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SYMPLECTIC AND CLUSTER EXCITATIONS IN NUCLEI: Evaluation of interaction matrix elements

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Abstract: A practical method is given for the evaluation of the matrix elements of a general two-body interaction in a mixed Sp(6, R) ⊃ U(3)-microscopic cluster model basis. A reduction formula expresses a matrix element connecting states of excitation $N\hbar\omega$ and $N'\hbar\omega$ in the same or in different symplectic bands in terms of matrix elements of unit SU(3) tensor operators between Sp(6, R) bandhead states. It also reduces the matrix element between a state of $N\hbar\omega$ excitation in a Sp(6, R) band and a general binary cluster model state to a simpler matrix element of pure cluster model type, so that all matrix elements have been reduced to pure shell or cluster model form. As a test of the new methods of calculation a comparison is made between the pure α-cluster model, the pure symplectic model and a calculation using a mixed α-cluster-symplectic basis for a very simple system, the ^{8}Be nucleus.

1. Introduction

In the past few years the symplectic group Sp(6, R) has emerged, through the pioneering contributions of Rosensteel and Rowe [1,2]), as the appropriate dynamical group for a many-body theory of nuclear collective motion. Since Sp(6, R) is also the dynamical group of the three-dimensional harmonic oscillator, with the Elliott SU(3) group as a natural subgroup, it has successfully incorporated core excitations into the shell model foundation of the nuclear collective model and has thus led to the possibility of detailed, fully microscopic calculations of nuclear collective phenomena [3,4]). Although the ultimate aim is a microscopic theory of heavy deformed nuclei the most detailed applications to date, [ref. [2])], have involved nuclei in the $A = 8-28$ mass range and mainly nuclei which have also been subjected to detailed study in terms of the microscopic nuclear cluster model [5]). The relationship between symplectic and cluster model wave functions was studied in ref. [6]) and has recently been extended in ref. [7]) to states of arbitrary excitation through a simple recursion formula. Although there are large overlaps between the lowest symplectic excitations

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and the corresponding cluster model states with the same SU(3) quantum numbers [6,7]), the cluster model and the symplectic model give complementary descriptions of core excitations in such nuclei. The cluster model generally underestimates E2 transition rates [7]) and overestimates α-widths. It also fails to predict certain observed core excited states which fall naturally into the framework of the symplectic model. The symplectic model, on the other hand, stresses quadrupole collectivity and may not fully develop the cluster correlations needed to account for observed α-widths. Both the microscopic cluster model and Sp(6, R) symmetry give us a means of selecting very specific physically relevant core excited states from the huge space of possible shell model excitations. To account both for the observed quadrupole collectivity and the required cluster correlations, a unified treatment including both cluster and symplectic excitations may give the most detailed description to date of the structure of light nuclei [7]).

The technology of the microscopic cluster model has been refined into a useful calculational tool, [see refs. [5,8]) for many earlier references]. Very recently also the mathematics of the group Sp($2d$, R) has been fully developed through the use of extended coherent state theory employing boson realizations of the symplectic algebras [9-14]). These methods have led to very useful explicit constructions for the needed discrete infinite-dimensional unitary-irreducible representations of Sp($2d$, R). For the Sp(6, R) representations of actual interest in nuclei it has also been shown that very simple and highly accurate approximation formulae [9,15,16]) can be used to advantage in the construction of Sp(6, R) basis states and should thus greatly facilitate calculations within the framework of the nuclear collective model. Despite these powerful mathematical advances the applications to nuclear spectroscopy have up to now been somewhat limited. Most of the applications to nuclear collective phenomena have employed model hamiltonians constructed from the Sp(6, R) generators themselves. Calculations have usually been restricted to a model space of a single Sp(6, R) irreducible representation or symplectic band [17]), and those calculations which have attempted some band mixing [18]) have not included all types of interband matrix elements. For a truly microscopic theory of deformed nuclei a model space spanning several symplectic bands may be required; and a detailed description of light nuclei may be improved by a treatment permitting the coupling of symplectic excitations to other degrees of freedom such as those emodied in the states of the nuclear cluster model.

In such applications a practical method is needed for the calculation of interaction matrix elements coupling a symplectic excitation in a particular Sp(6, R) irreducible representation to (1) a specific shell model state, or (2) a cluster model state, or (3) a symplectic excitation in the same or in a different Sp(6, R) band. Moreover, for a truly microscopic calculation of nuclear collective phenomena within the framework of Sp(6, R) symmetry such a tractable method of calculation must be able to accommodate the realistic effective interactions of the type used in conventional shell model or cluster model calculations. One method for achieving this goal

has been developed by Reske [19]) in his study of the giant E2 resonance in ^{24}Mg. In this method commutator and SU(3) recoupling techniques are used to reduce the matrix element of a two-body operator connecting excitations in the same or in different symplectic bands to symplectic bandhead (Sp(6, R) lowest weight state) matrix elements of simple shell model type. The method uses a recursive step-down procedure which leads to a family of nested coupled commutator operators. Although these can be reduced to one basic generic term the method involves a chain calculation and is somewhat computer intensive. Moreover, it does not yet take advantage of the recent theoretical advances in the construction of Sp(6, R) irreducible representation basis states.

It is the purpose of the present investigation to develop a simpler method of calculation of matrix elements of a general two-body operator in a Sp(6, R) basis. The combination of the new methods of constructing Sp(6, R) basis states [9-16]) with standard SU(3) recoupling techniques leads to a general formula which again reduces matrix elements connecting excitations in the same or in different symplectic bands to the corresponding symplectic bandhead (Sp(6, R) lowest weight) matrix elements and thus reduces the problem to a calculation of matrix elements of standard shell model type. The reduction formula is applicable to spin-orbit and tensor as well as to simple central interactions. The ingredients are SU(3) recoupling coefficients [20,21]) and some simple expansion coefficients common to all Sp(6, R) irreducible representations. These are tabulated in appendix A for symplectic excitations as high as $10\hbar\omega$. A very slight modification leads to a similar formula which reduces the two-body interaction matrix element between a Sp(6, R) basis state of arbitrary excitation and a general cluster model state to a matrix element connecting the general cluster model state to the symplectic bandhead state. The latter can in general be expressed in terms of a simple cluster model wave function. The general interaction matrix element is thus reduced to one which can readily be calculated by standard microscopic cluster model techniques. It is this version of the reduction formula which leads to a first application, a comparison of a pure α-cluster model calculation, a pure symplectic model calculation, and a calculation in a mixed α-cluster symplectic basis for a very simple system, the ^{8}Be nucleus.

