega(z; z') \quad , \end{aligned} \quad (5.4a)$$

with

$$P_{GCM}^{\Omega}(z; z') = \begin{cases} 1 \\ i [Pz^*, P'z'] \cdot S \\ 3\sqrt{10} [\mathcal{Y}_2(Pz^* + P'z') S^{(2)}]^{(0)} \end{cases} \quad \text{for } \Omega = \begin{cases} \text{central} \\ LS \\ \text{tensor} \end{cases} . \quad (5.4b)$$

The transformation of the Coulomb and kinetic energy kernels is easily obtained from that of $I^{exp}(z; z')$ and $I^N(z; z')$, but for later convenience we also give explicit forms of these GCM kernels as

$$I^{CL}(z; z') = I^N(z; z') \frac{2\sqrt{\nu}}{|Pz^* + P'z'|} \operatorname{erf} \left(\frac{1}{2} |Pz^* + P'z'| \right) ,$$

$$I^K(z; z') = I^N(z; z') \left\{ n - 1 - \frac{1}{3} (Tr({}^t z^* z^*) + Tr({}^t z' z')) + \frac{2}{3} Tr(z^* Q {}^t z') \right\} . \quad (5.4c)$$

We call these $I^{\Omega}(z; z')$ with parameters Q , P and P' the standard form of complex GCM kernels for (*0s*)-shell cluster systems and all the transformations in this and the following sections are carried out with respect to these forms.

The Bargmann integrals in Eq. (5.3) are most efficiently carried out by using some formulae which are specifically derived for this purpose involving many-dimensional Gaussian transformations. Since almost all these formulae can be straightforwardly obtained, only brief comments are made concerning their derivation. We first derive these for n -dimensional vectors $z \equiv (z_1, z_2, \dots, z_n)$, instead of $3(n - 1)$ dimensional ones $z = (z_1, \dots, z_{n-1})$, since the reduction to the case of our present interest is easily implemented. The starting point is a real Gaussian integral

$$\int_{-\infty}^{\infty} dx e^{-ax^2} = \left(\frac{\pi}{a} \right)^{\frac{1}{2}} \quad (a > 0) , \quad (5.5a)$$

or its extension

$$\int_{-\infty}^{\infty} dx e^{-a(x+u)^2} = \left(\frac{\pi}{a} \right)^{\frac{1}{2}} \quad (u \in \mathbf{C}, a > 0) , \quad (5.5b)$$

where u is an arbitrary complex number $u \in \mathbf{C}$. A standard procedure yields the following n -dimensional formula for Gaussian integrals ;

$$\int_{-\infty}^{\infty} dx_1 \dots dx_n e^{-{}^t x A x + 2{}^t u x} = \pi^{\frac{n}{2}} (\det A)^{-\frac{1}{2}} e^{{}^t u A^{-1} u} , \quad (5.6)$$

where $u = (u_1, \dots, u_n) \in \mathbf{C}^n$ is an arbitrary complex vector and A is a real symmetric matrix (${}^t A = A$) satisfying the positive-definiteness condition. Now we move to Bargmann integrals with one-dimensional Bargmann measure $d\mu(z) = \pi^{-1} e^{-z^* z} d(\Re z) d(\Im z)$ and their n -dimensional extension $d\mu(z) = d\mu(z_1) \dots d\mu(z_n)$. By applying the formula Eq. (5.6) to the real and imaginary parts, separately, we can easily prove²³

²³The formula Eq. (5.7) is well known, for example, in the Bargmann-Fock space approach to path integrals in the quantum field theory. See Eq. (9.56) in [109].

$$\int d\mu(z) e^{-{}^t z^*(C-1)z + {}^t u^* z + {}^t z^* v} = (\det C)^{-1} e^{{}^t u^* C^{-1} v} , \quad (5.7)$$

for arbitrary $u, v \in \mathbb{C}^n$ and a real, symmetric and positive-definite matrix C (${}^t C = C$). We can extend the formula in Eq. (5.7) to include ${}^t z^* A z^*$ and ${}^t z B z$ type terms also, by linearizing the z^* and z terms with the aid of Eq. (5.6). Namely, we use z^* and z for u in Eq. (5.6) and use Eq. (5.7) first and then integrate over x etc. by using Eq. (5.6) again. Through this procedure, we can get the following formula for n -dimensional Gaussian Bargmann integrals, which is most convenient for our purpose ;

$$\begin{aligned} & \int d\mu(z) \exp \left\{ -\frac{1}{2} {}^t z^* A z^* - \frac{1}{2} {}^t z B z - {}^t z^*(C-1)z + {}^t z^* u + {}^t v z \right\} \\ &= [\det (ACA^{-1}C - AB)]^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} {}^t u (CB^{-1}C - A)^{-1} u - \frac{1}{2} {}^t v (CA^{-1}C - B)^{-1} v \right. \\ & \quad \left. + {}^t u (C - BC^{-1}A)^{-1} v \right\} , \end{aligned} \quad (5.8a)$$

where $u, v \in \mathbb{C}^n$ and A, B and C are all $n \times n$ real and symmetric matrices. In the process of the proof, we have assumed that the matrix $A^{-1} - C^{-1}BC^{-1}$ is positive definite, which guarantees that the determinant in Eq. (5.8a) is non-zero ;

$$\det (ACA^{-1}C - AB) = \det (BCB^{-1}C - BA) \neq 0 . \quad (5.8b)$$

Note that this determinant is symmetric with respect to the interchange of A and B .

Now we can use the formula in Eq. (5.8) and the property of $\exp\{{}^t z^* z'\}$ as a reproducing kernel

$$\int d\mu(z) f(z) e^{{}^t z^* z'} = f(z') , \quad (5.9)$$

to derive

$$\begin{aligned} & \int d\mu(z) d\mu(z') A(R; z) A(R'; z')^* \exp\{{}^t z^* Q z' + {}^t z^* u + {}^t v z'\} \\ &= \left(\frac{2\sqrt{\gamma\gamma'}}{\pi} \right)^{\frac{1}{2}} D^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} {}^t \widehat{R} \left(A - \frac{1}{2} \right) \widehat{R} - \frac{1}{2} {}^t \widehat{R}' \left(A' - \frac{1}{2} \right) \widehat{R}' + {}^t \widehat{R} C \widehat{R}' \right. \\ & \quad \left. + {}^t \widehat{R} (Au - Cv) + {}^t (A'v - {}^t Cu) \widehat{R}' - \frac{1}{2} {}^t u Au - \frac{1}{2} {}^t v A'v + {}^t u Cv \right\} , \end{aligned} \quad (5.10a)$$

where $\widehat{R} = (2\sqrt{\gamma_1}R_1, \dots, 2\sqrt{\gamma_n}R_n)$ etc. and

$$\begin{aligned} D &= \det (1 - {}^t Q Q) = \det (1 - Q {}^t Q) \\ A &= (1 - Q {}^t Q)^{-1} , \quad A' = (1 - {}^t Q Q)^{-1} , \\ C &= Q(1 - {}^t Q Q)^{-1} = (1 - Q {}^t Q)^{-1} Q . \end{aligned} \quad (5.10b)$$

In Eq. (5.10a), we have assumed $(\gamma_1, \dots, \gamma_n)$ for the n -dimensional $A(R; z)$ and $(\gamma'_1, \dots, \gamma'_n)$ for $A(R'; z')$, and used a shorthand notation

$$\left(\frac{2\sqrt{\gamma\gamma'}}{\pi} \right)^{\frac{1}{2}} \equiv \prod_{i=1}^n \left(\frac{2\sqrt{\gamma_i\gamma'_i}}{\pi} \right)^{\frac{1}{2}} . \quad (5.10c)$$

At this stage, we move to the $3(n-1)$ dimensional parametrization $z_j \rightarrow z_{\alpha i}$ ($\alpha = x, y, z$ and $i = 1, \dots, n-1$) and $\widehat{R} = (2\sqrt{\gamma_1} \mathbf{R}_1, \dots, 2\sqrt{\gamma_{n-1}} \mathbf{R}_{n-1})$ etc., and use the property that $Q_{\alpha i, \beta j} \rightarrow \delta_{\alpha, \beta} Q_{i, j}$ yields $D = \det(\delta_{\alpha, \beta} \delta_{i, j} - ({}^t Q Q)_{i, j} \delta_{\alpha, \beta}) = \{\det(1 - {}^t Q Q)\}^3$. We also use the vector notation $\mathbf{z} = (\mathbf{z}_1, \dots, \mathbf{z}_{n-1})$ and $\mathbf{u} = (\mathbf{u}_1, \dots, \mathbf{u}_{n-1})$ etc., and their inner product $(\mathbf{u} \cdot \mathbf{z}^*) \equiv \sum_{i=1}^{n-1} (\mathbf{u}_i \cdot \mathbf{z}_i^*)$. Then by assuming the coefficients in Eq. (5.10b) for $(n-1) \times (n-1)$ matrix Q , we find that the Bargmann transformation of the GCM kernel, $\exp\{Tr(z^* Q^t z') + (\mathbf{u} \cdot \mathbf{z}^*) + (\mathbf{v} \cdot \mathbf{z}')\}$, is given by the same exponential form as in Eq. (5.10a) with $u \rightarrow \mathbf{u}$ and $v \rightarrow \mathbf{v}$, but a slight modification of the front factor into

$$\left(\frac{2\sqrt{\gamma\gamma'}}{\pi}\right)^{\frac{3}{2}} D^{-\frac{3}{2}} \quad \text{with} \quad \left(\frac{2\sqrt{\gamma\gamma'}}{\pi}\right)^{\frac{3}{2}} \equiv \prod_{i=1}^{n-1} \left(\frac{2\sqrt{\gamma_i \gamma'_i}}{\pi}\right)^{\frac{3}{2}}. \quad (5.10d)$$

In particular, if we set $\mathbf{u} = \mathbf{v} = 0$, it gives a transformation of the normalization kernel :

$$\begin{aligned} \mathcal{M}^N(R; R') &= \left(\frac{2\sqrt{\gamma\gamma'}}{\pi}\right)^{\frac{3}{2}} D^{-\frac{3}{2}} \\ &\times \exp\left\{-\frac{1}{2} {}^t \widehat{R} \left(A - \frac{1}{2}\right) \widehat{R} - \frac{1}{2} {}^t \widehat{R}' \left(A' - \frac{1}{2}\right) \widehat{R}' + {}^t \widehat{R} C \widehat{R}'\right\}. \end{aligned} \quad (5.11)$$

In order to derive transformation formulae for the interaction kernels, we first assume that the GCM kernel is given by

$$I(z; z') = I^N(z; z') \mathcal{F}_{GCM}(z; z'), \quad (5.12a)$$

with

$$\mathcal{F}_{GCM}(z; z') = \exp\left\{-\frac{\lambda}{2} (P\mathbf{z}^* + P'\mathbf{z}')^2 + (\mathbf{u} \cdot \mathbf{z}^*) + (\mathbf{v} \cdot \mathbf{z}')\right\}. \quad (5.12b)$$

Here again, we can use the Gaussian-integral representation

$$\exp\left\{-\frac{\lambda}{2} \boldsymbol{\rho}^2\right\} = (\pi\lambda)^{-\frac{3}{2}} \int d\mathbf{y} \exp\left\{-\frac{1}{\lambda} \mathbf{y}^2 + i\sqrt{2}(\boldsymbol{\rho} \cdot \mathbf{y})\right\} \quad (\lambda > 0), \quad (5.13)$$

to linearize the quadratic term of \mathbf{z}^* and \mathbf{z}' in Eq. (5.12b). Then we can use the formula in Eq. (5.10) again and carry out the \mathbf{y} -integral after that. From this procedure, we can show that the RGM kernel for $I^\Omega(z; z')$ in Eq. (5.12a) is given by

$$\mathcal{M}(R; R') = \mathcal{M}^N(R; R') \mathcal{F}(R; R') \quad (5.14a)$$

with

$$\begin{aligned} \mathcal{F}(R; R') &= \left(\frac{1}{1-\lambda\alpha}\right)^{\frac{3}{2}} \exp\left\{-\frac{1}{2} \frac{\lambda}{1-\lambda\alpha} \mathbf{V}^2 + {}^t(\widetilde{A}\widehat{R} - \widetilde{C}\widehat{R}') \mathbf{u}\right. \\ &\quad \left.+ {}^t \mathbf{v}(\widetilde{A}'\widehat{R}' - {}^t \widetilde{C}\widehat{R}) - \frac{1}{2} {}^t \mathbf{u} \widetilde{A} \mathbf{u} - \frac{1}{2} {}^t \mathbf{v} \widetilde{A}' \mathbf{v} + {}^t \mathbf{u} \widetilde{C} \mathbf{v}\right\}. \end{aligned} \quad (5.14b)$$

Here, various coefficients are given by

$$\begin{aligned}
f &= AP - CP' \quad , \quad g = A'P' - {}^tCP \quad ((n-1) \text{-dimensional vectors}) \quad , \\
\alpha &= {}^tPf + {}^tP'g = {}^tPAP + {}^tP'A'P' - 2{}^tPCP' \quad , \\
\mathbf{V} &= {}^t f \widehat{R} + {}^t g \widehat{R}' \quad , \quad (5.14c)
\end{aligned}$$

and

$$\begin{aligned}
\widetilde{A} &= A + \frac{\lambda}{1-\lambda\alpha} f {}^t f \quad , \quad \widetilde{A}' = A' + \frac{\lambda}{1-\lambda\alpha} g {}^t g \quad , \\
\widetilde{C} &= C - \frac{\lambda}{1-\lambda\alpha} f {}^t g \quad . \quad (5.14d)
\end{aligned}$$

In particular, $\mathbf{u} = \mathbf{v} = 0$ case in Eqs. (5.12) \sim (5.14) yields the RGM kernel for $I^{exp}(z; z')$ in Eq. (5.4a), which corresponds to the Gaussian central interaction.

We can extend the reduction of $\mathcal{F}_{GCM}(z; z')$ in Eq. (5.12b) a step further, to separate out the linear term $\mathcal{P}_{GCM}(z; z') = \exp\{(\mathbf{u} \cdot \mathbf{z}^*) + (\mathbf{v} \cdot \mathbf{z}')\}$ which serves as a generating function of the non-central polynomial terms. The corresponding RGM factor $\mathcal{P}(\widehat{R}; \widehat{R}')$ contains the coefficients \widetilde{A} , \widetilde{A}' and \widetilde{C} as is seen in Eq. (5.14b). However, the first-rank and second-rank tensorial properties of the LS and tensor factors greatly simplify the final expression due to the relationship in Eq. (5.14d). The final expressions of the RGM kernels in Eq. (5.3) are given by²⁴

$$\begin{aligned}
\mathcal{M}^{exp}(R; R') &= \mathcal{M}^N(R; R') \left(\frac{1}{1-\lambda\alpha} \right)^{\frac{3}{2}} \exp \left\{ -\frac{1}{2} \frac{\lambda}{1-\lambda\alpha} \mathbf{V}^2 \right\} \quad , \\
\mathcal{M}^\Omega(R; R') &= \mathcal{M}^{exp}(R; R') \mathcal{P}^\Omega(R; R') \quad , \quad (5.15a)
\end{aligned}$$

with

$$\mathcal{P}^\Omega(R; R') = \begin{cases} 1 \\ \left(\frac{1}{1-\lambda\alpha} \right) i \left[{}^tP(A\widehat{R} - C\widehat{R}'), {}^tP'(A'\widehat{R}' - {}^tC\widehat{R}') \right] \cdot \mathbf{s} \\ \left(\frac{1}{1-\lambda\alpha} \right)^2 3\sqrt{10} [\mathcal{Y}_2(\mathbf{V}) S^{(2)}]^{(0)} \end{cases}$$

$$\text{for } \Omega = \begin{cases} \text{central} \\ LS \\ \text{tensor} \end{cases} \quad . \quad (5.15b)$$

Besides the normalization kernel $\mathcal{M}^N(R; R')$ and its coefficients A , A' and C in Eqs. (5.11) and (5.10b), the necessary coefficients for the interaction kernels are given in Eq. (5.14c). The transformation of the Coulomb and the kinetic energy kernels in Eq. (5.4c) is given by

$$\begin{aligned}
\mathcal{M}^{CL}(R; R') &= \mathcal{M}^N(R; R') \frac{2\sqrt{\nu}}{|\mathbf{V}|} \operatorname{erf} \left(\frac{|\mathbf{V}|}{\sqrt{2(2-\alpha)}} \right) \quad , \\
\mathcal{M}^K(R; R') &= \mathcal{M}^N(R; R') \left\{ -(n-1) + 2Tr(A + A') - \frac{1}{3} \left[{}^t\widehat{R}(4A^2 - 3A)\widehat{R} \right. \right. \\
&\quad \left. \left. + {}^t\widehat{R}'(4A'^2 - 3A')\widehat{R}' - {}^t\widehat{R}(8AQA' - 2C)\widehat{R}' \right] \right\} \quad . \quad (5.15c)
\end{aligned}$$

²⁴This simple result of factorization in Eq. (5.15) was first obtained for 2-cluster systems in the RGM study of noncentral NN potentials in terms of a quark model. [110], [111]

§6. Gaussian Matrix Elements of RGM Kernels

For practical applications of the many-cluster RGM kernels derived in the preceding section, it is essential that we can easily carry out the angular-momentum projection to cope with many involved angular-momentum couplings of the relative wave functions due to cluster rearrangements. Although this procedure is well defined and contains no essential difficulties, it becomes quite tedious for the systems of more than three clusters. It is therefore very useful if we have some nice method to evaluate the RGM matrix elements with respect to basis states with some specific angular-momentum couplings for the relative motion. This is achieved by using Gaussian-type basis wave functions with arbitrary width parameters, in which the expression of the RGM matrix elements turns out to be given by only finite number of terms corresponding to the intermediate angular-momentum couplings. In fact, almost all the 3-cluster RGM calculations (and also multiconfiguration RGM calculations by Hackenbroich, Hofmann et al. [16], [20], [31]) up to the present have been performed in the variational method for scattering and bound-state problems with these Gaussian-type trial wave functions.

In this section, we combine the Bargmann-integration techniques for the kernel transformation with the theory of double Gel'fand polynomials developed for the representation theory of unitary groups [86], and derive a convenient formula for the Gaussian matrix elements of RGM kernels. The derivation is composed of three steps. First we introduce some kind of reduction rule from 3-dimensional complex vectors to 2-dimensional ones, which eliminates the O_3 -invariant polynomial terms of h.o. wave functions in the angular-momentum representation. This new technique is used to derive a transformation formula for Gaussian matrix elements directly from GCM kernels. Since the structure of this transformation is only slightly different from the one for GCM to RGM transformation, we can employ the full result in the preceding section in order to derive generating functions for Gaussian matrix elements. Finally, we expand these generating functions in terms of the double Gel'fand polynomials, and obtain the RGM matrix elements as the expansion coefficients.

6.1 Transformation Formula for Gaussian Matrix Elements

6.1.1 Two-Dimensional Reduction of Three-Dimensional Bargmann Variables

Suppose $\mathbf{R} = (R_x, R_y, R_z)$ and $\boldsymbol{\xi} = (\xi_1, \xi_2)$ are 3-dimensional and 2-dimensional complex variables, respectively, connected by a simple relationship

$$R_x = \frac{1}{2}(-\xi_1^2 + \xi_2^2) \ , \quad R_y = i \frac{1}{2}(\xi_1^2 + \xi_2^2) \ , \quad R_z = \xi_1 \xi_2 \ . \quad (6.1)$$

If we use the standard spherical tensor notation of real 3-dimensional vectors even for the complex vector \mathbf{R} , the relationship (6.1) can be expressed as

$$\begin{aligned} R_1 &= -\frac{1}{\sqrt{2}}(R_x + i R_y) = \frac{1}{\sqrt{2}} \xi_1^2 = v_{11}(\boldsymbol{\xi}) \ , \\ R_0 &= R_z = \xi_1 \xi_2 = v_{10}(\boldsymbol{\xi}) \ , \\ R_{-1} &= \frac{1}{\sqrt{2}}(R_x - i R_y) = \frac{1}{\sqrt{2}} \xi_2^2 = v_{-1}(\boldsymbol{\xi}) \ . \end{aligned} \quad (6.2)$$

Here, we have also used the Schwinger's spinor representation [112], [93] for angular-momentum states ;

$$v_{\ell m}(\boldsymbol{\xi}) = \frac{\xi_1^{\ell+m} \xi_2^{\ell-m}}{\sqrt{(\ell+m)!(\ell-m)!}} . \quad (6.3)$$

The essence of the transformation in Eq. (6.1) or (6.2) lies in the restriction of the six independent real variables of the complex \mathbf{R} to the four independent ones of $\boldsymbol{\xi}$, due to the simple property, $\mathbf{R}^2 = 0$, directly proved from Eq. (6.1). We call this $\mathbf{R} \downarrow \boldsymbol{\xi}$ reduction in the following. If we consider another 3-dimensional complex vector \mathbf{S} and its reduction $\boldsymbol{\eta}$ with $\mathbf{S} \downarrow \boldsymbol{\eta}$, we can easily show

$$(\mathbf{R}^* \cdot \mathbf{S}) = \frac{1}{2} (\boldsymbol{\xi}^* \cdot \boldsymbol{\eta})^2 , \quad (6.4a)$$

$$(\mathbf{R} \cdot \mathbf{S}) = -\frac{1}{2} \left| \begin{array}{cc} \xi_1 & \eta_1 \\ \xi_2 & \eta_2 \end{array} \right|^2 = -\frac{1}{2} | \det(\boldsymbol{\xi}, \boldsymbol{\eta}) |^2 . \quad (6.4b)$$

Now let us consider the h.o. expansion of the generating function $A_\gamma(\mathbf{r}, \mathbf{z})$ in Eq. (3.13) in the angular-momentum representation ;

$$\begin{aligned} A_\gamma(\mathbf{r}, \mathbf{z}) &= \left(\frac{2\gamma}{\pi} \right)^{\frac{3}{4}} \exp \left\{ -\gamma r^2 + 2\sqrt{\gamma} (\mathbf{r} \cdot \mathbf{z}) - \frac{\mathbf{z}^2}{2} \right\} \\ &= \sum_{N\ell m} V_{N\ell m}(\mathbf{r}, \gamma)^* U_{(N0)\ell m}(\mathbf{z}) , \end{aligned} \quad (6.5a)$$

where \mathbf{r} is a real vector, \mathbf{z} is complex, and

$$V_{N\ell m}(\mathbf{r}, \gamma) = R_{N\ell}(r, \gamma) Y_{\ell m}(\hat{\mathbf{r}}) , \quad (6.5b)$$

$$\begin{aligned} R_{N\ell m}(r, \gamma) &= \sqrt{4\pi} \left(\frac{2\gamma}{\pi} \right)^{\frac{3}{4}} \left[\frac{(N-\ell)!!}{(N+\ell+1)!!} \right]^{\frac{1}{2}} (2\sqrt{\gamma} r)^\ell L_n^{\ell+\frac{1}{2}}(2\gamma r^2) e^{-\gamma r^2} \\ &\quad \text{with } N = 2n + \ell , \end{aligned} \quad (6.5c)$$

$$U_{(N0)\ell m}(\mathbf{z}) = \left[\frac{(2\ell+1)!!}{(N-\ell)!!(N+\ell+1)!!} \right]^{\frac{1}{2}} (-\mathbf{z} \cdot \mathbf{z})^n \mathcal{Y}_{\ell m}(\mathbf{z}) . \quad (6.5d)$$

The spherical harmonic polynomial of order ℓ , $\mathcal{Y}_{\ell m}(\mathbf{z})$, is given in Eq. (3.63). We modify \mathbf{z} in Eq. (6.5) into \mathbf{R} and perform the reduction $\mathbf{R} \downarrow \boldsymbol{\xi}$. We can easily show that

$$U_{(N0)\ell m}(\mathbf{R}) = \delta_{n,0} \mathcal{Y}_{\ell m}(\mathbf{R}) , \quad \mathcal{Y}_{\ell m}(\mathbf{R}) = \sqrt{(2\ell-1)!!} v_{\ell m}(\boldsymbol{\xi}) \quad \text{for } \mathbf{R} \downarrow \boldsymbol{\xi} . \quad (6.6)$$

The last equation in Eq. (6.6) is the extension of $R_\mu = v_{1\mu}(\boldsymbol{\xi})$ in Eq. (6.2) and is shown as follows. We first use the angular-momentum C-G series

$$\left[Y_{\ell_1}(\widehat{\mathbf{R}}) Y_{\ell_2}(\widehat{\mathbf{R}}) \right]_{\ell m} = \frac{\widehat{\ell}_1 \widehat{\ell}_2}{\sqrt{4\pi \widehat{\ell}}} \langle \ell_1 0 \ell_2 0 | \ell 0 \rangle Y_{\ell m}(\widehat{\mathbf{R}}) \tag{6.7}$$

and show that the spherical harmonic polynomial is expressed as

$$\mathcal{Y}_{\ell m}(\mathbf{R}) = \frac{1}{\sqrt{\ell!}} \left[\cdots \left[[RR]_2 R \right]_3 \cdots \right]_{\ell m} . \tag{6.8}$$

Then, by $\mathbf{R} \downarrow \boldsymbol{\xi}$ reduction, we move to $R_\mu = v_{1\mu}(\boldsymbol{\xi})$ and use (see Eq. (5-3-11) of ref. [86])

$$\left[v_{\ell_1}(\boldsymbol{\xi}) v_{\ell_2}(\boldsymbol{\xi}) \right]_{\ell m} = \delta_{\ell, \ell_1 + \ell_2} \binom{2(\ell_1 + \ell_2)}{2\ell_1}^{\frac{1}{2}} v_{\ell_1 + \ell_2, m}(\boldsymbol{\xi}) . \tag{6.9}$$

Now going back to Eq. (6.5), the transformation $\mathbf{z} \rightarrow \mathbf{R} \downarrow \boldsymbol{\xi}$ yields

$$A_\gamma(\mathbf{r}, \mathbf{R})|_{\mathbf{R} \downarrow \boldsymbol{\xi}} = \left(\frac{2\gamma}{\pi} \right)^{\frac{3}{4}} e^{-\gamma r^2} e^{2\sqrt{\gamma}(\mathbf{r} \cdot \mathbf{R})}|_{\mathbf{R} \downarrow \boldsymbol{\xi}} = \sum_{\ell m} \chi_{\ell m}(\mathbf{r}, \gamma)^* \sqrt{(2\ell - 1)!!} v_{\ell m}(\boldsymbol{\xi}) , \tag{6.10a}$$

with

$$\begin{aligned} \chi_{\ell m}(\mathbf{r}, \gamma) &= V_{\ell m}(\mathbf{r}, \gamma) = \chi_\ell(r, \gamma) Y_{\ell m}(\widehat{\mathbf{r}}) , \\ \chi_\ell(r, \gamma) &= \left(\frac{2\gamma}{\pi} \right)^{\frac{3}{4}} \left[\frac{4\pi}{(2\ell + 1)!!} \right]^{\frac{1}{2}} (2\sqrt{\gamma} r)^\ell e^{-\gamma r^2} , \end{aligned} \tag{6.10b}$$

or

$$\chi_{\ell m}(\mathbf{r}, \gamma) = \left(\frac{2\gamma}{\pi} \right)^{\frac{3}{4}} \mathcal{Y}_{\ell m}(2\sqrt{\gamma} \mathbf{r}) e^{-\gamma r^2} . \tag{6.10c}$$

If we further express Eq. (6.10a) as

$$e^{2\sqrt{\gamma}(\mathbf{r} \cdot \mathbf{R})}|_{\mathbf{R} \downarrow \boldsymbol{\xi}} = \sum_{\ell m} \mathcal{Y}_{\ell m}(2\sqrt{\gamma} \mathbf{r})^* \sqrt{(2\ell - 1)!!} v_{\ell m}(\boldsymbol{\xi}) \tag{6.11}$$

and modify $2\sqrt{\gamma} \mathbf{r}$ into a complex variable \mathbf{S} , we obtain

$$e^{(\mathbf{R} \cdot \mathbf{S}^*)}|_{\mathbf{R} \downarrow \boldsymbol{\xi}} = \sum_{\ell m} \sqrt{(2\ell - 1)!!} v_{\ell m}(\boldsymbol{\xi}) \mathcal{Y}_{\ell m}(\mathbf{S})^* . \tag{6.12}$$

This is nothing but the $\mathbf{R} \downarrow \boldsymbol{\xi}$ reduction of the reproducing kernel in the Bargmann space ;

$$e^{(\mathbf{R} \cdot \mathbf{S}^*)} = \sum_{N \ell m} U_{(N0)\ell m}(\mathbf{R}) U_{(N0)\ell m}(\mathbf{S})^* . \tag{6.13}$$

6.1.2 Transformation Formula for One Variable

The Gaussian function we are going to deal with from now on is $\chi_\ell(r; \gamma)$ in Eq. (6.10b). In order to find the Bargmann image for this Gaussian function with an arbitrary width parameter γ , we first consider a simple Gaussian integral

$$\begin{aligned} & \int d\mathbf{r} A_\gamma(\mathbf{r}, \mathbf{z})^* A_{\gamma'}(\mathbf{r}, \mathbf{z}') \\ &= \left(\frac{2\sqrt{\gamma\gamma'}}{\gamma + \gamma'} \right)^{\frac{3}{2}} \exp \left\{ \frac{\gamma - \gamma'}{\gamma + \gamma'} \frac{1}{2} (\mathbf{z}^{*2} - \mathbf{z}'^2) + \frac{2\sqrt{\gamma\gamma'}}{\gamma + \gamma'} (\mathbf{z}^* \cdot \mathbf{z}') \right\} . \end{aligned} \quad (6.14)$$

If we set $\gamma \rightarrow \eta\gamma$, $\gamma' \rightarrow \gamma$ with $\eta > 0$, this can be expressed as

$$\begin{aligned} \int d\mathbf{r} A_{\eta\gamma}(\mathbf{r}, \mathbf{z})^* A_\gamma(\mathbf{r}, \mathbf{z}') &= (1 - \varepsilon^2)^{\frac{3}{4}} \exp \left\{ -\frac{\varepsilon}{2} (\mathbf{z}^{*2} - \mathbf{z}'^2) + \sqrt{1 - \varepsilon^2} (\mathbf{z}^* \cdot \mathbf{z}') \right\} \\ &\text{with } \varepsilon = \frac{1 - \eta}{1 + \eta} \quad \text{and} \quad -1 < \varepsilon < 1 . \end{aligned} \quad (6.15)$$

When $\eta = 1$ or $\varepsilon = 0$, Eq. (6.15) is reduced to the expression of the reproducing kernel. We set $\mathbf{z} \rightarrow \mathbf{R} \downarrow \boldsymbol{\xi}$ in Eq. (6.15) and use Eq. (6.10a) and (6.12). Then, by noting that $\mathcal{Y}_{\ell m}(\mathbf{z})$ is a homogeneous polynomial of order ℓ , we can easily find

$$\int d\mathbf{r} \chi_{\ell m}(\mathbf{r}, \eta\gamma) A_\gamma(\mathbf{r}, \mathbf{z}) = (1 - \varepsilon^2)^{\frac{1}{2}(\ell + \frac{3}{2})} \mathcal{Y}_{\ell m}(\mathbf{z}) e^{\frac{\varepsilon}{2}\mathbf{z}^2} \equiv \omega_{\ell m}(\mathbf{z}, \varepsilon) . \quad (6.16)$$

Namely, $\omega_{\ell m}(\mathbf{z}, \varepsilon)$ is the Bargmann image of $\chi_{\ell m}(\mathbf{r}, \eta\gamma)$.