To establish the notation, sect. 2 gives a very brief review of the new methods of constructing Sp(6, R) basis states. Sect. 3 then gives the derivation of the matrix element formula for a general translationally invariant two-body interaction between different symplectic excitations. As in ref. [19]), the present method requires an expansion of the interaction in terms of SU(3) irreducible tensor operators, and results are given for arbitrary two-body SU(3) unit tensor operators. Sect. 4 exhibits the modification of the reduction formula which gives the cluster model-symplectic excitation interaction matrix elements. Since these results are expressed in terms of matrix elements of two-body SU(3) unit tensor operators, matrix elements between two cluster states are also expressed in terms of the matrix elements of such operators, and sect. 5 shows how such matrix elements are derived by standard cluster model

techniques. It also gives some numerical results for a few simple cluster systems for the starting matrix elements needed for the evaluation of the cluster-symplectic interaction matrix elements of sect. 4. Sect. 6 gives the application to a very simple system, the ^{8}Be nucleus. This is the system in which the physical relevance of symplectic symmetry was first recognized by Arickx [22]). It has continued to serve as a proving ground for symplectic model techniques [23]). It is also one of the simplest and oldest systems [24]) studied by the microscopic cluster model. Our aim here is to establish the method of calculation. The results show the close parallel between the α-cluster model and symplectic symmetry. Since ^{8}Be *is* two α particles the calculation for the mixed α-cluster symplectic basis cannot be expected to make major changes in the pure α-cluster calculation. However, in the extension to heavier nuclei, the complementary character of symplectic and cluster model excitations can be expected to play a prominent role. Such applications form the basis of a future study, as indicated in a brief concluding section.

2. Construction of Sp(6, R) basis states

The states of a symplectic band in an Sp(6, R) $\supset$ U(3) basis are labeled by three types of U(3), or SU(3), quantum numbers: Γ_σ the symplectic bandhead or Sp(6, R) lowest weight U(3) symmetry, which labels the Sp(6, R) irreducible representation, Γ_n the U(3) symmetry of a raising polynomial, and Γ_ω the U(3) symmetry of the excited state in the symplectic band. It will be convenient to use the general shorthand label, Γ, for a U(3), or SU(3), representation label, and α for any convenient set of U(3) subgroup labels. Otherwise the notation will follow that of refs. [9,15]). Thus

$$\begin{aligned}
&\Gamma_n \equiv [n_1 n_2 n_3] \equiv (\lambda_n \mu_n) N \equiv (n_1 - n_2,\, n_2 - n_3) N = n_1 + n_2 + n_3 \,, \\
&\Gamma_\sigma \equiv [\sigma_1 \sigma_2 \sigma_3] \equiv (\lambda_\sigma \mu_\sigma) N_\sigma \equiv (\sigma_1 - \sigma_2,\, \sigma_2 - \sigma_3) N_\sigma = \sigma_1 + \sigma_2 + \sigma_3 \,, \\
&\Gamma_\omega \equiv [\omega_1 \omega_2 \omega_3] \equiv (\lambda_\omega \mu_\omega) N_\omega \equiv (\omega_1 - \omega_2,\, \omega_2 - \omega_3) N_\omega = \omega_1 + \omega_2 + \omega_3 \,. \qquad (1)
\end{aligned}$$

Here, the N's give the total number of squares in the U(3) Young tableaux, and $(\lambda\mu)$ are Elliott SU(3) labels [20,21]). The familiar realization of the Sp(6, R) algebra is given by the raising generators, $\boldsymbol{A}^\dagger$, of SU(3) symmetry (20), the hermitian conjugate lowering operators, $\boldsymbol{A}$, and the U(3) generators, C. These can be expressed in terms of oscillator creation and annihilation operators $b^\dagger_{si}$ and b_{si} with $A^\dagger_{ij} = \sum_s b^\dagger_{si} b^\dagger_{sj}$, $A_{ij} = \sum_s b_{si} b_{sj}$, and $C_{ij} = \frac{1}{2} \sum_s (b^\dagger_{si} b_{sj} + b_{sj} b^\dagger_{si})$ where $i, j = x, y, z$. The s-variables stand for a convenient set of Jacobi relative motion variables, with $s = 1, \ldots, A-1$; A = nucleon number. The Sp(6, R) state construction proceeds via the states

$$\begin{aligned}
|\Psi(\Gamma_\sigma \Gamma \rho \Gamma_\omega \alpha_\omega)\rangle &= [\boldsymbol{P}^{\Gamma_n}(\boldsymbol{A}^\dagger) \times |\Gamma_\sigma\rangle]^{\Gamma_\omega \rho}_{\alpha_\omega} \\
&= \sum_{\alpha_n \alpha_\sigma} \langle \Gamma_n \alpha_n \Gamma_\sigma \alpha_\sigma | \Gamma_\omega \alpha_\omega \rangle_\rho \boldsymbol{P}^{\Gamma_n}_{\alpha_n}(\boldsymbol{A}^\dagger) | \Gamma_\sigma \alpha_\sigma \rangle \,, \qquad (2)
\end{aligned}$$

where the square bracket denotes SU(3) coupling, and the multiplicity quantum number ρ which distinguishes multiple occurrence of Γ_ω in the SU(3) coupling $[\Gamma_n \times \Gamma_\sigma]$ is indicated by a subscript on the SU(3) Wigner coefficient. (The choice of ρ and the notations and phase conventions for SU(3) Wigner and recoupling coefficients follow those of refs. [20,21])). The raising polynomials are given by the parentage expansions

$$\boldsymbol{P}^{\Gamma_n}_{\alpha_n}(\boldsymbol{A}^\dagger) = \sum_{\Gamma_{n-2}} x^{\Gamma_n}(\Gamma_{n-2})[\boldsymbol{A}^{\dagger(20)} \times \boldsymbol{P}^{\Gamma_{n-2}}(\boldsymbol{A}^\dagger)]^{\Gamma_n}_{\alpha_n}, \tag{3}$$

with

$$x^{\Gamma_n}(\Gamma_{n'}) = \frac{1}{N}(n_1 n_2 n_3 \| \boldsymbol{a}^\dagger \| n_1' n_2' n_3'), \tag{4}$$

which follows from the bosonic character of the totally symmetric raising polynomials

$$[\boldsymbol{A}^{\dagger(20)} \times \boldsymbol{P}^{\Gamma_{n-2}}(\boldsymbol{A}^\dagger)]^{\Gamma_n}_{\alpha_n} = \boldsymbol{P}^{\Gamma_n}_{\alpha_n}(\boldsymbol{A}^\dagger)(\Gamma_n \| \boldsymbol{a}^\dagger \| \Gamma_{n-2}), \tag{5}$$

where the SU(3) reduced matrix elements of the six-dimensional boson operators, $\boldsymbol{a}^\dagger$, are given, e.g. by eq. (2.25) of ref. [9]) or eq. (12) of ref. [15]) and have the property $\sum_{n'}(\Gamma_n \| \boldsymbol{a}^\dagger \| \Gamma_{n'})^2 = N = n_1 + n_2 + n_3$. Since the labels Γ_n, ρ cannot be associated directly with the eigenvalues of a set of hermitian operators, the states $|\Psi(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega)\rangle$ form a non-orthonormal set. Their overlap matrix is the κ^2 matrix

$$\langle \Psi(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega) | \Psi(\Gamma_\sigma \Gamma_{n'} \rho' \Gamma_\omega \alpha_\omega)\rangle = (\kappa^2(\Gamma_\sigma, \Gamma_\omega))_{n\rho, n'\rho'}, \tag{6}$$