Let $I(\mathbf{z})$ be a term of GCM kernels, for which the corresponding RGM kernel is defined through

$$\mathcal{M}(\mathbf{r}) = \int d\mu(\mathbf{z}) A_\gamma(\mathbf{r}, \mathbf{z})^* I(\mathbf{z}) . \quad (6.17)$$

In the following, we find a convenient formula for calculating the RGM matrix element

$$M_{\ell m}(\eta) = \int d\mathbf{r} \chi_{\ell m}(\mathbf{r}, \eta\gamma) \mathcal{M}(\mathbf{r}) . \quad (6.18)$$

First, the formula in Eq. (6.16) shows that $M_{\ell m}(\eta)$ is given by the Bargmann integral

$$M_{\ell m}(\eta) = \int d\mu(\mathbf{z}) \omega_{\ell m}(\mathbf{z}^*, \varepsilon) I(\mathbf{z}) \quad \text{with } \varepsilon = \frac{1 - \eta}{1 + \eta} . \quad (6.19)$$

The essential point of the present approach is that we can replace this Bargmann integral with the original one in Eq. (6.17) with a small modification of coefficients. To show this, we extend \mathbf{r} in $A_\gamma(\mathbf{r}, \mathbf{z})$ to a complex \mathbf{R} and make a replacement

$$\mathbf{r} \rightarrow \frac{1}{2\sqrt{\gamma}} \frac{1}{\sqrt{-\varepsilon}} \mathbf{R} , \quad \mathbf{z} \rightarrow \sqrt{-\varepsilon} \mathbf{z} , \quad (6.20)$$

where $\sqrt{-\varepsilon}$ for $\varepsilon > 0$ should be understood as a principal value. Then, we perform $\mathbf{R} \downarrow \boldsymbol{\xi}$ reduction and use Eq. (6.12). From this procedure, we can easily show that

$$\begin{aligned}
 & A_\gamma \left(\frac{1}{\sqrt{-\varepsilon}} \frac{\mathbf{R}}{2\sqrt{\gamma}}, \sqrt{-\varepsilon} \mathbf{z} \right) \Big|_{\mathbf{R} \downarrow \xi} \\
 &= \left(\frac{2\gamma}{\pi} \right)^{\frac{3}{4}} \sum_{\ell m} \sqrt{(2\ell-1)!!} (1-\varepsilon^2)^{-\frac{1}{2}(\ell+\frac{3}{2})} v_{\ell m}(\xi) \omega_{\ell m}(\mathbf{z}^*, \varepsilon)^* . \quad (6.21)
 \end{aligned}$$

This expression yields

$$\begin{aligned}
 \omega_{\ell m}(\mathbf{z}^*, \varepsilon) &= (1-\varepsilon^2)^{\frac{1}{2}(\ell+\frac{3}{2})} \frac{1}{\sqrt{(2\ell-1)!!}} \left(\frac{\pi}{2\gamma} \right)^{\frac{3}{4}} \\
 &\quad \times \int d\mu(\xi) v_{\ell m}(\xi) A_\gamma \left(\frac{1}{\sqrt{-\varepsilon}} \frac{\mathbf{R}}{2\sqrt{\gamma}}, \sqrt{-\varepsilon} \mathbf{z} \right)^* \Big|_{\mathbf{R} \downarrow \xi} . \quad (6.22)
 \end{aligned}$$

If we use this representation for $\omega_{\ell m}(\mathbf{z}^*, \varepsilon)$ in Eq. (6.19), we obtain

$$M_{\ell m}(\eta) = (1-\varepsilon^2)^{\frac{1}{2}(\ell+\frac{3}{2})} \frac{1}{\sqrt{(2\ell-1)!!}} \int d\mu(\xi) v_{\ell m}(\xi) \widetilde{\mathcal{M}}(\mathbf{R}) \Big|_{\mathbf{R} \downarrow \xi} \quad (6.23)$$

with

$$\widetilde{\mathcal{M}}(\mathbf{R}) \equiv \left(\frac{\pi}{2\gamma} \right)^{\frac{3}{4}} \int d\mu(\mathbf{z}) A_\gamma \left(\frac{1}{\sqrt{-\varepsilon}} \frac{\mathbf{R}}{2\sqrt{\gamma}}, \sqrt{-\varepsilon} \mathbf{z} \right)^* I(\mathbf{z}) . \quad (6.24)$$

Here we further use a property of Bargmann integrals

$$\langle f(c\mathbf{z}) | g(\mathbf{z}) \rangle = \langle f(\mathbf{z}) | g(c^*\mathbf{z}) \rangle \quad \text{for } \forall c \in \mathbf{C} , \quad (6.25)$$

which is valid for arbitrary $f(z)$ and $g(z)$ in the Bargmann space. Thus we find

$$\widetilde{\mathcal{M}}(\mathbf{R}) = \left(\frac{\pi}{2\gamma} \right)^{\frac{3}{4}} \int d\mu(\mathbf{z}) A_\gamma \left(\frac{1}{\sqrt{-\varepsilon}} \frac{\mathbf{R}}{2\sqrt{\gamma}}, \mathbf{z} \right)^* I(\sqrt{-\varepsilon}^* \mathbf{z}) . \quad (6.26)$$

This implies that the RGM kernel $\widetilde{\mathcal{M}}(\mathbf{R})$ in Eq. (6.26) is easily obtained from the new GCM kernel $\widetilde{I}(\mathbf{z}) = I(\sqrt{-\varepsilon}^* \mathbf{z})$ by a simple replacement $\mathbf{R} \rightarrow (\mathbf{R}/2\sqrt{\gamma})^* (1/\sqrt{-\varepsilon})^*$ in the corresponding RGM kernel, as long as the transformation formula in Eq. (6.17) is explicitly known. The extra Bargmann integral for $v_{\ell m}(\xi)$ in Eq. (6.23) is usually unnecessary, since the expansion of $\widetilde{\mathcal{M}}(\mathbf{R}) \Big|_{\mathbf{R} \downarrow \xi}$ in the basis states $v_{\ell m}(\xi)$ yields much easier method to handle this process of angular-momentum projection.

6.1.3 Application to *n*-Cluster RGM Kernels

In *n*-cluster systems, we deal with angular-momentum coupled (*n* - 1)-body Gaussian trial functions defined through

$$\begin{aligned}
 \chi_\ell^{LM}(r; \eta) &= \left[\cdots \left[[\chi_{\ell_1}(\mathbf{r}_1, \eta_1 \gamma_1) \chi_{\ell_2}(\mathbf{r}_2, \eta_2 \gamma_2)]_{\ell_{12}} \chi_{\ell_3}(\mathbf{r}_3, \eta_3 \gamma_3) \right]_{\ell_{123}} \right. \\
 &\quad \left. \cdots \chi_{\ell_{n-1}}(\mathbf{r}_{n-1}, \eta_{n-1} \gamma_{n-1}) \right]_{LM} , \quad (6.27)
 \end{aligned}$$

and their RGM matrix elements²⁵

$$M_{\ell(LS); \ell'(L'S')}^{\Omega J}(\eta; \eta') = \left\langle [\chi_{\ell}^L(r; \eta) \xi_S]_{JM} \mid \mathcal{M}^{\Omega}(r; r') \mid [\chi_{\ell'}^{L'}(r'; \eta') \xi_{S'}']_{JM} \right\rangle . \quad (6.28)$$

Here, ℓ etc. denotes a set of angular-momentum couplings specified by the following Gel'fand pattern [86]

$$\begin{aligned} & | \ell ; L \rangle \equiv | [\cdots [[\ell_1 \ell_2] \ell_{12}, \ell_3] \ell_{123}, \cdots, \ell_{n-1}] L \rangle \\ & = \left(\begin{array}{ccccccc} \ell_1 + \cdots + \ell_{n-1} + L & \ell_1 + \cdots + \ell_{n-1} - L & 0 & \cdots & \cdots & \cdots & 0 \\ & \ddots & & \ddots & & \ddots & \\ & \ell_1 + \ell_2 + \ell_3 + \ell_{123} & \ell_1 + \ell_2 + \ell_3 - \ell_{123} & 0 & & & \\ & & \ell_1 + \ell_2 + \ell_{12} & \ell_1 + \ell_2 - \ell_{12} & & & \\ & & & 2\ell_1 & & & \end{array} \right) , \end{aligned} \quad (6.29)$$

We use the same notation for $2 \times (n-1)$ double Gel'fand (DG) polynomials [86] ;

$$\begin{aligned} v_{\ell}^{LM}(\xi) & \equiv \varphi_{r, \ell}^{(2n-1)(\lambda\mu)}(\xi) \\ & = \left[\cdots [[v_{\ell_1}(\xi_1) v_{\ell_2}(\xi_2)]_{\ell_{12}} v_{\ell_3}(\xi_3)]_{\ell_{123}} \cdots v_{\ell_{n-1}}(\xi_{n-1}) \right]_{LM} , \end{aligned} \quad (6.30)$$

where $\lambda + 2\mu = 2(\ell_1 + \ell_2 + \cdots + \ell_{n-1})$, $\lambda/2 = L$ and $\lambda/2 - r = M$. If we use a shorthand notation $|\ell| = \ell_1 + \ell_2 + \cdots + \ell_{n-1}$, the relationship between $(\lambda\mu)r$ and LM is given by

$$\lambda = 2L \quad , \quad \mu = |\ell| - L \quad , \quad r = L - M \quad . \quad (6.31)$$

We extend the formula in Eqs. (6.23) ~ (6.26) to the $(n-1)$ -dimensional angular-momentum coupled states, and apply it to the RGM matrix element in Eq. (6.28). Then, we find

$$\begin{aligned} M_{\ell(LS); \ell'(L'S')}^{\Omega J}(\eta; \eta') & = (1 - \varepsilon^2)^{\frac{1}{2}(\ell + \frac{3}{2})} (1 - \varepsilon'^2)^{\frac{1}{2}(\ell' + \frac{3}{2})} \left[\frac{1}{(2\ell - 1)!! (2\ell' - 1)!!} \right]^{\frac{1}{2}} \\ & \times \left\langle [v_{\ell}^L(\xi) \xi_S]_{JM} \mid \widetilde{\mathcal{M}}^{\Omega}(R; R') \mid_{\mathbf{R} \downarrow \xi, \mathbf{R}' \downarrow \xi'} \left[v_{\ell'}^{L'}(\xi') \xi_{S'}' \right]_{JM} \right\rangle , \end{aligned} \quad (6.32)$$

where the matrix element is taken for the Bargmann integrals over $d\mu(\xi) d\mu(\xi')$ and

$$\begin{aligned} \widetilde{\mathcal{M}}^{\Omega}(R; R') & = \left(\frac{\pi}{2\gamma} \right)^{\frac{3}{4}} \left(\frac{\pi}{2\gamma'} \right)^{\frac{3}{4}} \int d\mu(\mathbf{z}) d\mu(\mathbf{z}') A \left(\frac{1}{\sqrt{-\varepsilon}} \frac{R}{2\sqrt{\gamma}} ; z \right) \\ & \times A \left(\frac{1}{\sqrt{-\varepsilon'}} \frac{R'}{2\sqrt{\gamma'}} ; z' \right)^* I^{\Omega} \left(\sqrt{-\varepsilon}^* z ; \sqrt{-\varepsilon'}^* z' \right) . \end{aligned} \quad (6.33)$$

In Eqs. (6.32) and (6.33), we have used some shorthand notations through

²⁵In Eq. (6.28). ξ_S and $\xi_{S'}'$ are the ‘‘formal’’ spin-isospin wave functions and should not be confused with the $2 \times (n-1)$ Bargmann variables $\xi = (\xi_1, \cdots, \xi_{n-1})$.

$$\begin{aligned}
 (1 - \varepsilon^2)^{\frac{1}{2}(\ell + \frac{3}{2})} &= \prod_{i=1}^{n-1} (1 - \varepsilon_i^2)^{\frac{1}{2}(\ell_i + \frac{3}{2})} \quad \text{with} \quad \varepsilon_i = \frac{1 - \eta_i}{1 + \eta_i} , \\
 (2\ell - 1)!! &= \prod_{i=1}^{n-1} (2\ell_i - 1)!! , \quad \left(\frac{\pi}{2\gamma}\right)^{\frac{3}{4}} = \prod_{i=1}^{n-1} \left(\frac{\pi}{2\gamma_i}\right)^{\frac{3}{4}} , \quad (6.34)
 \end{aligned}$$

and $\sqrt{-\varepsilon}$ is supposed to be an $(n-1) \times (n-1)$ diagonal matrix; $\sqrt{-\varepsilon} = ((\sqrt{-\varepsilon})_{ij}) = (\delta_{i,j} \sqrt{-\varepsilon_i})$ etc. The modification $z^* \rightarrow \sqrt{-\varepsilon} z^*$ and $z' \rightarrow \sqrt{-\varepsilon'} z'$ in Eq. (5.4) implies

$$Q \rightarrow \tilde{Q} = \sqrt{-\varepsilon} Q \sqrt{-\varepsilon'}^* , \quad P \rightarrow \tilde{P} = \sqrt{-\varepsilon} P , \quad \tilde{P}' = \sqrt{-\varepsilon'}^* P' . \quad (6.35)$$

We set the coefficients of the corresponding RGM kernel in Eqs. (5.10b) and (5.14c) as $\tilde{D}, \tilde{A}, \tilde{A}', \tilde{C}, \tilde{f}, \tilde{g}$ and $-\tilde{\alpha}$,²⁶ and further make a replacement $\hat{R} \rightarrow R/\sqrt{-\varepsilon}$, $\hat{R}' \rightarrow R'*/\sqrt{-\varepsilon'}^*$ and define

$$\begin{aligned}
 \hat{A} &= \frac{1}{\sqrt{-\varepsilon}} (1 - \tilde{A}) \frac{1}{\sqrt{-\varepsilon}} , \quad \hat{A}' = \frac{1}{\sqrt{-\varepsilon'}^*} (1 - \tilde{A}') \frac{1}{\sqrt{-\varepsilon'}^*} , \\
 \hat{C} &= \frac{1}{\sqrt{-\varepsilon}} \tilde{C} \frac{1}{\sqrt{-\varepsilon'}^*} , \quad \hat{f} = \frac{1}{\sqrt{-\varepsilon}} \tilde{f} , \quad \hat{g} = \frac{1}{\sqrt{-\varepsilon'}^*} \tilde{g} . \quad (6.36)
 \end{aligned}$$

From this procedure, $\tilde{\mathcal{M}}(R; R')$ in Eq. (6.33) is derived as

$$\begin{aligned}
 \tilde{\mathcal{M}}^N(R; R') &= \tilde{D}^{-\frac{3}{2}} \exp \left\{ \frac{1}{2} {}^t \mathbf{R} \left(\hat{A} + \frac{1}{2\varepsilon} \right) \mathbf{R} + \frac{1}{2} {}^t \mathbf{R}'^* \left(\hat{A}' + \frac{1}{2\varepsilon'} \right) \mathbf{R}'^* + {}^t \mathbf{R} \hat{C} \mathbf{R}'^* \right\} , \\
 \tilde{\mathcal{M}}^{exp}(R; R') &= \tilde{\mathcal{M}}^N(R; R') \left(\frac{1}{1 + \lambda \tilde{\alpha}} \right)^{\frac{3}{2}} \exp \left\{ -\frac{1}{2} \frac{\lambda}{1 + \lambda \tilde{\alpha}} \tilde{\mathbf{V}}^2 \right\} , \\
 \tilde{\mathcal{M}}^\Omega(R; R') &= \tilde{\mathcal{M}}^{exp}(R; R') \tilde{\mathcal{P}}^\Omega(R; R') , \quad (6.37a)
 \end{aligned}$$

with

$$\tilde{\mathcal{P}}^\Omega(R; R') = \begin{cases} 1 \\ \left(\frac{1}{1 + \lambda \tilde{\alpha}}\right) i \left[{}^t \hat{P} \mathbf{R} + {}^t \hat{P}' \mathbf{R}'^* + {}^t \hat{P}' \mathbf{R}'^* + {}^t \hat{P}' \mathbf{R} \right] \cdot \mathbf{S} \\ \left(\frac{1}{1 + \lambda \tilde{\alpha}}\right)^2 3\sqrt{10} \left[\mathcal{Y}_2(\tilde{\mathbf{V}}) S^{(2)} \right]^{(0)} \end{cases} . \quad (6.37b)$$

Here, we have explicitly shown the 3-dimensional vector character of R by $R = \mathbf{R} = (\mathbf{R}_1, \dots, \mathbf{R}_{n-1})$. In Eqs. (6.37a) and (6.37b), the coefficients for the normalization kernel is given by

$$\begin{aligned}
 \tilde{D} &= \det(1 - \varepsilon {}^t Q \varepsilon Q) = \det(1 - Q \varepsilon {}^t Q \varepsilon) , \\
 \tilde{C} &= Q(1 - \varepsilon {}^t Q \varepsilon Q)^{-1} = (1 - Q \varepsilon {}^t Q \varepsilon)^{-1} Q , \\
 \hat{A} &= \hat{C} \varepsilon {}^t Q = (1 - Q \varepsilon {}^t Q \varepsilon)^{-1} Q \varepsilon {}^t Q , \\
 \hat{A}' &= {}^t Q \varepsilon \hat{C} = {}^t Q \varepsilon Q (1 - \varepsilon {}^t Q \varepsilon Q)^{-1} , \quad (6.37c)
 \end{aligned}$$

²⁶Note that the notation \tilde{A}, \tilde{A}' and \tilde{C} in Eq. (5.14d) is differently used from that here.

and, for the interaction kernels,

$$\begin{aligned}
\widehat{P} &= (1 + \widehat{A}\varepsilon)P , & \widehat{P}' &= (1 + \widehat{A}'\varepsilon')P' , \\
\widetilde{P} &= {}^t\widehat{C}\varepsilon P , & \widetilde{P}' &= \widehat{C}\varepsilon' P' , \\
\widehat{f} &= \widehat{P} + \widetilde{P}' , & \widehat{g} &= \widehat{P}' + \widetilde{P} , \\
\widetilde{\alpha} &= {}^tP\varepsilon\widehat{f} + {}^tP'\varepsilon'\widehat{g} , & \widetilde{\mathbf{V}} &= {}^t\widehat{f}\mathbf{R} + {}^t\widehat{g}\mathbf{R}'^* .
\end{aligned} \tag{6.37d}$$

Note that \widehat{A} and \widehat{A}' are the symmetric matrices ; i.e., ${}^t\widehat{A} = \widehat{A}$ and ${}^t\widehat{A}' = \widehat{A}'$.