which is central to the Sp(6, R) state construction, where κ^2 is diagonal in Γ_σ and Γ_ω and independent of U(3) subgroup labels α_ω, with rows and columns labeled by Γ_n and ρ (or $n\rho$ for short). Very recently it has been shown that the matrix κ^2 can be evaluated from a generating kernel for which a closed analytic expression can be given [13,14]). To obtain the required κ^2 matrix elements this kernel must still be expanded in the appropriate SU(3)-coupled basis polynomials of an associated Bargmann space of complex variables. Alternately, the κ^2 matrix elements can be evaluated through a set of recursion relations [9,15]). It may also be useful to define normalized states, (denoted by a $\bar{\Psi}$),

$$|\bar{\Psi}(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega)\rangle = \mathcal{N}_{\sigma n \rho \omega} |\Psi(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega)\rangle, \tag{7}$$

where the normalization constants $\mathcal{N}_{\sigma n \rho \omega}$ are given by $[(\kappa^2)_{n\rho, n\rho}]^{-1/2}$. The overlap matrices of the $\bar{\Psi}$ states then have (by definition) diagonal matrix elements of unity. Their off-diagonal matrix elements are of order $(1/\bar{\sigma})$, a convenient parameter of smallness [9]) for the nuclear applications. Here $\bar{\sigma} = \frac{2}{3}[\lambda_\sigma + 2\mu_\sigma + 3(\sigma_3 + \frac{1}{2}(A-1))]$; (cf. eq. (1)). Although small, (e.g. of order 0.03 in ^{20}Ne), these off-diagonal matrix elements are by no means negligible.

Since, by definition, κ^2 is hermitian and non-negative, the hermitian square root matrix κ is always well-defined and can be used [9-11]) to transform the states (2)

from a mere labelling scheme into an orthonormal basis for a unitary irreducible representation of Sp(6, R) by means of

$$|\Psi(\Gamma_\sigma \Gamma_{n_i} \rho_i \Gamma_\omega \alpha_\omega)\rangle = \sum_{n_j \rho_j} (\kappa(\Gamma_\sigma, \Gamma_\omega))_{n_i \rho_i, n_j \rho_j} |\Gamma_\sigma \Gamma_{n_j} \rho_j \Gamma_\omega \alpha_\omega\rangle \,. \tag{8a}$$

Here, $|\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega\rangle$, without the symbol Ψ, denotes the orthonormal basis states. Due to the smallness of the off-diagonal matrix elements of κ^2 the orthonormal basis states can also be tagged by the labels $\Gamma_{n_j} \rho_j$ which correspond to the dominant values of $\Gamma_n \rho$ in these states.

The diagonalization of the κ^2 matrices enables us to get the needed matrix elements of κ. The matrix elements of κ can also be evaluated directly by an approximation formula [16]), valid for small values of $(1/\bar{\sigma})$. The orthonormal states $|\Gamma_\sigma \Gamma_n \rho_\omega \alpha_\omega\rangle$ can thus be constructed explicitly in terms of polynomials in the raising generators acting on the symplectic bandhead states. Combining the inverse of eq. (8) with eq. (5) after an SU(3) recoupling transformation, the SU(3) reduced matrix element of the raising generator $\boldsymbol{A}^\dagger$ is given by

$$\begin{aligned}
&\langle \Gamma_\sigma \Gamma_{n'} \rho' \Gamma_{\omega'} \| \boldsymbol{A}^{\dagger(20)} \| \Gamma_\sigma \Gamma_n \rho \Gamma_\omega \rangle \\
&\quad = \sum_{\alpha_\omega \alpha_2} \langle \Gamma_\omega \alpha_\omega (20) \alpha_2 | \Gamma_{\omega'} \alpha_{\omega'} \rangle \langle \Gamma_\sigma \Gamma_{n'} \rho' \Gamma_{\omega'} \alpha_{\omega'} | A^{\dagger(20)}_{\alpha_2} | \Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega \rangle \\
&\quad = (-1)^{\Gamma_\omega - \Gamma_{\omega'}} \sum_{n_2 \rho_2} \sum_{n_1 \rho_1} (\kappa(\Gamma_\sigma, \Gamma_{\omega'}))_{n_2 \rho_2, n' \rho'} (\Gamma_{n_2} \| \boldsymbol{a}^\dagger \| \Gamma_{n_1}) \\
&\qquad \times U((20) \Gamma_{n_1} \Gamma_{\omega'} \Gamma_\sigma; \Gamma_{n_2} - \rho_2; \Gamma_\omega \rho_1 -) (\kappa^{-1}(\Gamma_\sigma, \Gamma_\omega))_{n\rho, n_1 \rho_1} \,.
\end{aligned} \tag{9}$$

The phase factor $(-1)^\Gamma$ is an abbreviation to be used throughout:

$$(-1)^\Gamma = (-1)^{\lambda + \mu} \,. \tag{10}$$

For the states of actual interest in the nuclear physics applications, with small values of $(1/\bar{\sigma})$, these reduced matrix elements are also given by an approximation formula [9,15])

$$\begin{aligned}
&\langle \Gamma_\sigma \Gamma_{n'} \rho' \Gamma_{\omega'} \| \boldsymbol{A}^{\dagger(20)} \| \Gamma_\sigma \Gamma_n \rho \Gamma_\omega \rangle \\
&\quad \simeq (-1)^{\Gamma_\omega - \Gamma_{\omega'}} [\Omega(\sigma n' \omega') - \Omega(\sigma n \omega)]^{1/2} (\Gamma_{n'} \| a^\dagger \| \Gamma_n) \\
&\qquad \times U((20) \Gamma_n \Gamma_{\omega'} \Gamma_\sigma; \Gamma_{n'} - \rho'; \Gamma_\omega \rho_-) \,.
\end{aligned} \tag{11}$$

The $\Omega(\sigma n \omega)$ are eigenvalues of a U(3)-scalar operator given, e.g., by eq. (2.16) of ref. [9]). The differences of eigenvalues have been put into convenient form in eq. (10b) of ref. [16]). For simple states for which Γ_n and ρ are uniquely determined by Γ_σ, Γ_ω, so that the κ matrix is 1-dimensional, eq. (11) is exact. This is a common case for many of the lower excitations in the symplectic band. In the general case eq. (11) has been shown to be of a high degree of accuracy [9,15]).

In the very special case when one of the eigenvalues of κ^2 is zero, the κ^2 method automatically reveals that there is a problem of overcompleteness. In this case the orthonormal states can best be defined through

$$|\Gamma_\sigma \Gamma_{n_i} \rho_i \Gamma_\omega \alpha_\omega\rangle = \sum_j \lambda_i^{-1/2} U_{ij} |\Psi(\Gamma_\sigma \Gamma_{n_j} \rho_j \Gamma_\omega \alpha_\omega)\rangle \,, \tag{8b}$$

where the λ_i are the nonzero eigenvalues of κ^2 and U is the matrix which diagonalizes κ^2, $\lambda = U\kappa^2 U^\dagger$. In the general case, with all $\lambda_i > 0$, transformation (8b) can be followed with a further unitary transformation, $U^\dagger$, leading to the hermitian transformation matrix, $\kappa^{-1} = U^\dagger \lambda^{-1/2} U$ used in refs. [9-11]). Either the choice $\kappa = U^\dagger \lambda^{1/2}$ with $\kappa^{-1} = \lambda^{-1/2} U$; or alternately $\kappa = U^\dagger \lambda^{1/2} U$ with $\kappa^{-1} = U^\dagger \lambda^{-1/2} U$ could be made. The first accommodates the very special case with zero eigenvalues more readily. However, since this very special case does not occur for nuclei with $A > 6$, as shown by Rowe, Wybourne, and Butler [31]) we shall adhere to the second.

3. Interaction matrix elements between symplectic states

For a general translationally invariant two-body operator of the type used in shell model or cluster model calculations

$$V = \sum_{i<j} V_{ij}, \tag{12a}$$

with

$$V_{12} = V(\boldsymbol{r}_1 - \boldsymbol{r}_2, \boldsymbol{p}_1 - \boldsymbol{p}_2; \boldsymbol{\sigma}_1, \tau_1, \boldsymbol{\sigma}_2, \tau_2), \tag{12b}$$

a matrix element between totally antisymmetric A-particle states follows from the matrix element for a particular V_{ij}, e.g. V_{12}. To apply SU(3) recoupling techniques it will be necessary to expand V_{12} in terms of SU(3) irreducible tensor operators, $V^{\Gamma_0}_{\alpha_0}$, with SU(3)-reduced (double-barred) matrix elements given by, (see also eq. (9)),

$$\langle \Gamma'\alpha' | V^{\Gamma_0}_{\alpha_0} | \Gamma\alpha \rangle = \sum_{\rho_0} \langle \Gamma' \| V^{\Gamma_0} \| \Gamma \rangle_{\rho_0} \langle \Gamma\alpha\Gamma_0\alpha_0 | \Gamma'\alpha' \rangle_{\rho_0}. \tag{13}$$

The operator $V^{\Gamma_0}_{\alpha_0}$ can be defined in terms of the full set of its reduced matrix elements in the oscillator basis of its own (dimensionless) variable

$$\boldsymbol{r} = \left(\frac{m\omega}{2\hbar}\right)^{1/2} (\boldsymbol{r}_1 - \boldsymbol{r}_2) \equiv \boldsymbol{x}_{s=1}. \tag{14}$$

For a gaussian interaction, e.g., with

$$V_{12} = V_0(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \tau_1, \tau_2) \exp(-\beta r^2), \tag{15}$$

the tensor decomposition is given by [25])

$$\begin{aligned}
&\langle (q'0) \| V^{(\lambda_0\mu_0)} \| (q0) \rangle \\
&\quad = V_0 \frac{(-1)^{\min(\lambda_0/2, \mu_0/2)} (-1)^{(q'-q)/2} (\frac{1}{2}\beta)^{(\lambda_0+\mu_0)/2}}{2(1+\beta)^{(q'+q+3)/2}} \left[\frac{\dim(\lambda_0\mu_0)}{\dim(q'0)}\right]^{1/2} \\
&\qquad \times [(\lambda_0+\mu_0+2)(q-\mu_0)!(\lambda_0+q+2)!]^{1/2} \\
&\qquad \times \sum_{m=0}^{[(q-\mu_0)/2]} \left(\frac{\beta}{2}\right)^{2m} \frac{1}{m!(q-\mu_0-2m)![\frac{1}{2}(\lambda_0+\mu_0+2)+m]!}.
\end{aligned} \tag{16}$$

The formula is reproduced here to illustrate its simplicity, but also because the last factor, written correctly here as $[\frac{1}{2}(\lambda_0+\mu_0+2)+m]$, contains a typographic error in ref. [25]); (compare eqs. (40) and (41) or ref. [25]); note also that the SU(3)-reduced matrix element is defined through a slightly different convention in ref. [25]), leading to the additional ratio of SU(3) dimension factors $[\dim(\lambda_0\mu_0)/\dim(q'0)]^{1/2}$ in eq. (16).)

For the practical applications in a basis of several symplectic bands, SU(3)-reduced matrix elements of the operators $V^{\Gamma_0}_{\alpha_0^0}$ are needed. Between the orthonormal basis states of the type $|\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\alpha_\omega\rangle$, defined through eq. (8), such a reduced matrix element can be expressed by

$$\begin{aligned}\langle\Gamma_{\sigma'}\Gamma_{n'}\rho'\Gamma_{\omega'}\|V^{\Gamma_0}\|\Gamma_\sigma\Gamma_{n_1}\rho_1\Gamma_\omega\rangle_{\rho_0}&\\ =\sum_{n\rho}(\kappa^{-1}(\Gamma_\sigma,\Gamma_\omega))_{n_1\rho_1,n\rho}&\sum_{\alpha_\omega\alpha_0}\langle\Gamma_\omega\alpha_\omega\Gamma_0\alpha_0|\Gamma_{\omega'}\alpha_{\omega'}\rangle_{\rho_0}\\ \times\langle\Gamma_{\sigma'}\Gamma_{n'}\rho'\Gamma_{\omega'}\alpha_{\omega'}|V^{\Gamma_0}_{\alpha_0^0}&[\boldsymbol{P}^{\Gamma_n}(\boldsymbol{A}^\dagger)\times|\Gamma_\sigma\rangle]^{\Gamma_\omega\rho}_{\alpha_\omega}\,.\end{aligned}\tag{17}$$

Since $V^{\Gamma_0}_{\alpha_0^0}$ is a function only of $\boldsymbol{r}=\boldsymbol{x}_{s=1}$, the first of a set of $A-1$ Jacobi variables, (cf. eq. (14)), it is useful to separate the sum over s in the defining relation for $\boldsymbol{A}^\dagger$ into two parts and rewrite

$$\begin{aligned}A^\dagger_{\alpha_{ij}}&=\sqrt{2}\,P^{(20)}_{\alpha_{ij}}(\boldsymbol{b}^\dagger_{s=1})+\mathscr{A}^\dagger_{\alpha_{ij}}\\ &=\sqrt{2}\,P^{(20)}_{\alpha_{ij}}(\boldsymbol{b}^\dagger_{s=1})+\sum_{s=2}^{A-1}b^\dagger_{si}b^\dagger_{sj}\,,\end{aligned}\tag{18}$$

where $\mathscr{A}^\dagger$ is independent of the Jacobi variable $\boldsymbol{x}_{s=1}$ and where use has been made of the relation

$$[P^{(q_1 0)}(\boldsymbol{b}^\dagger_{s=1})\times P^{(q_2 0)}(\boldsymbol{b}^\dagger_{s=1})]^{(\lambda\mu)}_\alpha=\delta_{(\lambda\mu)(q_1+q_2,0)}\left[\frac{(q_1+q_2)!}{q_1!\,q_2!}\right]^{1/2}P^{(q_1+q_2,0)}_\alpha(\boldsymbol{b}^\dagger_{s=1})\,,\tag{19}$$

valid for the normalized Moshinsky polynomial [26]) in the single 3-dimensional oscillator creation operator. It is then useful to expand the $\boldsymbol{P}^{\Gamma_n}_{\alpha_n^n}(\boldsymbol{A}^\dagger)$ of eq. (3) in terms of the two types of operators of eq. (18)

$$\boldsymbol{P}^{\Gamma_n}_{\alpha_n^n}(\boldsymbol{A}^\dagger)=\sum_{q,\Gamma}c^{\Gamma_n}_q(\Gamma)[P^{(q0)}\times\mathscr{P}^\Gamma(\mathscr{A}^\dagger)]^{\Gamma_n}_{\alpha_n^n}\,,\tag{20}$$