The first step to derive the matrix elements in Eq. (6.32) is to make $\mathbf{R} \downarrow \boldsymbol{\xi}$ and $\mathbf{R}' \downarrow \boldsymbol{\xi}'$ reductions. In the central kernel $\widetilde{\mathcal{M}}^{exp}(R; R')$ in Eq. (6.37a), we expand $\widetilde{\mathbf{V}}^2$ term and use the property

$$\begin{aligned}
{}^t\mathbf{R} \frac{1}{2\varepsilon} \mathbf{R} &= \sum_{i=1}^{n-1} \frac{1}{2\varepsilon_i} \mathbf{R}_i^2 = 0 , \\
\frac{1}{2} {}^t\mathbf{R} \mathbf{A} \mathbf{R} &= \sum_{i<j}^{n-1} A_{ij} (\mathbf{R}_i \cdot \mathbf{R}_j) = -\frac{1}{2} \sum_{i<j}^{n-1} A_{ij} (\delta_{ij})^2 , \\
\frac{1}{2} {}^t\mathbf{R}'^* \mathbf{A}' \mathbf{R}'^* &= \sum_{i<j}^{n-1} A'_{ij} (\mathbf{R}'_i{}^* \cdot \mathbf{R}'_j{}^*) = -\frac{1}{2} \sum_{i<j}^{n-1} A'_{ij} (\delta'_{ij})^2 , \\
{}^t\mathbf{R} \mathbf{C} \mathbf{R}'^* &= \sum_{i,j=1}^{n-1} C_{ij} (\mathbf{R}_i \cdot \mathbf{R}'_j{}^*) = \frac{1}{2} \sum_{i,j=1}^{n-1} C_{ij} (\boldsymbol{\xi}_i \cdot \boldsymbol{\xi}'_j{}^*)^2 ,
\end{aligned} \tag{6.38}$$

with $\delta_{ij} = \det(\boldsymbol{\xi}_i, \boldsymbol{\xi}_j)$ and $\delta'_{ij} = \det(\boldsymbol{\xi}'_i, \boldsymbol{\xi}'_j)$ from Eq. (6.4). Then, we find

$$\widetilde{\mathcal{M}}^{exp}(R; R')|_{\mathbf{R} \downarrow \boldsymbol{\xi}, \mathbf{R}' \downarrow \boldsymbol{\xi}'} = D^{-\frac{3}{2}} I(\boldsymbol{\xi}; \boldsymbol{\xi}') ,$$

$$I(\boldsymbol{\xi}; \boldsymbol{\xi}') \equiv \exp \left\{ -\frac{1}{2} \sum_{i<j}^{n-1} A_{ij} (\delta_{ij})^2 - \frac{1}{2} \sum_{i<j}^{n-1} A'_{ij} (\delta'_{ij})^2 + \frac{1}{2} \sum_{i,j=1}^{n-1} C_{ij} (\boldsymbol{\xi}_i \cdot \boldsymbol{\xi}'_j{}^*)^2 \right\} , \tag{6.39a}$$

where the coefficients D , A , A' and C are given by

$$\begin{aligned}
D &= \widetilde{D} (1 + \lambda\widetilde{\alpha}) , & C &= \widehat{C} - \frac{\lambda}{1 + \lambda\widetilde{\alpha}} \widehat{f} {}^t\widehat{g} , \\
A &= \widehat{A} - \frac{\lambda}{1 + \lambda\widetilde{\alpha}} \widehat{f} {}^t\widehat{f} , & A' &= \widehat{A}' - \frac{\lambda}{1 + \lambda\widetilde{\alpha}} \widehat{g} {}^t\widehat{g} .
\end{aligned} \tag{6.39b}$$

On the other hand, for the LS and tensor kernels, we use

$$\begin{aligned}
[ab]_{00} &= -\frac{1}{\sqrt{3}} (\mathbf{a} \cdot \mathbf{b}) , & [ab]_{1\mu} &= i \frac{1}{\sqrt{2}} [\mathbf{a} \times \mathbf{b}]_{\mu} , \\
a_{\mu} &= \sqrt{\frac{4\pi}{3}} a Y_{1\mu}(\widehat{\mathbf{a}}) = \mathcal{Y}_{1\mu}(\mathbf{a}) ,
\end{aligned} \tag{6.40}$$

and define their reduced matrix elements by separating the spin part,²⁷

²⁷In this paper, we have assumed the reduced matrix elements of \mathbf{S} and $S^{(2)}$ for the total system unity; $\langle S \parallel \mathbf{S} \parallel S' \rangle = \langle S \parallel S^{(2)} \parallel S' \rangle = 1$. However, they are explicitly shown here for the later convenience.

$$M_{\ell(LS); \ell'(L'S')}^{\Omega J}(\eta; \eta') = (1 - \varepsilon^2)^{\frac{1}{2}(\ell + \frac{3}{2})} (1 - \varepsilon'^2)^{\frac{1}{2}(\ell' + \frac{3}{2})} D^{-\frac{3}{2}}$$

$$\times \left\{ \begin{array}{ll} \delta_{L,L'} \delta_{S,S'} \widetilde{M}_{\ell L; \ell' L}^C(\eta; \eta') & \text{for } \textit{central} \\ \left[\begin{array}{ccc} L' & S' & J \\ 1 & 1 & 0 \\ L & S & J \end{array} \right] \langle S \parallel \mathbf{S} \parallel S' \rangle (-\sqrt{6}) \left(\frac{1}{1 + \lambda \widetilde{\alpha}} \right) \widetilde{M}_{\ell L; \ell' L}^{LS}(\eta; \eta') & \text{for } LS \\ \left[\begin{array}{ccc} L' & S' & J \\ 2 & 2 & 0 \\ L & S & J \end{array} \right] \langle S \parallel S^{(2)} \parallel S' \rangle 3\sqrt{10} \left(\frac{1}{1 + \lambda \widetilde{\alpha}} \right)^2 \widetilde{M}_{\ell L; \ell' L}^T(\eta; \eta') & \text{for } \textit{tensor} . \end{array} \right. \quad (6.41a)$$

Here, $\widetilde{M}_{\ell L; \ell' L}^{\Omega}(\eta; \eta')$ are given by

$$\widetilde{M}_{\ell L; \ell' L}^{\Omega}(\eta; \eta') = \left[\frac{1}{(2\ell - 1)!! (2\ell' - 1)!!} \right]^{\frac{1}{2}} \left\langle v_{\ell}^L(\xi) \parallel I(\xi; \xi') \widetilde{\mathcal{P}}^{\Omega}(\xi; \xi') \parallel v_{\ell'}^{L'}(\xi') \right\rangle , \quad (6.41b)$$

with $\widetilde{\mathcal{P}}^C = 1$ and

$$\begin{aligned} \widetilde{\mathcal{P}}^{LS}(\xi; \xi') &= \left[\mathcal{Y}_1({}^t \widehat{P} \mathbf{R} + {}^t \widetilde{P} \mathbf{R}'^*) \mathcal{Y}_1({}^t \widetilde{P}' \mathbf{R} + {}^t \widehat{P}' \mathbf{R}'^*) \right]_{1\mu} |_{\mathbf{R} \downarrow \xi, \mathbf{R}' \downarrow \xi'} , \\ \widetilde{\mathcal{P}}^T(\xi; \xi') &= \mathcal{Y}_{2\mu}({}^t \widehat{f} \mathbf{R} + {}^t \widehat{g} \mathbf{R}'^*) |_{\mathbf{R} \downarrow \xi, \mathbf{R}' \downarrow \xi'} . \end{aligned} \quad (6.41c)$$

The central factor $I(\xi; \xi')$ in Eq. (6.41b) is given in Eq. (6.39a). The reduction of the polynomial terms in Eq. (6.41c) is given in §6.2.2.

6.2 Expansion by Double Gel'fand Polynomials

6.2.1 Central Matrix Elements

In order to derive the matrix elements $\widetilde{M}_{\ell L; \ell' L}^C(\eta; \eta')$ in Eq. (6.41b), we expand $I(\xi; \xi')$ in Eq. (6.39a) as

$$I(\xi; \xi') = \sum_{L, \ell, \ell'} \frac{1}{N_H(\lambda\mu) N_H(\lambda\mu')} I_{\ell, \ell'}^L(C; A, A') \sum_{r=0}^{\lambda} \varphi_{r, \ell}^{(2n-1)(\lambda\mu)}(\xi) \varphi_{r, \ell'}^{(2n-1)(\lambda\mu')}(\xi')^* , \quad (6.42)$$

where $\varphi_{r, \ell}^{(2n-1)(\lambda\mu)}(\xi)$ is the $2 \times (n-1)$ DG polynomials defined in Eq. (6.30). In Eq. (6.42), $I_{\ell, \ell'}^L(C; A, A')$ is a function of C_{ij} ($i, j = 1 \sim n-1$), A_{ij} and A'_{ij} ($1 \leq i < j \leq n-1$), and λ, μ and μ' are related to $L, |\ell|$ and $|\ell'|$ through $\lambda = 2L, \mu = |\ell| - L, \mu' = |\ell'| - L$ (see Eq. (6.31)). Furthermore, $N_H(\lambda\mu)$ is the normalization constant of the highest-weight state for 2×2 DG polynomials, and is given by [86]

$$N_H(\lambda\mu) = \left[\frac{\lambda + 1}{(\lambda + \mu + 1)! \mu!} \right]^{\frac{1}{2}} . \quad (6.43)$$

Once the expansion Eq. (6.42) is obtained, the matrix elements are easily obtained through the orthogonality of the DG polynomials. They are given by

$$\widetilde{M}_{\ell L; \ell' L}^C(\eta; \eta') = \left[\frac{1}{(2\ell - 1)!! (2\ell' - 1)!!} \right]^{\frac{1}{2}} \frac{1}{N_H(\lambda\mu) N_H(\lambda\mu')} I_{\ell, \ell'}^L(C; A, A') . \quad (6.44)$$

Let us first consider the expansion of SU_2 -scalar part in $I(\xi; \xi')$. We set $V_{ij} = (\xi_i \cdot \xi_j^*)$ or $V = {}^t \xi \xi'^*$ in $(n-1) \times (n-1)$ matrix form and expand it in powers of V ;

$$\exp \left\{ \frac{1}{2} \sum_{i,j=1}^{n-1} C_{ij} (\xi_i \cdot \xi_j^*)^2 \right\} = \prod_{i,j=1}^{n-1} \sum_{k_{ij}=0}^{\infty} \frac{1}{2^{k_{ij}} k_{ij}!} C_{ij}^{k_{ij}} V_{ij}^{2k_{ij}} \equiv \sum_k \frac{1}{2^k k!} C^k V^{2k} . \quad (6.45)$$

In the last equation in Eq. (6.45), we have used an abbreviated notation for the repeated indices $C^k \equiv \prod_{i,j=1}^{n-1} C_{ij}^{k_{ij}}$ etc. In order to expand V^{2k} in Eq. (6.45) further, we employ the polynomial expansion of $(n-1) \times (n-1)$ DG polynomials [81]

$$\varphi_{a,b}^{(n-1 \ n-1)[f]}(V) = \sum_k \begin{bmatrix} [f] & b \\ a & k \end{bmatrix} \frac{V^k}{\sqrt{k!}} , \quad (6.46a)$$

or its inverse expansion

$$\frac{V^k}{\sqrt{k!}} = \sum_{[f],a,b} \begin{bmatrix} [f] & b \\ a & k \end{bmatrix} \varphi_{a,b}^{(n-1 \ n-1)[f]}(V) , \quad (6.46b)$$

which can be derived by the orthogonality relationship

$$\left\langle \frac{V^k}{\sqrt{k!}} \left| \frac{V^{k'}}{\sqrt{k'}} \right. \right\rangle = \delta_{k,k'} . \quad (6.46c)$$

We can also use the product formula [86] of the DG polynomials; i.e.,

$$\varphi_{a,b}^{(n-1 \ n-1)[f]}(V) = \varphi_{a,b}^{(n-1 \ n-1)[f]}({}^t \xi \xi'^*) = \frac{1}{N_H[f]} \sum_c \varphi_{c,a}^{(2 \ n-1)[f]}(\xi) \varphi_{c,b}^{(2 \ n-1)[f]}(\xi')^* . \quad (6.47)$$

We note that the irreducible representation label $[f]$ is actually a two-row partition $[f] = [\lambda + \mu, \mu, 0, \dots, 0] = (\lambda\mu)$ for $2 \times (n-1)$ DG polynomials. We also use r , instead of c , for the SU_2 internal quantum-number label, and the parametrization by ℓ in Eq. (6.29) for a etc. Following these procedures, we find

$$\begin{aligned} & \exp \left\{ \frac{1}{2} \sum_{i,j=1}^{n-1} C_{ij} (\xi_i \cdot \xi_j^*)^2 \right\} \\ &= \sum_{(\lambda\mu) \ell, \ell'} \frac{1}{N_H(\lambda\mu)} F_{\ell, \ell'}^{(\lambda\mu)}(C) \sum_{r=0}^{\lambda} \varphi_{r, \ell}^{(2 \ n-1)(\lambda\mu)}(\xi) \varphi_{r, \ell'}^{(2 \ n-1)(\lambda\mu)}(\xi')^* , \end{aligned} \quad (6.48)$$

where $F_{\ell, \ell'}^{(\lambda \mu)}(C)$ are homogeneous polynomials of C_{ij} ($i, j = 1 \sim n - 1$) of order $\lambda/2 + \mu = |\ell| = |\ell'|$ and are given by

$$F_{\ell, \ell'}^{(\lambda \mu)}(C) = \sum_k \left[\frac{(2k - 1)!!}{(2k)!!} \right]^{\frac{1}{2}} \begin{bmatrix} (\lambda \mu) & \ell' \\ \ell & 2k \end{bmatrix} C^k \quad (6.49a)$$

Note that the polynomial $F_{\ell, \ell'}^{(\lambda \mu)}(C)$ has a very similar structure to the DG polynomials in Eq. (6.46a). However, the factors $k = (k_{ij})$ are doubled and satisfy the weight condition

$$\sum_{i=1}^{n-1} k_{ij} = \ell'_j, \quad \sum_{j=1}^{n-1} k_{ij} = \ell_i, \quad k_{ij} = \text{non-negative integers}, \quad (6.49b)$$

and $\lambda = \text{even only}$. The appearance of the factor of the type $[(2k - 1)!!/(2k)!!]^{1/2}$, instead of $1/\sqrt{k!}$, is a typical feature of this modification of the DG polynomials.