where $\mathscr{P}^\Gamma_\alpha(\mathscr{A}^\dagger)$ is defined through the analogue of eq. (3), and the abbreviated notation $P^{(q0)}$ will be used henceforth for $P^{(q0)}(b^\dagger_1)$. Note also that $P^{(20)}_{\alpha_2}(\boldsymbol{A}^\dagger)=\sqrt{\frac{1}{2}}\,A^\dagger_{\alpha_2}$. The expansion coefficients $c^{\Gamma_n}_q(\Gamma)$ are common to all Sp(6, R) irreducible representations and are easily calculated by a recursive process. They are tabulated in appendix A for all states with $N\leqslant 10$. For the special case with $\Gamma_n=(N0)$, and any N, they have the simple value

$$c^{(N0)}_q(\Gamma)=\delta_{\Gamma,(N-q,0)}\left[\frac{(\frac{1}{2}N)!\,q!}{(\frac{1}{2}N-\frac{1}{2}q)!\,2^{q/2}}\right]^{1/2}\frac{1}{(\frac{1}{2}q)!}\,.\tag{21}$$

Note also that $c^{\Gamma_n}_0(\Gamma)=\delta_{\Gamma,\Gamma_n}$.

A specific term in the expansion of eq. (17) can then be put in the form

$$\langle \Gamma_{\sigma'}\Gamma_{n'}\rho'\Gamma_{\omega'}\alpha_{\omega'}| V^{\Gamma_0}_{\alpha_0} \boldsymbol{P}^{\Gamma_n}_{\alpha_n}(\boldsymbol{A}^\dagger)|\Gamma_\sigma\alpha_\sigma\rangle$$
$$= \langle \Gamma_{\sigma'}\Gamma_{n'}\rho'\Gamma_{\omega'}\alpha_{\omega'}|\{\boldsymbol{P}^{\Gamma_n}_{\alpha_n}(\boldsymbol{A}^\dagger)\, V^{\Gamma_0}_{\alpha_0} + \sum_{q=2}^{N}\sum_{\Gamma} c^{\Gamma_n}_q(\Gamma)$$
$$\times \sum_{\alpha_q,\alpha} \langle (q0)\alpha_q\Gamma\alpha|\Gamma_n\alpha_n\rangle \boldsymbol{\mathscr{P}}^{\Gamma}_{\alpha}(\boldsymbol{\mathscr{A}}^\dagger)[\, V^{\Gamma_0}_{\alpha_0},\, P^{(q0)}_{\alpha_q}]\}|\Gamma_\sigma\alpha_\sigma\rangle\,, \tag{22}$$

using the fact that $\boldsymbol{\mathscr{A}}^\dagger$ commutes with $V^{\Gamma_0}_{\alpha_0}$. Since it is possible, without loss of generality, to arrange all symplectic-symplectic matrix elements such that $N' \leq N$, the first term of eq. (22) is identically zero unless $N' = N$, (which follows from the bandhead property $\langle \Gamma_{\sigma'}\alpha_{\sigma'}|\boldsymbol{A}^\dagger = 0$). In the second term it will be useful to use the inverse of eq. (18) to re-express $\boldsymbol{\mathscr{P}}(\boldsymbol{\mathscr{A}}^\dagger)$ in terms of $\boldsymbol{P}(\boldsymbol{A}^\dagger)$:

$$\mathscr{A}^\dagger_{\alpha_{ij}} = -\sqrt{2}\, P^{(20)}_{\alpha_{ij}} + A^\dagger_{\alpha_{ij}}\,, \tag{23}$$

leading to

$$\boldsymbol{\mathscr{P}}^{\Gamma}_{\alpha}(\boldsymbol{\mathscr{A}}^\dagger) = \sum_{\bar{q},\bar{\Gamma}} c^{\Gamma}_{\bar{q}}(\bar{\Gamma})(-1)^{\bar{q}/2}[P^{(\bar{q}0)} \times \boldsymbol{\mathscr{P}}^{\bar{\Gamma}}(\boldsymbol{A}^\dagger)]^{\Gamma}_{\alpha}\,. \tag{24}$$

The degree of the various polynomials is given by $N_\Gamma = N - q$, $N_{\bar{\Gamma}} = N - q - \bar{q}$. Note also that the representations Γ_n, $(q0)$, Γ, $(\bar{q}0)$, $\bar{\Gamma}$ are all even, in the sense $(-1)^\Gamma = +1$, cf. eq. (10); so that the order of the symmetric couplings in eqs. (20) and (24) can be reversed. A specific term in the expansion of eq. (17) can then be further put in the form

$$\langle \Gamma_{\sigma'}\Gamma_{n'}\rho'\Gamma_{\omega'}\alpha_{\omega'}| V^{\Gamma_0}_{\alpha_0} \boldsymbol{P}^{\Gamma_n}_{\alpha_n}(\boldsymbol{A}^\dagger)|\Gamma_\sigma\alpha_\sigma\rangle$$
$$= \langle \Gamma_{\sigma'}\Gamma_{n'}\rho'\Gamma_{\omega'}\alpha_{\omega'}|\Big\{ \boldsymbol{P}^{\Gamma_n}_{\alpha_n}(\boldsymbol{A}^\dagger)\mathbb{1}\delta_{N'N} V^{\Gamma_0}_{\alpha_0}$$
$$+ \sum_{q=2}^{N}\sum_{\Gamma} c^{\Gamma_n}_q(\Gamma) \sum_{\bar{q}=N-N'-q}^{N-q}\sum_{\bar{\Gamma}} c^{\Gamma}_{\bar{q}}(\bar{\Gamma})(-1)^{\bar{q}/2} \sum_{\alpha_q,\alpha}\sum_{\alpha_{\bar{q}},\bar{\alpha}} \boldsymbol{P}^{\bar{\Gamma}}_{\bar{\alpha}}(\boldsymbol{A}^\dagger)\mathbb{1}$$
$$\times \langle (q0)\alpha_q\Gamma\alpha|\Gamma_n\alpha_n\rangle\langle(\bar{q}0)\alpha_{\bar{q}}\bar{\Gamma}\bar{\alpha}|\Gamma\alpha\rangle$$
$$\times P^{(\bar{q}0)}_{\alpha_{\bar{q}}}[\, V^{\Gamma_0}_{\alpha_0},\, P^{(q0)}_{\alpha q}]\Big\}|\Gamma_\sigma\alpha_\sigma\rangle\,. \tag{25}$$

Note that $N_{\bar{\Gamma}}$, the degree of $\bar{\Gamma}$, must be $\leq N'$, the degree of $\Gamma_{n'}$; and therefore $\bar{q}$ must be $\geq N - N' - q$. Recall that N' was chosen such that $N' \leq N$. Also, a $c^{\Gamma}_{q}(\bar{\Gamma})$ with negative q will be defined to be identically zero. The unit operator, $\mathbb{1}$, to the right of $\boldsymbol{P}^{\bar{\Gamma}}_{\bar{\alpha}}(\boldsymbol{A}^\dagger)$ in this eq. can now be put in the form

$$\mathbb{1} = \sum_{\Gamma_{\omega''}\alpha_{\omega''}}\sum_{n''\rho''}\sum_{n'''\rho'''} |\Gamma_{\sigma'}\Gamma_{n'''}\rho'''\Gamma_{\omega''}\alpha_{\omega''}\rangle(\kappa^{-1}(\Gamma_{\sigma'}, \Gamma_{\omega''}))_{n''\rho'',n'''\rho'''}\langle \Psi(\Gamma_{\sigma'}\Gamma_{n''}\rho''\Gamma_{\omega''}\alpha_{\omega''})|\,, \tag{26}$$

where the degrees of $\Gamma_{n''}$, $\Gamma_{n'''}$ are restricted for each value of $\Gamma_{\omega''}$. Eq. (9) or (11) can then be used to evaluate the left hand terms of eq. (25). The corresponding unit

operator to the right of $P^{\Gamma_n}_{\alpha_n}(A^\dagger)$, needed only for $N'=N$, is simply given by $\mathbb{1}=\sum_{\alpha_{\sigma'}}|\Gamma_{\sigma'}\alpha_{\sigma'}\rangle\langle\Gamma_{\sigma'}\alpha_{\sigma'}|$. Finally, the operators which are functions only of the single Jacobi variable $x_{s=1}$, or its derivative, can be expressed in terms of unit operators acting in the space spanned by oscillator functions in the variable $x_{s=1}$. With

$$|(a0)\alpha_a\rangle = P^{(a0)}_{\alpha_a}(b^\dagger_{s=1})|0\rangle\,, \tag{27}$$

a unit irreducible tensor operator, $\mathcal{U}^{\Gamma_0}_{\alpha_0}(b,a)$, in this space is defined by

$$\langle(b'0)\alpha_b|\mathcal{U}^{\Gamma_0}_{\alpha_0}(b,a)|(a'0)\alpha_a\rangle = \delta_{a'a}\delta_{b'b}\langle(a0)\alpha_a\Gamma_0\alpha_0|(b0))\alpha_b\rangle\,, \tag{28a}$$

or through its SU(3) reduced matrix elements

$$\langle(b'0)\|\mathcal{U}^{\Gamma_0}(b,a)\|(a'0)\rangle = \delta_{a'a}\delta_{b'b}\,, \tag{28b}$$

where the possible Γ_0 are given by the Kronecker product $(b0)\times(0a)$. Note also that the operators $P^{(q0)}$ and V^{Γ_0} can be expressed in terms of such unit operators by

$$P^{(q0)}_{\alpha_q} = \sum_{a=0}^{\infty}\left[\frac{(q+a)!}{q!\,a!}\right]^{1/2}\mathcal{U}^{(q0)}_{\alpha_q}(q+a,a)\,, \tag{29a}$$

$$V^{\Gamma_0}_{\alpha_0} = \sum_{a,b}\langle(b0)\|V^{\Gamma_0}\|(a0)\rangle\mathcal{U}^{\Gamma_0}_{\alpha_0}(b,a)\,. \tag{29b}$$

The $x_{s=1}$-dependent operators in eq. (25) can be expressed in terms of such unit operators.

$$\begin{aligned}
&P^{(\bar q 0)}_{\alpha_{\bar q}}[V^{\Gamma_0}_{\alpha_0}, P^{(q0)}_{\alpha_q}] \\
&\quad=\sum_{ab}\sum_{\Gamma'_0\alpha'_0}\sum_{\Gamma_{q+\bar q},\alpha_{q+\bar q}}\sum_{\bar\rho_0}(-1)^{\sigma(\Gamma_{q+\bar q},\alpha_{q+\bar q})}\langle(\bar q 0)\alpha_{\bar q}(q0)\alpha_q|\Gamma_{q+\bar q}\alpha_{q+\bar q}\rangle \\
&\qquad\times\langle\tilde\Gamma_{q+\bar q}\tilde\alpha_{q+\bar q}\Gamma'_0\alpha'_0|\Gamma_0\alpha_0\rangle_{\bar\rho_0}\left[\frac{d(\Gamma'_0)}{d(\Gamma_0)}\right]^{1/2}\mathcal{U}^{\Gamma'_0}_{\alpha'_0}(b,a)F(\Gamma_0 q\bar q;\,\Gamma'_0\Gamma_{q+\bar q}\bar\rho_0;\,ab)\,,
\end{aligned} \tag{30}$$

where $\tilde\Gamma$ stands for the conjugate of the SU(3) representation Γ, that is $\tilde\Gamma=(\mu,\lambda)$ if $\Gamma=(\lambda,\mu)$; and $d(\Gamma)$ is a shorthand notation for the dimension of the SU(3) representation, dim $(\lambda\mu)$. The phase factor [20]), given by σ, is related to the conjugation of the SU(3) basis functions

$$(\Psi^\Gamma_\alpha)^* = (-1)^{\sigma(\Gamma,\alpha)}\Psi^{\tilde\Gamma}_{\tilde\alpha}\,.$$

In eq. (30) the F factor is given by

$$\begin{aligned}
&F(\Gamma_0 q\bar q;\,\Gamma'_0\Gamma_{q+\bar q}\bar\rho_0;\,ab) \\
&\quad=\left[\frac{(q+a)!\,b!}{q!\,a!\,\bar q!(b-\bar q)!}\right]^{1/2}\langle(b-\bar q,0)\|V^{\Gamma_0}\|(q+a,0)\rangle \\
&\qquad\times\begin{bmatrix}(0\bar q) & (0q) & \tilde\Gamma_{q+\bar q} & - \\ (b0) & (0a) & \Gamma'_0 & - \\ (b-\bar q,0) & (0,q+a) & \Gamma_0 & - \\ - & - & \bar\rho_0 & \end{bmatrix}-\delta_{\Gamma_{q+\bar q},(q+\bar q,0)}\left[\frac{b!}{q!\,\bar q!(b-q-\bar q)!}\right]^{1/2} \\
&\qquad\times\langle(b-q-\bar q,0)\|V^{\Gamma_0}\|(a0)\rangle U((0,q+\bar q)(b0)\Gamma_0(0a);\,(b-q-\bar q,0)\Gamma'_0)\,,
\end{aligned} \tag{31a}$$

where the SU(3) reduced matrix elements of V^{Γ_0} are given by expressions such as eq. (16). The combination of eqs. (17), (25), (26) and (30) then leads, after straightforward but somewhat lengthy SU(3) recoupling transformations, to the final expression