Now we proceed to the non- SU_3 -scalar part of $I(\xi; \xi')$ in Eq. (6.39a), and consider expansion of $(\delta_{ij})^2$ part :

$$\begin{aligned} \exp \left\{ -\frac{1}{2} \sum_{i < j}^{n-1} A_{ij} (\delta_{ij})^2 \right\} &= \prod_{i < j}^{n-1} \sum_{m_{ij}=0}^{\infty} \left(-\frac{1}{2} \right)^{m_{ij}} \frac{1}{m_{ij}!} A_{ij}^{m_{ij}} (\delta_{ij})^{2m_{ij}} \\ &= \sum_{m=0}^{\infty} \left(-\frac{1}{2} \right)^m \sum_{\sum_{i < j} m_{ij}=m} \frac{1}{m!} A^m \delta^{2m}, \end{aligned} \quad (6.50)$$

where we have again used the abbreviated notation for the multi-dimensional index m . Since δ^{2m} is an SU_2 -scalar polynomial, we can expand it by $\varphi_{0, \ell''}^{(2 \ n-1) (0 \ 2m)}(\xi)$ with $|\ell''| = 2m$. Thus we expand Eq. (6.50) as

$$\begin{aligned} &\exp \left\{ -\frac{1}{2} \sum_{i < j}^{n-1} A_{ij} (\delta_{ij})^2 \right\} \\ &= \sum_{m=0}^{\infty} \left(-\frac{1}{2} \right)^m \frac{1}{N_H(0 \ 2m)} \sum_{\ell''} G_{\ell''}^{(0 \ 2m)}(A) \varphi_{0, \ell''}^{(2 \ n-1) (0 \ 2m)}(\xi). \end{aligned} \quad (6.51)$$

Note that, for a small value of n , the coefficient polynomial $G_{\ell''}^{(0 \ 2m)}(A)$ takes a very simple form due to the condition $1 \leq i < j \leq n - 1$. For 2-cluster systems with $n = 2$, this term does not exist. For 3-cluster systems with $n = 3$, the explicit expression of 2×2 DG polynomials [86] yields

$$G_0^{(0 \ 2m)}(A) = \frac{1}{m!} A_{12}^m, \quad (6.52a)$$

where we have used the SU_2 notation $r = 0$ for the Gel'fand pattern ℓ'' in Eq. (6.51) :

$$|\ell''\rangle = \begin{bmatrix} \lambda + \mu & \mu \\ \lambda + \mu - r & \end{bmatrix} = \begin{bmatrix} 2m & 2m \\ 2m & \end{bmatrix} = \begin{bmatrix} \ell_1 + \ell_2 & \ell_1 + \ell_2 \\ & 2\ell_1 \end{bmatrix}, \quad (6.52b)$$

with $\ell = 2L = 0$, $\mu = \ell_1 + \ell_2 = 2m$, and $\ell_1 = \ell_2 = m$. Even in 4-cluster systems, we only need to deal with polynomials of δ_{12} , δ_{13} and δ_{23} and the explicit expression of 2×3 DG polynomials [86] yields $G_{\ell''}^{(0 \ 2m)}(A)$ given by

$$G_{0 \ q \ r}^{(0 \ 2m)}(A) = \left[\frac{(2m - q - 1)!! (q - r - 1)!! (r - 1)!!}{(2m - 1)!! m! (m - \frac{q}{2})! (\frac{q-r}{2})! (\frac{r}{2})!} \right]^{\frac{1}{2}} A_{12}^{m-\frac{q}{2}} A_{13}^{\frac{q-r}{2}} A_{23}^{\frac{r}{2}}, \quad (6.53a)$$

where the SU_3 quantum numbers $q = 0 \sim 2m$, $r = 0 \sim q$ are even only and are related to ℓ'' through

$$\begin{aligned} |\ell''\rangle &= \left| \begin{array}{ccc} \lambda + \mu & \mu & 0 \\ \lambda + \mu - p & \mu - q & \\ \lambda + \mu - p - r & & \end{array} \right\rangle = \left| \begin{array}{ccc} 2m & 2m & 0 \\ 2m & 2m - q & \\ 2m - r & & \end{array} \right\rangle \\ &= \left| \begin{array}{ccc} \ell_1 + \ell_2 + \ell_3 & \ell_1 + \ell_2 + \ell_3 & 0 \\ & \ell_1 + \ell_2 + \ell_3 & \ell_1 + \ell_2 - \ell_3 \\ & & 2\ell_1 \end{array} \right\rangle, \quad (6.53b) \end{aligned}$$

with $\lambda = 2L = 0$, $\mu = \ell_1 + \ell_2 + \ell_3 = 2m$ (even only) and $p = 0$. Note that this coupling scheme is related to the SU_2 -scalar state $[[v_{\ell_1}(\xi_1) v_{\ell_2}(\xi_2)]_{\ell_3} v_{\ell_3}(\xi_3)]_0$.

In order to derive a general expression for $G_{\ell''}^{(0 \ 2m)}(A)$ for an arbitrary n , we employ Eq. (6.48) by assuming $C = (-1/2)A$ and $\xi'^* = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \xi \equiv \epsilon \xi$. By this assignment, the relationship $(\xi_i \cdot \xi_j^*) = ({}^t \xi \epsilon \xi)_{ij} = \det(\xi_i, \xi_j) = \delta_{ij}$ yields

$$\begin{aligned} &\exp \left\{ -\frac{1}{2} \sum_{i < j}^{n-1} A_{ij} (\delta_{ij})^2 \right\} \\ &= \sum_{(\lambda\mu) \ell, \ell'} \frac{1}{N_H(\lambda\mu)} F_{\ell, \ell'}^{(\lambda\mu)} \left(-\frac{1}{2} A \right) \sum_{r=0}^{\lambda} \varphi_{r, \ell}^{(2 \ n-1) (\lambda\mu)}(\xi) \varphi_{r, \ell'}^{(2 \ n-1) (\lambda\mu)}(\epsilon \xi), \quad (6.54) \end{aligned}$$

where we have modified the (usually non-zero) diagonal matrix elements A_{ii} into 0 ; i.e., $A_{ii} = 0$ ($i = 1 \sim n - 1$). First we use the fact that $F_{\ell, \ell'}^{(\lambda\mu)}(C)$ in Eq. (6.49a) is a homogeneous polynomials of C_{ij} with the order $\lambda/2 + \mu$ ($\lambda = 2L = \text{even}$), and find

$$F_{\ell, \ell'}^{(\lambda\mu)} \left(-\frac{1}{2} A \right) = \left(-\frac{1}{2} \right)^{\frac{\lambda}{2} + \mu} F_{\ell, \ell'}^{(\lambda\mu)}(A). \quad (6.55)$$

Further, we can use the product formula of DG polynomials and use $\varphi_{r, r'}^{(22) (\lambda)\mu}(\epsilon) = \delta_{r', \lambda-r} (-1)^r N_H(\lambda\mu)$ to derive

$$\varphi_{r, \ell'}^{(2 \ n-1) (\lambda\mu)}(\epsilon \xi) = \frac{1}{N_H(\lambda\mu)} \sum_{r'} \varphi_{r, r'}^{(22) (\lambda)\mu}(\epsilon) \varphi_{r', \ell'}^{(2 \ n-1) (\lambda\mu)}(\xi) = (-1)^r \varphi_{\lambda-r, \ell'}^{(2 \ n-1) (\lambda\mu)}(\xi). \quad (6.56)$$

Then, by using the SU_2 C-G coefficients $\langle \lambda/2(\lambda/2 - r) \lambda/2 - (\lambda/2 - r) | 00 \rangle = (-1)^r (1/\sqrt{\lambda + 1})$ and the C-G series for $2 \times (n - 1)$ DG polynomials [86], we find

$$\begin{aligned} & \sum_{r=0}^{\lambda} \varphi_{r,\ell}^{(2\ n-1)(\lambda\mu)}(\xi) \varphi_{r,\ell'}^{(2\ n-1)(\lambda\mu)}(\epsilon\xi) = \sqrt{\lambda + 1} \left[\varphi_{*,\ell}^{(2\ n-1)(\lambda\mu)}(\xi) \varphi_{*,\ell'}^{(2\ n-1)(\lambda\mu)}(\xi) \right]_0^{(0)} \\ & = \sqrt{\lambda + 1} \frac{N_H(\lambda\mu)^2}{N_H(0\ \lambda + 2\mu)} \sum_{\ell''} \langle (\lambda\mu)\ell(\lambda\mu)\ell' | (0\ \lambda + 2\mu)\ell'' \rangle_{n-1} \varphi_{0,\ell''}^{(2\ n-1)(0\ \lambda+2\mu)}(\xi) \ , \end{aligned} \tag{6.57}$$

where we have used the two-row SU_{n-1} C-G coefficients $\langle (\lambda\mu)\ell(\lambda\mu)\ell' | (0\ \lambda + 2\mu)\ell'' \rangle_{n-1}$. These two-row SU_{n-1} C-G coefficients are discussed in §6.2.3, together with the polynomial functions $F_{\ell,\ell'}^{(\lambda\mu)}(C)$. Finally, we combine Eqs. (6.54), (6.55) and (6.57) and compare it with Eq. (6.51). Then we find that $G_{\ell'', 2m}^{(0\ 2m)}(A)$ is given by

$$G_{\ell'', 2m}^{(0\ 2m)}(A) = \sum_{\substack{(\lambda\mu)\ell,\ell' \\ \lambda+2\mu=2m}} \sqrt{\lambda + 1} N_H(\lambda\mu) \langle (\lambda\mu)\ell(\lambda\mu)\ell' | (0\ \lambda + 2\mu)\ell'' \rangle_{n-1} F_{\ell,\ell'}^{(\lambda\mu)}(A) \ , \tag{6.58}$$

where ${}^tA = A$ with $A_{11} = \dots = A_{n-1,n-1} = 0$.

We use the same procedure for another non- SU_2 -scalar part in $I(\xi; \xi')$. By combining these, we find

$$\begin{aligned} I(\xi; \xi') &= \sum_{\substack{(\lambda\mu)\tilde{\ell},\tilde{\ell}' \\ \tilde{\ell}'',\tilde{\ell}'''}} \sum_{m,m'} \left(-\frac{1}{2}\right)^{m+m'} \frac{1}{N_H(\lambda\mu) N_H(0\ 2m) N_H(0\ 2m')} \\ &\times F_{\tilde{\ell},\tilde{\ell}'}^{(\lambda\mu)}(C) G_{\tilde{\ell}'', 2m}^{(0\ 2m)}(A) G_{\tilde{\ell}''', 2m'}^{(0\ 2m')}(A') \\ &\times \sum_r \left(\varphi_{r,\tilde{\ell}}^{(2\ n-1)(\lambda\mu)}(\xi) \varphi_{0,\tilde{\ell}''}^{(2\ n-1)(0\ 2m)}(\xi) \right) \left(\varphi_{r,\tilde{\ell}'}^{(2\ n-1)(\lambda\mu)}(\xi') \varphi_{0,\tilde{\ell}'''}^{(2\ n-1)(0\ 2m')}(\xi') \right)^* \ , \end{aligned} \tag{6.59}$$

where we have changed the notation $\ell \rightarrow \tilde{\ell}$, $\ell' \rightarrow \tilde{\ell}'$ etc., to reserve ℓ and ℓ' for the later use. We again use the C-G series to combine two DG polynomials. After some alteration of notation to fix the polynomial powers, we finally obtain

$$\begin{aligned} & I_{\tilde{\ell},\tilde{\ell}'}^L(C; A, A') \\ &= \sum_{\substack{\mu_0=0\ \text{or}\ 1 \\ (\text{mod}\ 2)}}^{\min\{\mu,\mu'\}} \left(-\frac{1}{2}\right)^{\frac{\mu+\mu'}{2}-\mu_0} N_H(\lambda\mu_0) \sum_{\tilde{\ell},\tilde{\ell}',\tilde{\ell}'',\tilde{\ell}'''} \langle (\lambda\mu_0)\tilde{\ell}(0\ \mu - \mu_0)\tilde{\ell}'' | (\lambda\mu)\ell \rangle_{n-1} \\ &\times \langle (\lambda\mu_0)\tilde{\ell}'(0\ \mu' - \mu_0)\tilde{\ell}''' | (\lambda\mu')\ell' \rangle_{n-1} F_{\tilde{\ell},\tilde{\ell}'}^{(\lambda\mu_0)}(C) G_{\tilde{\ell}'', \mu-\mu_0}^{(0)}(A) G_{\tilde{\ell}''', \mu'-\mu_0}^{(0)}(A') \ , \end{aligned} \tag{6.60}$$

where $\lambda = 2L$, $\mu = |\ell| - L$ and $\mu' = |\ell'| - L$.

6.2.2 Noncentral Matrix Elements

In order to evaluate the noncentral matrix elements, we need some preparation to reduce the polynomial parts in Eq. (6.41c). The first formula is with respect to 3-dimensional vectors, $\mathbf{R}_1, \dots, \mathbf{R}_{n-1}$, and reads

$$\mathcal{Y}_{\ell m} \left(\sum_{i=1}^{n-1} \mathbf{R}_i \right) = \sum_{\ell_1 + \dots + \ell_{n-1} = \ell} \left[\frac{\ell!}{\ell_1! \dots \ell_{n-1}!} \right]^{\frac{1}{2}} \times \left[\dots [\mathcal{Y}_{\ell_1}(\mathbf{R}_1) \mathcal{Y}_{\ell_2}(\mathbf{R}_2)]_{\ell_1 + \ell_2} \dots \mathcal{Y}_{\ell_{n-1}}(\mathbf{R}_{n-1}) \right]_{\ell m}, \quad (6.61)$$

where all the intermediate couplings are stretched ones ; i.e., $\ell_{12\dots s} = \ell_1 + \ell_2 + \dots + \ell_s$ ($s = 1 \sim n - 2$) and $L = \ell_1 + \dots + \ell_{n-1} = \ell$ in the Gel'fand pattern (6.29). This well-known formula is easily proved by using the generating function of $\mathcal{Y}_{\ell m}(\mathbf{R})$ in Eq. (6.12) and the reduction formula in Eq. (6.9). By using this formula, one can prove

$$\mathcal{Y}_{\ell m}({}^t f \mathbf{R}) |_{\mathbf{R} \downarrow \xi} = \mathcal{Y}_{\ell m} \left(\sum_{i=1}^{n-1} f_i \mathbf{R}_i \right) \Big|_{\mathbf{R} \downarrow \xi} = \sqrt{(2\ell)!!} \sum_{|\ell_s| = \ell} F_{0, \ell_s}^{(2\ell \ 0)}(f) v_{\ell_s}^{\ell m}(\xi), \quad (6.62a)$$

where

$$F_{0, \ell_s}^{(2\ell \ 0)}(f) = \left[\frac{(2\ell_s - 1)!!}{(2\ell_s)!!} \right]^{\frac{1}{2}} f^{\ell_s} \quad (6.62b)$$

and ℓ_s denotes the stretched Gel'fand pattern ℓ . For example, if we write Eq. (6.62a) explicitly, it means that

$$\mathcal{Y}_{\ell m} \left(\sum_{i=1}^{n-1} f_i \mathbf{R}_i \right) \Big|_{\mathbf{R} \downarrow \xi} = \sqrt{(2\ell)!!} \sum_{\ell_1 + \dots + \ell_{n-1} = \ell} \left[\frac{(2\ell_1 - 1)!! \dots (2\ell_{n-1} - 1)!!}{(2\ell_1)!! \dots (2\ell_{n-1})!!} \right]^{\frac{1}{2}} \times f_1^{\ell_1} \dots f_{n-1}^{\ell_{n-1}} \left[\dots [v_{\ell_1}(\xi_1) v_{\ell_2}(\xi_2)]_{\ell_1 + \ell_2} \dots v_{\ell_{n-1}}(\xi_{n-1}) \right]_{\ell m}. \quad (6.62c)$$

The third formula we need for LS factors is

$$\left[\mathcal{Y}_1({}^t f \mathbf{R}) \mathcal{Y}_1({}^t g \mathbf{R}) \right]_{1m} |_{\mathbf{R} \downarrow \xi} = 2\sqrt{2} \sum_{\ell} F_{1, \ell}^{(21)}(f, g) v_{\ell}^{1m}(\xi), \quad (6.63a)$$

where

$$F_{1, \ell}^{(21)}(f, g) = \frac{1}{2} \sum_{|\ell_s| = |\ell'_s| = 1} \langle (20)\ell_s (20)\ell'_s | (21)\ell \rangle_{n-1} f^{\ell_s} g^{\ell'_s}. \quad (6.63b)$$