$$
\begin{aligned}
&\langle \Gamma_{\sigma'}\Gamma_{n'}\rho'\Gamma_{\omega'} \| V^{\Gamma_0} \| \Gamma_\sigma \Gamma_{n_1}\rho_1\Gamma_\omega\rangle_{\rho_0} \\
&\quad = \delta_{N'N} \sum_{n\rho} \sum_{\rho''} \sum_{\rho_{00}} (\kappa(\Gamma_{\sigma'}, \Gamma_{\omega'}))_{n\rho'',n'\rho'} (\kappa^{-1}(\Gamma_\sigma, \Gamma_\omega))_{n_1\rho_1,n\rho} \\
&\qquad \times \langle \Gamma_{\sigma'} \| V^{\Gamma_0} \| \Gamma_\sigma \rangle_{\rho_{00}} U(\Gamma_n \Gamma_\sigma \Gamma_{\omega'} \Gamma_0; \Gamma_\omega \rho \rho_0; \Gamma_{\sigma'} \rho_{00} \rho'') \\
&\qquad + \sum_{\Gamma_{\omega''}} \sum_{n''\rho''} \sum_{n'''\rho'''} \sum_{n\rho} (\kappa^{-1}(\Gamma_{\sigma'}, \Gamma_{\omega''}))_{n''\rho'',n'''\rho'''} (\kappa^{-1}(\Gamma_\sigma, \Gamma_\omega))_{n_1\rho_1,n\rho} \\
&\qquad \times \sum_{q=2}^{N} \sum_{\Gamma} \sum_{\bar{q}=N-N'-q}^{N-q} \sum_{\bar{\Gamma}} c_q^{\Gamma_n}(\Gamma) c_{\bar{q}}^{\Gamma}(\bar{\Gamma}) (-1)^{\bar{q}/2} \\
&\qquad \times \sum_{\bar{\rho}} \langle \Gamma_{\sigma'}\Gamma_{n'}\rho'\Gamma_{\omega'}\alpha_{\omega'} | [\boldsymbol{P}^{\bar{\Gamma}}(\boldsymbol{A}^\dagger) \times | \Gamma_{\sigma'}\Gamma_{n'''}\rho'''\Gamma_{\omega''}\rangle]^{\Gamma_{\omega'},\bar{\rho}}_{\alpha_{\omega'}} \\
&\qquad \times \sum_{\Gamma_0'\rho_0'} \sum_{ab} \left[\frac{\mathrm{d}(\Gamma_0')\,\mathrm{d}(\Gamma_n)}{\mathrm{d}(\Gamma_0)\,\mathrm{d}(\bar{\Gamma})} \right]^{1/2} \langle \Psi(\Gamma_{\sigma'}\Gamma_{n''}\rho''\Gamma_{\omega''}) \| \mathcal{U}^{\Gamma_0'}(b,a) \| \Gamma_\sigma \rangle_{\rho_0'} \\
&\qquad \times \sum_{\Gamma_{q+\bar{q}}} \sum_{\tilde{\rho}_0\tilde{\rho}} (-1)^{\Gamma_{q+\bar{q}}} U(\bar{\Gamma}(\bar{q}0)\Gamma_n(q0); \Gamma_{--}; \Gamma_{q+\bar{q}-}\tilde{\bar{\rho}}) \\
&\qquad \times \begin{bmatrix} \Gamma_n & \tilde{\bar{\Gamma}}_{q+\bar{q}} & \bar{\Gamma} & \bar{\rho} \\ \Gamma_\sigma & \Gamma_0' & \Gamma_{\omega''} & \rho_0' \\ \Gamma_\omega & \Gamma_0 & \Gamma_{\omega'} & \rho_0 \\ \rho & \bar{\rho}_0 & \bar{\rho} & \end{bmatrix} F(\Gamma_0 q\bar{q}; \Gamma_0'\Gamma_{q+\bar{q}}\bar{\rho}_0; ab) \,. \qquad (31b)
\end{aligned}
$$

The SU(3) Racah or U-coefficients and the SU(3) $9-\Gamma$ coefficients in eq. (31b) are given in unitary form [20]). (Where not needed, multiplicity labels ρ are replaced by a dash or simply omitted altogether). In the first term of eq. (31b), only needed when $N' = N$, the reduced matrix elements of V^{Γ_0} between bandhead states Γ_σ and $\Gamma_{\sigma'}$ can be expressed in terms of known reduced matrix elements, (see eq. (29b))

$$
\langle \Gamma_{\sigma'} \| V^{\Gamma_0} \| \Gamma_\sigma \rangle_{\rho_{00}} = \sum_{ab} \langle (b0) \| V^{\Gamma_0} \| (a0) \rangle \langle \Gamma_{\sigma'} \| \mathcal{U}^{\Gamma_0}(b,a) \| \Gamma_\sigma \rangle_{\rho_{00}} \,. \qquad (31c)
$$

The quantities

$$
\langle \Gamma_{\sigma'}\Gamma_{n'}\rho'\Gamma_{\omega'}\alpha_{\omega'} | [\boldsymbol{P}^{\bar{\Gamma}}(\boldsymbol{A}^\dagger) \times | \Gamma_{\sigma'}\Gamma_{n'''}\rho'''\Gamma_{\omega''}\rangle]^{\Gamma_{\omega'},\bar{\rho}}_{\alpha_{\omega'}} \,,
$$

needed for the second term of eq. (31b), can be evaluated through the transformation coefficients $B(\Gamma_1\Gamma_2, \Gamma_3\rho)$ given in appendix B.

The final ingredients needed for the full evaluation of eq. (31b) are the reduced matrix elements of the unit operators $\langle \Psi(\Gamma_{\sigma'}\Gamma_{n''}\rho''\Gamma_{\omega''}) \| \mathcal{U}^{\Gamma_0'}(b,a) \| \Gamma_\sigma \rangle_{\rho_0'}$. If the degree of $\Gamma_{n''}$, $N'' \neq 0$, these can be reduced to matrix elements between simple bandhead states using eq. (31b). Hermitian conjugation gives

$$
\langle \Gamma_{\omega''} \| \mathcal{U}^{\Gamma_0'}(b,a) \| \Gamma_\sigma \rangle_{\rho_0'} = (-1)^{a+b+\Gamma_{\omega''}+\Gamma_\sigma} \left[\frac{\mathrm{d}(b0)\,\mathrm{d}(\Gamma_\sigma)}{\mathrm{d}(a0)\,\mathrm{d}(\Gamma_{\omega''})} \right]^{1/2} \langle \Gamma_\sigma \| \mathcal{U}^{\bar{\Gamma}_0'}(a,b) \| \Gamma_{\omega''} \rangle^*_{\rho_0'} \,,
$$