We note that the coupling by the two-row SU_{n-1} C-G coefficients in Eq. (6.63b) corresponds to the outer product of two $(n-1)$ -dimensional vectors f_i and g_i . In fact, these C-G coefficients show up in the C-G series of the DG polynomials in

$$\left[v_{\ell_s}^1(\xi) v_{\ell'_s}^1(\xi) \right]_{1m} = \sqrt{2} \sum_{\ell} \langle (20)\ell_s (20)\ell'_s | (21)\ell \rangle_{n-1} v_{\ell}^{1m}(\xi). \quad (6.64)$$

Since $|\ell_s| = |\ell'_s| = 1$ means that ℓ_s and ℓ'_s just specify the vector components ξ_{ℓ_s} and $\xi_{\ell'_s}$, for example, we can rather use the ordered combination $\{\ell_s \ell'_s\}$, in order to specify the Gel'fand pattern ℓ for $(\lambda\mu) = (21)$. Namely, we define, for $|\ell_s| = |\ell'_s| = 1$,

$$v_{\{\ell_s \ell'_s\}}^{1m}(\xi) \equiv \left[v_{\ell_s}^1(\xi) v_{\ell'_s}^1(\xi) \right]_{1m} = \left[v_1(\xi_{\ell_s}) v_1(\xi_{\ell'_s}) \right]_{1m} , \quad (6.65a)$$

from which we can show

$$v_{\{\ell_s \ell'_s\}}^{1m}(\xi) = -v_{\{\ell'_s \ell_s\}}^{1m}(\xi) , \quad v_{\{\ell_s \ell_s\}}^{1m}(\xi) = 0 . \quad (6.65b)$$

By using this identification $\ell \equiv \{\ell_s \ell'_s\}$, the formula in Eq. (6.63a) is expressed as

$$\left[\mathcal{Y}_1({}^t f \mathbf{R}) \mathcal{Y}_1({}^t g \mathbf{R}) \right]_{1m} |_{\mathbf{R} \downarrow \xi} = \sum_{|\ell_s|=|\ell'_s|=1} f^{\ell_s} g^{\ell'_s} v_{\{\ell_s \ell'_s\}}^{1m}(\xi) . \quad (6.66)$$

Now, we can use the formulae in Eqs. (6.61), (6.62) and (6.66), in order to reduce the polynomial factors in Eq. (6.41c). We find

$$\begin{aligned} \tilde{\mathcal{P}}_{1\mu}^{LS}(\xi; \xi') = & \sum_{|\ell_s|=|\ell'_s|=1} \left\{ \hat{P}^{\ell_s} \tilde{P}'^{\ell'_s} v_{\{\ell_s \ell'_s\}}^{1\mu}(\xi) + \tilde{P}^{\ell_s} \hat{P}'^{\ell'_s} w_{\{\ell_s \ell'_s\}}^{1\mu}(\xi'^*) \right. \\ & \left. - \left(\hat{P}^{\ell_s} \hat{P}'^{\ell'_s} - \tilde{P}^{\ell_s} \tilde{P}'^{\ell'_s} \right) \left[v_{\ell_s}^1(\xi) w_{\ell'_s}^1(\xi'^*) \right]_{1\mu} \right\} , \end{aligned} \quad (6.67a)$$

$$\begin{aligned} \tilde{\mathcal{P}}_{2\mu}^T(\xi; \xi') = & 2\sqrt{2} \sum_{|\ell_s|=2} \left[\frac{(2\ell_s - 1)!!}{(2\ell_s)!!} \right]^{\frac{1}{2}} \left\{ \hat{f}^{\ell_s} v_{\ell_s}^{2\mu}(\xi) + \hat{g}^{\ell_s} w_{\ell_s}^{2\mu}(\xi'^*) \right\} \\ & - \sqrt{2} \sum_{|\ell_s|=|\ell'_s|=1} \hat{f}^{\ell_s} \hat{g}'^{\ell'_s} \left[v_{\ell_s}^1(\xi) w_{\ell'_s}^1(\xi'^*) \right]_{2\mu} , \end{aligned} \quad (6.67b)$$

where we have used the conjugate spinor functions

$$w_{\ell m}(\xi'^*) = (-1)^{\ell+m} v_{\ell, -m}(\xi)^* \quad (6.68)$$

and their extension to $2 \times (n - 1)$ DG polynomials $w_{\ell}^{LM}(\xi'^*)$ like $v_{\ell}^{LM}(\xi)$ in Eq. (6.30). Through these procedures, we only need to calculate the reduced matrix elements of $I(\xi; \xi') \mathcal{P}^{(\kappa)}(\xi; \xi')$ with respect to the tensor factors

$$\mathcal{P}_{\mu}^{(\kappa)}(\xi; \xi') = \left[v_{\ell}^{\ell_0}(\xi) w_{\ell'}^{\ell'_0}(\xi'^*) \right]_{\kappa\mu} \quad (6.69)$$

with $\kappa = 1$ and 2 . The full expression is obtained through a simple superposition of different types. The final result is given by

$$\begin{aligned} M_{\ell(LS); \ell'(L'S')}^{\Omega J}(\eta; \eta') = & \left[\frac{(|\ell| + L + 1)! (|\ell| - L)! (|\ell'| + L' + 1)! (|\ell'| - L')!}{(2L + 1)(2\ell - 1)!! (2L' + 1)(2\ell' - 1)!!} \right]^{\frac{1}{2}} \\ & \times (1 - \varepsilon^2)^{\frac{1}{2}(\ell + \frac{3}{2})} (1 - \varepsilon'^2)^{\frac{1}{2}(\ell' + \frac{3}{2})} \left(\frac{1}{D} \right)^{\frac{3}{2}} \end{aligned}$$

$$\times \begin{cases} \delta_{L,L'} \delta_{S,S'} I_{\ell,\ell'}^L(C; A, A') & \text{for } \textit{central} \\ \langle \mathbf{L} \cdot \mathbf{S} \rangle_{LS,L'S'}^J \left(\frac{1}{1+\lambda\tilde{\alpha}} \right) I_{\ell L; \ell' L'}^{(LS)}(C; A, A'; \hat{P}, \tilde{P}, \hat{P}', \tilde{P}') & \text{for } \textit{LS} \\ \langle S_{12} \rangle_{LS,L'S'}^J \left(\frac{1}{1+\lambda\tilde{\alpha}} \right)^2 I_{\ell L; \ell' L'}^{(T)}(C; A, A'; \hat{f}, \hat{g}) & \text{for } \textit{Tensor} . \end{cases} \quad (6.70a)$$

with

$$\langle \mathbf{L} \cdot \mathbf{S} \rangle_{LS,L'S'}^J = \begin{bmatrix} L' & S' & J \\ 1 & 1 & 0 \\ L & S & J \end{bmatrix} \langle S \parallel \mathbf{S} \parallel S' \rangle \sqrt{6} (-1)^{L'} \frac{1}{\sqrt{2L+1}} , \quad (6.70b)$$

$$\langle S_{12} \rangle_{LS,L'S'}^J = \begin{bmatrix} L' & S' & J \\ 2 & 2 & 0 \\ L & S & J \end{bmatrix} \langle S \parallel S^{(2)} \parallel S' \rangle \sqrt{30} (-1)^{L'} \frac{1}{\sqrt{2L+1}} . \quad (6.70c)$$

The LS and tensor factors in Eqs. (6.70b) and (6.70c) are symmetric with respect to the interchange of LS and $L'S'$. In Eq. (6.70a), the central factor $I_{\ell,\ell'}^L(C; A, A')$ is given in Eq. (6.60). The LS and tensor factors are expressed in terms of these central factors as follows :

$$\begin{aligned} & I_{\ell L; \ell' L'}^{(LS)}(C; A, A'; \hat{P}, \tilde{P}, \hat{P}', \tilde{P}') \\ &= (-1)^{L'+1} \frac{\hat{L}}{2\sqrt{2}} \sum_{\tilde{\ell}} I_{\tilde{\ell}, \tilde{\ell}'}^{L'}(C; A, A') \sum_{|\ell_s|=|\ell'_s|=1} \hat{P}^{\ell_s} \tilde{P}'^{\ell'_s} \langle (\lambda\tilde{\mu}) \tilde{\ell} (21) \{ \ell_s \ell'_s \} | (\lambda\mu) \ell \rangle_{n-1} \\ &+ (-1)^L \frac{\hat{L}'}{2\sqrt{2}} \sum_{\tilde{\ell}'} I_{\tilde{\ell}, \tilde{\ell}'}^{L'}(C; A, A') \sum_{|\ell_s|=|\ell'_s|=1} \tilde{P}^{\ell_s} \hat{P}'^{\ell'_s} \langle (\lambda\tilde{\mu}') \tilde{\ell}' (21) \{ \ell_s \ell'_s \} | (\lambda'\mu') \ell' \rangle_{n-1} \\ &+ \sum_{\tilde{L}} (-1)^{\tilde{L}} \frac{\hat{\tilde{L}} \hat{\tilde{L}'}}{2\hat{\tilde{L}}} U(L' 1 L 1; \tilde{L} 1) \sum_{\tilde{\ell}, \tilde{\ell}'} I_{\tilde{\ell}, \tilde{\ell}'}^{\tilde{L}}(C; A, A') \sum_{|\ell_s|=|\ell'_s|=1} \left(\hat{P}^{\ell_s} \hat{P}'^{\ell'_s} - \tilde{P}^{\ell_s} \tilde{P}'^{\ell'_s} \right) \\ &\times \langle (\tilde{\lambda}\tilde{\mu}) \tilde{\ell} (20) \ell_s | (\lambda\mu) \ell \rangle_{n-1} \langle (\tilde{\lambda}\tilde{\mu}') \tilde{\ell}' (20) \ell'_s | (\lambda'\mu') \ell' \rangle_{n-1} , \end{aligned} \quad (6.70d)$$

$$\begin{aligned} & I_{\ell L; \ell' L'}^{(T)}(C; A, A'; \hat{f}, \hat{g}) \\ &= (-1)^{L'} \hat{L} \sum_{\tilde{\ell}} I_{\tilde{\ell}, \tilde{\ell}'}^{L'}(C; A, A') \sum_{|\ell_s|=2} \left[\frac{(2\ell_s - 1)!!}{(2\ell_s)!!} \right]^{\frac{1}{2}} \hat{f}^{\ell_s} \langle (\lambda\tilde{\mu}) \tilde{\ell} (40) \ell_s | (\lambda\mu) \ell \rangle_{n-1} \\ &+ (-1)^L \hat{L}' \sum_{\tilde{\ell}'} I_{\tilde{\ell}, \tilde{\ell}'}^{L'}(C; A, A') \sum_{|\ell'_s|=2} \left[\frac{(2\ell'_s - 1)!!}{(2\ell'_s)!!} \right]^{\frac{1}{2}} \hat{g}^{\ell'_s} \langle (\lambda\tilde{\mu}') \tilde{\ell}' (40) \ell'_s | (\lambda'\mu') \ell' \rangle_{n-1} \end{aligned}$$

$$\begin{aligned}
 & + \sum_{\tilde{L}} (-1)^{\tilde{L}} \sqrt{\frac{3}{2}} \left(\begin{matrix} \widehat{L} \widehat{L}' \\ \widehat{\tilde{L}} \end{matrix} \right) U(L' 1 L 1; \tilde{L} 2) \sum_{\tilde{\ell}, \tilde{\ell}'} I_{\tilde{\ell}, \tilde{\ell}'}^{\tilde{L}}(C; A, A') \\
 & \times \sum_{|\ell_s|=|\ell'_s|=1} \widehat{f}^{\ell_s} \widehat{g}^{\ell'_s} \langle (\tilde{\lambda} \tilde{\mu}) \tilde{\ell}(20) \ell_s | (\lambda \mu) \ell \rangle_{n-1} \langle (\tilde{\lambda} \tilde{\mu}') \tilde{\ell}'(20) \ell'_s | (\lambda' \mu') \ell' \rangle_{n-1} \quad , \quad (6.70e)
 \end{aligned}$$

where $\lambda = 2L, \mu = |\ell| - L, \lambda' = 2L', \mu' = |\ell'| - L'$, and $\tilde{\lambda} = 2\tilde{L}$. In the first and second terms of Eqs. (6.70d) and (6.70e), the non-negative values $\tilde{\mu}$ and $\tilde{\mu}'$ are given by $\tilde{\mu} = |\ell| - L' - 2$ and $\tilde{\mu}' = |\ell'| - L - 2$, while in the third terms these are $\tilde{\mu} = |\ell| - \tilde{L} - 1$ and $\tilde{\mu}' = |\ell'| - \tilde{L} - 1$. Furthermore, $U(L' 1 L 1; \tilde{L} 1)$ etc. denote the unitary form of the angular-momentum Racah coefficients.

6.2.3 Two-Row SU_{n-1} C-G Coefficients and the Expansion Coefficients of $F_{\ell, \ell'}^{(\lambda \mu)}(C)$

The expressions of the central, *LS* and tensor matrix elements in Eqs. (6.60) and (6.70) would be useless, if it were not possible to evaluate the SU_{n-1} C-G coefficients and the coefficients of polynomial functions $F_{\ell, \ell'}^{(\lambda \mu)}(C)$. Fortunately, these are all of the two-row type, and can be obtained from the standard angular-momentum Wigner coefficients.²⁸

Let us first consider the two-row SU_{n-1} C-G coefficients. We start from the C-G series of $2 \times (n - 1)$ DG polynomials [86]

$$\begin{aligned}
 & \left[\varphi_{*, \ell}^{(2 \ n-1)(\lambda \mu)}(\xi) \varphi_{*, \ell'}^{(2 \ n-1)(\lambda' \mu')}(\xi) \right]_{L'', L''-r''} \\
 & = \frac{N_H(\lambda \mu) N_H(\lambda' \mu')}{N_H(\lambda'' \mu'')} \sum_{\ell''} \langle (\lambda \mu) \ell (\lambda' \mu') \ell' | (\lambda'' \mu'') \ell'' \rangle_{n-1} \varphi_{r'', \ell''}^{(2 \ n-1)(\lambda'' \mu'')}(\xi) \quad , \quad (6.71)
 \end{aligned}$$

where the two-row condition is $\lambda + 2\mu + \lambda' + 2\mu' = \lambda'' + 2\mu''$. We use the vector-coupling expression in Eq. (6.30), and reduce the left-hand side of Eq. (6.71) by the aid of the angular-momentum recouplings and the reduction formula in Eq. (6.9). From this procedure, we find

$$\begin{aligned}
 & \langle (\lambda \mu) \ell (\lambda' \mu') \ell' | (\lambda'' \mu'') \ell'' \rangle_{n-1} \\
 & = \frac{N_H(\lambda'' \mu'')}{N_H(\lambda \mu) N_H(\lambda' \mu')} \left[\begin{matrix} (2\ell''_1) \\ (2\ell_1) \end{matrix} \begin{matrix} (2\ell''_2) \\ (2\ell_2) \end{matrix} \dots \begin{matrix} (2\ell''_{n-1}) \\ (2\ell_{n-1}) \end{matrix} \right]^{\frac{1}{2}} \\
 & \times \begin{bmatrix} \ell_1 & \ell_2 & \ell_{12} \\ \ell'_1 & \ell'_2 & \ell'_{12} \\ \ell''_1 & \ell''_2 & \ell''_{12} \end{bmatrix} \begin{bmatrix} \ell_{12} & \ell_3 & \ell_{123} \\ \ell'_{12} & \ell'_3 & \ell'_{123} \\ \ell''_{12} & \ell''_3 & \ell''_{123} \end{bmatrix} \dots \begin{bmatrix} \ell_{12\dots n-2} & \ell_{n-1} & L \\ \ell'_{12\dots n-2} & \ell'_{n-1} & L' \\ \ell''_{12\dots n-2} & \ell''_{n-1} & L'' \end{bmatrix} \quad , \quad (6.72)
 \end{aligned}$$

where $\lambda = 2L, \mu = |\ell| - L, \lambda' = 2L', \mu' = |\ell'| - L', \lambda'' = 2L'', \mu'' = |\ell''| - L''$, and $\ell_i + \ell'_i = \ell''_i$ ($i = 1 \sim n - 1$) (stretched). Here, the square bracket means the unitary

²⁸This is natural, since we are essentially dealing with the algebra of angular-momentum projections.

form of the 9-*j* coefficients. Furthermore, $N_H(\lambda\mu)$ is given in Eq. (6.43). The first 9-*j* coefficient in Eq. (6.72) is stretched for 2 columns, so that it is expressed by a single C-G coefficient (see Eq. (5-3-13) of [86]). Namely, we can show

$$\begin{aligned} \begin{bmatrix} \ell_1 & \ell_2 & \ell_{12} \\ \ell'_1 & \ell'_2 & \ell'_{12} \\ \ell''_1 & \ell''_2 & \ell''_{12} \end{bmatrix} &= \frac{N_H(2\ell_{12}, \ell_1 + \ell_2 - \ell_{12}) N_H(2\ell'_{12}, \ell'_1 + \ell'_2 - \ell'_{12})}{N_H(2\ell''_{12}, \ell_1 + \ell_2 + \ell'_1 + \ell'_2 - \ell''_{12})} \left[\begin{pmatrix} 2\ell''_1 \\ 2\ell_1 \end{pmatrix} \begin{pmatrix} 2\ell''_2 \\ 2\ell_2 \end{pmatrix} \right]^{-\frac{1}{2}} \\ &\times \langle \ell_{12} \ell_1 - \ell_2 \ell'_{12} \ell'_1 - \ell'_2 | \ell''_{12} \ell_1 - \ell_2 + \ell'_1 - \ell'_2 \rangle \\ &\text{for } \ell_1 + \ell'_1 = \ell''_1 \quad \text{and} \quad \ell_2 + \ell'_2 = \ell''_2 . \end{aligned} \tag{6.73}$$

If $(\lambda\mu)\ell$ and $(\lambda'\mu')\ell'$ are both stretched angular-momentum couplings with $\lambda = 2L = 2(\ell_1 + \dots + \ell_{n-1})$, $\mu = 0$, $\ell_{12\dots s} = \ell_1 + \ell_2 + \dots + \ell_s$ ($s = 1 \sim n - 1$) and $\lambda' = 2L' = 2(\ell'_1 + \dots + \ell'_{n-1})$, $\mu' = 0$, $\ell'_{12\dots s} = \ell'_1 + \ell'_2 + \dots + \ell'_s$, respectively, all the 9-*j* coefficients are of this type. For the C-G coefficients $\langle (\lambda'\tilde{\mu})\tilde{\ell}(21)\{\ell_s\ell'_s\} | (\lambda\mu)\ell \rangle_{n-1}$ etc. with $|\ell_s| = |\ell'_s| = 1$ in Eq. (6.70d), we can use

$$\begin{aligned} &\langle (\lambda'\tilde{\mu})\tilde{\ell}(21)\{\ell_s\ell'_s\} | (\lambda\mu)\ell \rangle_{n-1} \\ &= \sqrt{2} \sum_{\ell'} \langle (\lambda'\tilde{\mu})\tilde{\ell}(21)\ell' | (\lambda\mu)\ell \rangle_{n-1} \langle (20)\ell_s(20)\ell'_s | (21)\ell' \rangle_{n-1} \end{aligned} \tag{6.74}$$

from Eqs. (6.64) and (6.65a).

Next, let us consider the polynomial functions $F_{\ell,\ell'}^{(\lambda\mu)}(C)$ in Eq. (6.49a). We only need to consider the expansion coefficients $\begin{bmatrix} (\lambda\mu) & \ell' \\ \ell & 2k \end{bmatrix}$. These are easily obtained from the vector coupling expression of the $(n - 1) \times (n - 1)$ DG polynomials given in Eq. (2-2-15a) of ref. [86]. We find

$$\begin{aligned} \begin{bmatrix} (\lambda\mu) & \ell' \\ \ell & 2k \end{bmatrix} &= \sum_{\tilde{\ell}_{12}, \dots, \tilde{\ell}_{12\dots n-2}} \langle (2\ell_1 0) k_{1*} (2\ell_2 0) k_{2*} | (2\ell_{12} \mu_{12}) \tilde{\ell}_{12} \rangle_{n-1} \\ &\times \langle (2\ell_{12} \mu_{12}) \tilde{\ell}_{12} (2\ell_3 0) k_{3*} | (2\ell_{123} \mu_{123}) \tilde{\ell}_{123} \rangle_{n-1} \\ &\times \dots \dots \dots \\ &\times \langle (2\ell_{12\dots n-2} \mu_{12\dots n-2}) \tilde{\ell}_{12\dots n-2} (2\ell_{n-1} 0) k_{n-1*} | (\lambda\mu)\ell' \rangle_{n-1} , \end{aligned} \tag{6.75}$$

where $k_{i*} = (k_{i1}, \dots, k_{i,n-1})$ ($i = 1 \sim n - 1$) specifies internal quantum numbers of the one-row SU_{n-1} state with $(2\ell_i 0)$ through

$$|k_{i*}; \ell_i\rangle = \left| \begin{array}{ccccccc} 2(k_{i1} + \dots + k_{i,n-1}) & 0 & \dots & \dots & \dots & 0 & \\ & \ddots & & \ddots & & \ddots & \\ & & 2(k_{i1} + k_{i2} + k_{i3}) & 0 & & 0 & \\ & & & 2(k_{i1} + k_{i2}) & & 0 & \\ & & & & & 2k_{i1} & \end{array} \right\rangle . \tag{6.76}$$

Note that k_{ij} are non-negative integers which satisfy the weight condition (6.49b). Furthermore, $\mu_{12} = \ell_1 + \ell_2 - \ell_{12}$, $\mu_{123} = \ell_1 + \ell_2 + \ell_3 - \ell_{123}$, \dots , $\mu_{12\dots n-2} = \ell_1 + \dots + \ell_{n-2} - \ell_{12\dots n-2}$ from the two-row conditions, and $\lambda = 2L$ and $\mu = \ell_1 + \ell_2 + \dots + \ell_{n-1} - L$. The expression of $F_{\ell,\ell'}^{(\lambda\mu)}(C)$ is also obtained from the original expression of Eq. (6.48) directly by using Eqs. (6.12), (6.9), (6.62a) and the C-G series in Eq. (6.71).

6.3 Examples for 2- and 3-Cluster Systems

6.3.1 2-Cluster Systems

For 2-cluster systems, the SU_{n-1} C-G coefficients in Eqs. (6.60) and (6.70) become simply Kronecker delta's for the conservation of weights and no C-G coefficient appears for the central matrix elements. The expansion coefficient of $F_{\ell,\ell'}^{(\lambda\mu)}(C)$ in Eq. (6.75) is unity and the polynomial $G_{\ell'}^{(0,2m)}(A)$ in Eq. (6.58) is not necessary. In this particular case, it is convenient to introduce the standard angular-spin wave functions

$$\mathcal{Y}_{LS}^{JM}(\hat{\mathbf{r}}; spin) \equiv [Y_L(\hat{\mathbf{r}}) \xi_S]_{JM} \quad , \quad (6.77)$$

and define the LS and tensor factors in Eqs. (6.70b) and (6.70c) in a little different way. Namely, we define

$$\begin{aligned} (\mathbf{L} \cdot \mathbf{S})_{LS,L'S'}^J &\equiv \langle \mathcal{Y}_{LS}^{JM}(\hat{\mathbf{r}}; spin) | (\mathbf{L} \cdot \mathbf{S}) | \mathcal{Y}_{L'S'}^{JM}(\hat{\mathbf{r}}; spin) \rangle \\ &= \delta_{L,L'} \begin{bmatrix} L & S' & J \\ 1 & 1 & 0 \\ L & S & J \end{bmatrix} (-\sqrt{3}) \sqrt{L(L+1)} \langle S \parallel \mathbf{S} \parallel S' \rangle \quad , \end{aligned} \quad (6.78a)$$

$$\begin{aligned} (S_{12})_{LS,L'S'}^J &\equiv \langle \mathcal{Y}_{LS}^{JM}(\hat{\mathbf{r}}; spin) | S_{12} | \mathcal{Y}_{L'S'}^{JM}(\hat{\mathbf{r}}; spin) \rangle \\ &= \begin{bmatrix} L' & S' & J \\ 2 & 2 & 0 \\ L & S & J \end{bmatrix} \sqrt{30} \langle L020 | L'0 \rangle \langle S \parallel S^{(2)} \parallel S' \rangle \quad , \end{aligned} \quad (6.78b)$$

where the LS factor is non-zero only for $L = L'$ due to the parity conservation, and the tensor factor S_{12} is defined through $S_{12} = \sqrt{24\pi} [Y_2(\hat{\mathbf{r}}) S^{(2)}]^{(0)}$ (see Eq. (3.62)). When both clusters have spin 1/2 and are identical, these definitions reduce to the ordinary spin and tensor factors, usually adopted in the study of NN interaction through $\mathbf{S} = (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)/2$, $S_\mu^{(2)} = 2[SS]_\mu^{(2)} = [\sigma_1\sigma_2]_\mu^{(2)}$ (see Eqs. (4.18) and (4.19)) :

$$(\mathbf{L} \cdot \mathbf{S})_{LS,L'S'}^J = \delta_{L,L'} \delta_{S,S'} \delta_{S,1} \frac{1}{2} \left[J(J+1) - L(L+1) - S(S+1) \right] \quad , \quad (6.79a)$$

and

$$(S_{12})_{LS,L'S'}^J = \delta_{S,S'} \delta_{S,1} (S_{12})_{L,L'}^J \quad (6.79b)$$

with

$$\begin{aligned}
(S_{12})_{J,J}^J &= 2 \quad , \quad (S_{12})_{J-1,J+1}^J = (S_{12})_{J+1,J-1}^J = \frac{6\sqrt{J(J+1)}}{2J+1} \quad , \\
(S_{12})_{J-1,J-1}^J &= \frac{2(1-J)}{2J+1} \quad , \quad (S_{12})_{J+1,J+1}^J = -\frac{2(J+2)}{2J+1} \quad . \quad (6.79c)
\end{aligned}$$

In this case, we should carefully divide the spin-isospin factors in Eq. (4.27) with the reduced matrix elements $\langle 1 \parallel \mathbf{S} \parallel 1 \rangle = \sqrt{2}$ and $\langle 1 \parallel S^{(2)} \parallel 1 \rangle = 2\sqrt{5/3}$ (see Eq. (4.21)). By using these notations, the matrix elements in Eq. (6.70) are expressed as

$$\begin{aligned}
M_{(LS);(L'S')}^{\Omega J}(\eta; \eta') &= (1 - \varepsilon^2)^{\frac{1}{2}(L + \frac{3}{2})} (1 - \varepsilon'^2)^{\frac{1}{2}(L' + \frac{3}{2})} \left(\frac{1}{D} \right)^{\frac{3}{2}} \\
&\times \begin{cases} \delta_{L,L'} \delta_{S,S'} C^L & \text{for } \textit{central} \\ -\delta_{L,L'} (\mathbf{L} \cdot \mathbf{S})_{LS,LS'}^J C^{L-1} h & \text{for } \textit{LS} \\ (S_{12})_{LS,L'S'}^J \left\{ \delta_{L,L'+2} \sqrt{(2L-1)(2L+1)} C^{L'} f^2 + \delta_{L+2,L'} \sqrt{(2L'-1)(2L'+1)} \right. \\ \quad \left. \times C^L g^2 + \delta_{L,L'} (2L+3) C^{L-1} f g \right\} & \text{for } \textit{tensor} \quad , \end{cases} \quad (6.80)
\end{aligned}$$

where the coefficients, D , C , f , g and h , are given by

$$\begin{aligned}
D &= \tilde{D} (1 + \lambda \tilde{\alpha}) \quad , \quad \tilde{D} = 1 - \varepsilon \varepsilon' Q^2 \quad , \\
\tilde{\alpha} &= \frac{1}{\tilde{D}} (\varepsilon P^2 + \varepsilon' P'^2 + 2\varepsilon \varepsilon' Q P P') \quad , \\
C &= \frac{Q - \lambda P P'}{D} \quad , \quad h = \frac{P P'}{D} \quad , \quad f = \frac{P + \varepsilon' Q P'}{D} \quad , \quad g = \frac{P' + \varepsilon Q P}{D} \quad . \quad (6.81)
\end{aligned}$$

Note that Q , P and P' are the coefficients of the GCM kernels defined through Eq. (5.4), and are explicitly given by $Q = 1 - x/\mu$, $P = p/\sqrt{\mu}$ and $P' = q/\sqrt{\mu}$ with $\mu = A_1 A_2 / (A_1 + A_2)$, $x = 0 \sim \min\{A_1, A_2\}$ and $p, q = 0$ or ± 1 . Furthermore, ε and ε' are defined through $\varepsilon = (1 - \eta)/(1 + \eta)$ and $\varepsilon' = (1 - \eta')/(1 + \eta')$. The Coulomb and kinetic-energy matrix elements which correspond to the GCM kernels in Eq. (5.4c) are obtained from the central matrix elements in Eq. (6.80) by a slight modification with $D \rightarrow \tilde{D}$ and

$$C^L \rightarrow 2\sqrt{\frac{\nu}{\pi}} \sqrt{\frac{2}{2 + \tilde{\alpha}}} \sum_{r=0}^L \frac{(-1)^r}{2r+1} \binom{L}{r} (\hat{C})^{L-r} \left(\frac{\hat{f} \hat{g}}{2 + \tilde{\alpha}} \right)^r \quad \text{for } \textit{Coulomb} \quad , \quad (6.82a)$$

$$\rightarrow (\hat{C})^L \frac{2}{3} \left(L + \frac{3}{2} \right) \frac{1 - \varepsilon - \varepsilon' + \varepsilon \varepsilon' Q^2}{\tilde{D}} \quad \text{for } \textit{kinetic-energy} \quad , \quad (6.82b)$$

where \hat{C} , \hat{f} , \hat{g} and \tilde{D} and the coefficients C , f , g and D for $\lambda = 0$, respectively ; i.e.,

$$\hat{C} = \frac{Q}{\tilde{D}} \quad , \quad \hat{f} = \frac{P + \varepsilon' Q P'}{\tilde{D}} \quad , \quad \hat{g} = \frac{P' + \varepsilon Q P}{\tilde{D}} \quad . \quad (6.82c)$$

For the derivation of the Coulomb matrix elements, a simple integration formula

$$\int_0^1 dx (1 + \beta x^2)^{-(r+\frac{3}{2})} x^{2r} = \frac{1}{2r+1} (1 + \beta)^{-(r+\frac{1}{2})} \tag{6.83}$$

is employed.

6.3.2 3-Cluster Systems

In 3-cluster systems with $n=3$, the SU_{n-1} C-G coefficients in Eq. (6.72) are nothing but the angular-momentum C-G coefficients. The explicit correspondence is given by

$$\langle (\lambda\mu)\ell(\lambda'\mu')\ell' | (\lambda''\mu'')\ell'' \rangle_2 = \langle L \ell_1 - \ell_2 \ L' \ell'_1 - \ell'_2 | L'' \ell_1 - \ell_2 + \ell'_1 - \ell'_2 \rangle \tag{6.84a}$$

with

$$\begin{aligned} \lambda &= 2L \ , \quad \mu = \ell_1 + \ell_2 - L \ , \quad \ell_1 + \ell'_1 = \ell''_1 \ , \\ \lambda' &= 2L' \ , \quad \mu' = \ell'_1 + \ell'_2 - L' \ , \quad \ell_2 + \ell'_2 = \ell''_2 \ , \\ \lambda'' &= 2L'' \ , \quad \mu'' = \ell''_1 + \ell''_2 - L'' = \ell_1 + \ell_2 + \ell'_1 + \ell'_2 - L'' \ . \end{aligned} \tag{6.84b}$$

The function $F_{\ell,\ell'}^{(\lambda\mu)}(C)$ in Eq. (6.49a) is therefore very simple. It is given by

$$\begin{aligned} F_{\ell,\ell'}^{(\lambda\mu)}(C) &= \sum_{[k]} \left[\frac{(2k-1)!!}{(2k)!!} \right]^{\frac{1}{2}} \\ &\times \langle k_{11} + k_{12} \ k_{11} - k_{12} \ k_{21} + k_{22} \ k_{21} - k_{22} | L \ k_{11} - k_{12} + k_{21} - k_{22} \rangle C^k \ , \end{aligned} \tag{6.85}$$

where the summation over k_{ij} ($i, j = 1, 2$) is only for the non-negative integers which satisfy the weight condition (6.49b). By using this expression and $G_0^{(0 \ 2m)}(A)$ in Eq. (6.52a), we can explicitly write down the factors for the central matrix elements in Eq. (6.60) as follows :

$$\begin{aligned} I_{\ell_1\ell_2,\ell'_1\ell'_2}^L(C; A, A') &= \sum_{[k],m,m'} \left(-\frac{1}{2} \right)^{m+m'} \frac{1}{m!m'} \left[\frac{(2L+1)(2k-1)!!}{(|k|+L+1)! (|k|-L)! (2k)!!} \right]^{\frac{1}{2}} \\ &\times \langle k_{11} + k_{12} \ k_{11} - k_{12} \ k_{21} + k_{22} \ k_{21} - k_{22} | L \ k_{11} - k_{12} + k_{21} - k_{22} \rangle \\ &\times C^k (A_{12})^m (A'_{12})^{m'} \ , \end{aligned} \tag{6.86a}$$

where we have again used the shorthand notation $|k| = k_{11} + \dots + k_{22}$, $(2k)!! = (2k_{11})!! \dots (2k_{22})!!$, $C^k = C_{11}^{k_{11}} \dots C_{22}^{k_{22}}$ etc. The weight condition in Eq. (6.86a) is

$$\begin{aligned} k_{11} + k_{12} + m &= \ell_1 \ , \quad k_{11} + k_{21} + m' = \ell'_1 \ , \\ k_{21} + k_{22} + m &= \ell_2 \ , \quad k_{12} + k_{22} + m' = \ell'_2 \ . \end{aligned} \tag{6.86b}$$

The coefficients, C , A and A' , are given in Eq. (6.39b) with \widehat{C} , \widehat{A} and \widehat{A}' being those for the normalization kernel. The expressions in Eq. (6.37c) are further simplified for 3-cluster systems by using the cofactor matrix $\delta_O = |O|^t O^{-1}$. From here on, we use

the notation $|O|$ to denote the determinant of O ; $|O| = (\det O)$. For arbitrary 2×2 matrices, O, A, B etc., we can show a number of simple relationships such as

$$\begin{aligned} O + {}^t\delta_O &= (Tr O) e , & O {}^t\delta_O &= {}^t\delta_O O = |O| e , \\ |e - O| &= 1 - (Tr O) + |O| , \\ {}^tAB + {}^t\delta_B\delta_A &= (Tr {}^tAB) e = (Tr {}^t\delta_B\delta_A) e , \\ \delta_{e-{}^tAB} &= e - {}^t\delta_A\delta_B , & \delta_{AB} &= \delta_A\delta_B , \end{aligned} \quad (6.87)$$

where e is the 2×2 unit matrix. By using these, we can easily show

$$\begin{aligned} \tilde{D} &= 1 - Tr(\varepsilon' {}^tQ\varepsilon Q) + |\varepsilon||\varepsilon'| |Q|^2 = 1 - \sum_{i,j=1}^2 \varepsilon_i \varepsilon'_j Q_{ij}^2 + \varepsilon_1 \varepsilon_2 \varepsilon'_1 \varepsilon'_2 |Q|^2 , \\ \hat{C} &= \frac{\tilde{C}}{\tilde{D}} , & \hat{A} &= \frac{\tilde{A}}{\tilde{D}} , & \hat{A}' &= \frac{\tilde{A}'}{\tilde{D}} , \\ \tilde{C} &= Q - \delta_\varepsilon \delta_Q \delta_{\varepsilon'} |Q| = \begin{pmatrix} Q_{11} - \varepsilon_2 \varepsilon'_2 Q_{22} |Q| & Q_{12} + \varepsilon_2 \varepsilon'_1 Q_{21} |Q| \\ Q_{21} + \varepsilon_1 \varepsilon'_2 Q_{12} |Q| & Q_{22} - \varepsilon_1 \varepsilon'_1 Q_{11} |Q| \end{pmatrix} , \\ \tilde{A} &= Q\varepsilon' {}^tQ - \delta_\varepsilon |\varepsilon'| |Q|^2 , & \tilde{A}_{12} &= \varepsilon'_1 Q_{11} Q_{21} + \varepsilon'_2 Q_{12} Q_{22} , \\ \tilde{A}' &= {}^tQ\varepsilon Q - \delta_{\varepsilon'} |\varepsilon| |Q|^2 , & \tilde{A}'_{12} &= \varepsilon_1 Q_{11} Q_{12} + \varepsilon_2 Q_{21} Q_{22} . \end{aligned} \quad (6.88)$$

Here, we have newly defined the polynomial factors \tilde{C} , \tilde{A} and \tilde{A}' , which are useful for numerical calculations. The 2×2 matrix Q for particular nucleon exchange is given in Eq. (3.43) or Eq. (3.107) through an appropriate transformation for the selected Jacobi coordinates. On the other hand, the factors \hat{P} , \tilde{P} , \hat{P}' and \tilde{P}' for the interaction kernels are obtained through Eq. (6.37d) by assigning P_1, P_2, P'_1 and P'_2 to those in Table IV for each interaction type. (See Eq. (3.116).)

In order to derive the Coulomb matrix elements, we again employ the integral representation of the error function and the integration formula in Eq. (6.83). They are given by a simple modification of the norm-kernel matrix elements through Eqs. (6.70a) and (6.86a). Namely, in $I_{\ell_1 \ell_2, \ell'_1 \ell'_2}^L(\hat{C}; \hat{A}, \hat{A}')$, we should modify

$$\begin{aligned} \hat{C}^k \left(\hat{A}_{12} \right)^m \left(\hat{A}'_{12} \right)^{m'} &\rightarrow 2\sqrt{\frac{\nu}{\pi}} \sqrt{\frac{2}{2+\tilde{\alpha}}} \sum_{r_{11}=0}^{k_{11}} \cdots \sum_{r_{22}=0}^{k_{22}} \sum_{s=0}^m \sum_{s'=0}^{m'} \frac{(-1)^{|r|+s+s'}}{2(|r|+s+s'+1)} \\ &\times \binom{k_{11}}{r_{11}} \cdots \binom{k_{22}}{r_{22}} \binom{m}{s} \binom{m'}{s'} \left(\hat{C}_{11} \right)^{k_{11}-r_{11}} \cdots \left(\hat{C}_{22} \right)^{k_{22}-r_{22}} \left(\hat{A}_{12} \right)^{m-s} \left(\hat{A}'_{12} \right)^{m'-s'} \\ &\times \left(\frac{\hat{f}_1}{\sqrt{2+\tilde{\alpha}}} \right)^{r_{11}+r_{12}+s} \left(\frac{\hat{f}_2}{\sqrt{2+\tilde{\alpha}}} \right)^{r_{21}+r_{22}+s} \left(\frac{\hat{g}_1}{\sqrt{2+\tilde{\alpha}}} \right)^{r_{11}+r_{21}+s'} \left(\frac{\hat{g}_2}{\sqrt{2+\tilde{\alpha}}} \right)^{r_{12}+r_{22}+s'} , \end{aligned} \quad (6.89)$$

where $|r| = r_{11} + \cdots + r_{22}$. For the derivation of the kinetic-energy matrix elements, we need some algebra of transforming the coefficient matrices with the aid of the formulae in Eq. (6.87). The final result is given by modifying Eq. (6.86a) as

$$\widehat{C}^k \left(\widehat{A}_{12} \right)^m \left(\widehat{A}'_{12} \right)^{m'} \rightarrow \widetilde{C}^k \left(\widehat{A}_{12} \right)^m \left(\widehat{A}'_{12} \right)^{m'} \\ \times \frac{2}{3} \left\{ \frac{3 + |\ell| + |\ell'|}{2} \frac{\widetilde{X}}{\widetilde{D}} + \sum_{i,j=1}^2 k_{ij} \left(1 - \frac{\widetilde{Z}_{ij}}{\widetilde{C}_{ij}} \right) - m \frac{\widetilde{Y}_{12}}{\widetilde{A}_{12}} - m' \frac{\widetilde{Y}'_{12}}{\widetilde{A}'_{12}} \right\}, \quad (6.90a)$$

where $|\ell| = \ell_1 + \ell_2$ etc. and the new coefficients, \widetilde{X} , \widetilde{Z} , \widetilde{Y} and \widetilde{Y}' , are given through²⁹

$$\begin{aligned} \widetilde{X} &= 2 - Tr(\varepsilon + \varepsilon') + |\varepsilon'| Tr({}^t Q \varepsilon Q) + |\varepsilon| Tr(Q \varepsilon' {}^t Q) - 2|\varepsilon| |\varepsilon'| |Q|^2 \\ &= 2 - \varepsilon_1 - \varepsilon_2 - \varepsilon'_1 - \varepsilon'_2 + (\varepsilon_2 + \varepsilon'_2) \varepsilon_1 \varepsilon'_1 Q_{11}^2 + (\varepsilon_2 + \varepsilon'_1) \varepsilon_1 \varepsilon'_2 Q_{12}^2 \\ &\quad + (\varepsilon_1 + \varepsilon'_2) \varepsilon_2 \varepsilon'_1 Q_{21}^2 + (\varepsilon_1 + \varepsilon'_1) \varepsilon_2 \varepsilon'_2 Q_{22}^2 - 2\varepsilon_1 \varepsilon_2 \varepsilon'_1 \varepsilon'_2 |Q|^2, \\ \widetilde{Z} &= 2Q - \delta_\varepsilon Q - Q \delta_{\varepsilon'} = \begin{pmatrix} (2 - \varepsilon_2 - \varepsilon'_2) Q_{11} & (2 - \varepsilon_2 - \varepsilon'_1) Q_{12} \\ (2 - \varepsilon_1 - \varepsilon'_2) Q_{21} & (2 - \varepsilon_1 - \varepsilon'_1) Q_{22} \end{pmatrix}, \\ \widetilde{Y} &= e - \delta_\varepsilon Tr(Q \varepsilon' {}^t Q) + 2\delta_\varepsilon |\varepsilon'| |Q|^2 - |\varepsilon'| Q {}^t Q, \\ \widetilde{Y}_{12} &= -\varepsilon'_1 \varepsilon'_2 (Q_{11} Q_{21} + Q_{12} Q_{22}), \\ \widetilde{Y}' &= e - \delta_{\varepsilon'} Tr({}^t Q \varepsilon Q) + 2\delta_{\varepsilon'} |\varepsilon| |Q|^2 - |\varepsilon| {}^t Q Q, \\ \widetilde{Y}'_{12} &= -\varepsilon_1 \varepsilon_2 (Q_{11} Q_{12} + Q_{21} Q_{22}). \end{aligned} \quad (6.90b)$$

Finally, we show the factors for *LS* and tensor matrix elements in Eqs. (6.70d) and (6.70e) with respect to the 3-cluster systems. These are given by

$$\begin{aligned} &I_{\ell_1 \ell_2 L; \ell'_1 \ell'_2 L'}^{(LS)}(C; A, A'; \widehat{P}, \widetilde{P}, \widehat{P}', \widetilde{P}') \\ &= (-1)^{L'+1} \frac{1}{2\sqrt{2}} \widehat{L} I_{\ell'_1-1, \ell_2-1; \ell'_1, \ell'_2}^{L'}(C; A, A') \langle L' \ell'_1 - \ell_2 \ 10 | L \ell_1 - \ell_2 \rangle \left(\widehat{P}_1 \widetilde{P}'_2 - \widetilde{P}_2 \widehat{P}'_1 \right) \\ &+ (-1)^L \frac{1}{2\sqrt{2}} \widetilde{L} I_{\ell_1, \ell_2; \ell'_1-1, \ell'_2-1}^{L'}(C; A, A') \langle L \ell'_1 - \ell'_2 \ 10 | L' \ell'_1 - \ell'_2 \rangle \left(\widetilde{P}_1 \widehat{P}'_2 - \widehat{P}_2 \widetilde{P}'_1 \right) \\ &+ \sum_{\widetilde{L}} (-1)^{\widetilde{L}} \frac{\widehat{L} \widetilde{L}'}{2\widetilde{L}} U(L' \ 1 \ L \ 1; \widetilde{L} \ 1) \sum_{\ell_s=0}^1 \sum_{\ell'_s=0}^1 I_{\ell_1-\ell_s, \ell_2+\ell_s-1; \ell'_1-\ell'_s, \ell'_2+\ell'_s-1}^{\widetilde{L}}(C; A, A') \\ &\quad \times \langle \widetilde{L} \ell_1 - \ell_2 - 2\ell_s + 1 \ 1 \ 2\ell_s - 1 | L \ell_1 - \ell_2 \rangle \langle \widetilde{L} \ell'_1 - \ell'_2 - 2\ell'_s + 1 \ 1 \ 2\ell'_s - 1 | L' \ell'_1 - \ell'_2 \rangle \\ &\quad \times \left(\widehat{P}_{2-\ell_s} \widehat{P}'_{2-\ell'_s} - \widetilde{P}'_{2-\ell_s} \widetilde{P}_{2-\ell'_s} \right), \end{aligned} \quad (6.91a)$$

$$\begin{aligned} &I_{\ell_1 \ell_2 L; \ell'_1 \ell'_2 L'}^{(T)}(C; A, A'; \widehat{f}, \widehat{g}) \\ &= (-1)^{L'} \widehat{L} \sum_{\ell_s=0}^2 I_{\ell_1-\ell_s, \ell_2+\ell_s-2; \ell'_1, \ell'_2}^{L'}(C; A, A') \end{aligned}$$

²⁹Note that \widetilde{A}_{12} , \widetilde{A}'_{12} , \widetilde{Y}_{12} and \widetilde{Y}'_{12} in [51] are defined with an opposite sign to the one adopted here. Furthermore, the difference of \widetilde{X} is due to the trivial factor $(n-1)$ in Eq. (5.4c), which means that we have included all the relative kinetic-energy contributions between clusters in the present formula.

$$\begin{aligned}
 & \times \frac{1}{2} \left(\frac{3}{2}\right)^{\frac{1}{2}|\ell_s-1|} \langle L' \ell_1 - \ell_2 - 2(\ell_s - 1) \ 2 \ 2(\ell_s - 1) | L \ell_1 - \ell_2 \rangle (\widehat{f}_1)^{\ell_s} (\widehat{f}_2)^{2-\ell_s} \\
 & + (-1)^L \widehat{L}' \sum_{\ell'_s=0}^2 I_{\ell_1, \ell_2; \ell'_1-\ell'_s, \ell'_2+\ell'_s-2}^L(C; A, A') \\
 & \times \frac{1}{2} \left(\frac{3}{2}\right)^{\frac{1}{2}|\ell'_s-1|} \langle L' \ell'_1 - \ell'_2 - 2(\ell'_s - 1) \ 2 \ 2(\ell'_s - 1) | L' \ell'_1 - \ell'_2 \rangle (\widehat{g}_1)^{\ell'_s} (\widehat{g}_2)^{2-\ell'_s} \\
 & + \sum_{\widetilde{L}} (-1)^{\widetilde{L}} \sqrt{\frac{3}{2}} \left(\frac{\widehat{L}\widehat{L}'}{\widetilde{L}}\right) U(L' \ 1 \ L \ 1; \widetilde{L} \ 2) \sum_{\ell_s=0}^1 \sum_{\ell'_s=0}^1 I_{\ell_1-\ell_s, \ell_2+\ell_s-1; \ell'_1-\ell'_s, \ell'_2+\ell'_s-1}^{\widetilde{L}}(C; A, A') \\
 & \times \langle \widetilde{L} \ell_1 - \ell_2 - 2\ell_s + 1 \ 1 \ 2\ell_s - 1 | L \ell_1 - \ell_2 \rangle \langle \widetilde{L} \ell'_1 - \ell'_2 - 2\ell'_s + 1 \ 1 \ 2\ell'_s - 1 | L' \ell'_1 - \ell'_2 \rangle \\
 & \times \widehat{f}_{2-\ell_s} \widehat{g}_{2-\ell'_s} . \tag{6.91b}
 \end{aligned}$$

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