and eq. (31b) then yields

$$
\begin{aligned}
&\langle \Psi(\Gamma_{\sigma'}\Gamma_{n''}\rho''\Gamma_{\omega''})\| \mathcal{U}^{\Gamma_0'}(b,a)\|\Gamma_\sigma\rangle_{\rho_0'} \\
&\quad = \sum_{q=2}^{N''} c_q^{\Gamma_{n''}}((N''-q,0))(-1)^{(N''-q)/2}\left[\frac{(N''-q)!}{(\frac{1}{2}N''-\frac{1}{2}q)!\,2^{(N''-q)/2}}\right]^{1/2} \\
&\qquad \times(-1)^{a+b+\Gamma_\sigma+\Gamma_{\sigma'}} \sum_{\Gamma_0''\rho_0''\tilde\rho_0}\left[\frac{\mathrm{d}(b0)\,\mathrm{d}(\Gamma_\sigma)\,\mathrm{d}(\Gamma_0'')}{\mathrm{d}(a0)\,\mathrm{d}(\Gamma_{\sigma'})\,\mathrm{d}(\Gamma_0')}\right]^{1/2} \sum_{\rho'''}\begin{bmatrix} (00) & \Gamma_{n''} & \Gamma_{n''} & - \\ \Gamma_{\sigma'} & (00) & \Gamma_{\sigma'} & - \\ \Gamma_{\sigma'} & \Gamma_{n''} & \Gamma_{\omega''} & \rho''' \\ - & - & \rho'' & \end{bmatrix} \\
&\qquad \times U(\Gamma_{\omega''}\tilde\Gamma_{n''}\Gamma_\sigma\Gamma_0'';\Gamma_{\sigma'}\rho'''\rho_0'';\tilde\Gamma_0'\tilde\rho_0\rho_0') \\
&\qquad \times\Bigg\{\left[\frac{b!(N''-q+a)!}{q!(b-q)!\,a!(N''-q)!}\right]^{1/2}\langle\Gamma_\sigma\|\mathcal{U}^{\Gamma_0''}(N''-q+a,b-q)\|\Gamma_{\sigma'}\rangle_{\rho_0''}^{*} \\
&\qquad\quad \times\begin{bmatrix} (0,N''-q) & (0q) & \tilde\Gamma_{n''} & - \\ (N''-q+a,0) & (0,b-q) & \Gamma_0'' & - \\ (a0) & (0b) & \tilde\Gamma_0' & - \\ - & - & \tilde\rho_0 & \end{bmatrix} \\
&\qquad\quad -\delta_{\Gamma_{n''},(N''0)}\left[\frac{(N''+a)!}{q!(N''-q)!\,a!}\right]^{1/2}\langle\Gamma_\sigma\|\mathcal{U}^{\Gamma_0''}(N''+a,b)\|\Gamma_{\sigma'}\rangle_{\rho_0''}^{*} \\
&\qquad\quad \times U((0N'')(N''+a,0)\tilde\Gamma_0'(0b);(a0)\Gamma_0'')\Bigg\}. \qquad (31d)
\end{aligned}
$$

In this case the bandhead property $\langle\Gamma_\sigma\alpha_\sigma|A_\alpha^\dagger=0$ eliminates many terms, e.g., in the polynomial $\mathscr{P}_\alpha^\Gamma(\mathscr{A}^\dagger)$ in the analog of eq. (22), where the degree of Γ is $N''-q$, only the first term, with $\bar q=N''-q$, survives in the inverse expansion of eq. (24). This also limits Γ to the single representation $\Gamma=(N''-q,0)$. In the derivation of eqs. (31a-d), the simple symmetry properties of the SU(3) Wigner coefficients have been used (see eq. (35) of ref. [20])). The 9-Γ coefficient with (00) in the 1 and 4 position in eq. (31d) is an efficient way to express the needed nonsimple symmetry property

$$
\langle\Gamma_{n''}\alpha_{n''}\Gamma_{\sigma'}\alpha_{\sigma'}|\Gamma_{\omega''}\alpha_{\omega''}\rangle_{\rho''} = \sum_{\rho'''}\langle\Gamma_{\sigma'}\alpha_{\sigma'}\Gamma_{n''}\alpha_{n''}|\Gamma_{\omega''}\alpha_{\omega''}\rangle_{\rho'''}\begin{bmatrix} (00) & \Gamma_{n''} & \Gamma_{n''} & - \\ \Gamma_{\sigma'} & (00) & \Gamma_{\sigma'} & - \\ \Gamma_{\sigma'} & \Gamma_{n''} & \Gamma_{\omega''} & \rho''' \\ - & - & \rho'' & \end{bmatrix}. \qquad (32)
$$

Note that in the very common case when the product $\Gamma_{n''} \times \Gamma_{\sigma'} \to \Gamma_{\omega''}$ is free of multiplicity this simple $9-\Gamma$ coefficient collapses to a unit matrix with value given by the simple phase factor

$$(-1)^{\Gamma_{n''}+\Gamma_{\sigma'}-\Gamma_{\omega''}}.$$

Note also that the sum over ρ''' in eq. (31d) can be reduced to

$$\sum_{\rho'''} \begin{bmatrix} (00) & \Gamma_{n''} & \Gamma_{n''} & - \\ \Gamma_{\sigma'} & (00) & \Gamma_{\sigma'} & - \\ \Gamma_{\sigma'} & \Gamma_{n''} & \Gamma_{\omega''} & \rho''' \\ - & - & \rho'' & \end{bmatrix} U(\Gamma_{\omega''}\tilde{\Gamma}_{n''}\Gamma_{\sigma}\Gamma_0''; \Gamma_{\sigma'}\rho'''\rho_0''; \tilde{\Gamma}_0'\bar{\rho}_0\rho_0')$$

$$= (-1)^{\Gamma_{\sigma'}+\Gamma_{n''}+\Gamma_{\omega''}} \left[\frac{\mathrm{d}(\Gamma_{\sigma'})\,\mathrm{d}(\Gamma_{n''})}{\mathrm{d}(\Gamma_{\omega''})}\right]^{1/2} \begin{bmatrix} \Gamma_{n''} & \tilde{\Gamma}_{n''} & (00) & - \\ \Gamma_{\sigma'} & \Gamma_0'' & \Gamma_{\sigma} & \rho_0'' \\ \Gamma_{\omega''} & \tilde{\Gamma}_0' & \Gamma_{\sigma} & \rho_0' \\ \rho'' & \bar{\rho}_0 & - & \end{bmatrix}. \qquad (31e)$$

To summarize, eqs. (31a-e) give a formula for a straightforward evaluation of the matrix elements of a two-body interaction, $V = \sum_{i<j} V_{ij}$, in a Sp(6, R) basis. The formula (31) is a reduction formula which expresses the matrix element connecting states of arbitrary excitations N and N' in the same symplectic band or in different symplectic bands, (if $\Gamma_{\sigma'} \neq \Gamma_{\sigma}$), in terms of the matrix elements of simple unit operators connecting the bandhead states, $\langle \Gamma_{\sigma'} \| \mathcal{U}^{\Gamma_0''}(a', b') \| \Gamma_{\sigma} \rangle_{\rho_0}$. Since the bandhead states $|\Gamma_{\sigma}\alpha_{\sigma}\rangle$ are generally simple shell model states or expressible in terms of simple shell model configurations in most real applications, the problem has been reduced to an evaluation of matrix elements of standard shell model type. Since the reduction formula (31) is a formula for SU(3) reduced matrix elements, and therefore independent of SU(3) subgroup labels, it applies equally to tensor or spin-orbit as well as to central interactions. The additional angular momentum coupling needed for the full matrix elements in the case of tensor or vector interactions is thus also pushed into the domain of the bandhead matrix elements of simple shell model type. Since the unit operator, $\mathcal{U}^{\Gamma_0''}(a', b')$, acts only in the space of the relative motion variable $\sqrt{\frac{1}{2}}(\boldsymbol{r}_1 - \boldsymbol{r}_2)$, the evaluation of its matrix elements between bandhead states of shell model type involves standard cfp techniques by which particles labelled 1 and 2, (alternately A and $A-1$), are uncoupled from the rest, and Moshinsky-Talmi transformations to two-particle relative and cm motion variables (see, e.g., refs. [19,27])). Since the states are SU(3)-coupled states, the needed Moshinsky brackets are simple angular momentum, SU(2) d-functions. Also, since the bandhead states generally involve simple shell model configurations, the quantum numbers a' and b' in $\mathcal{U}^{\Gamma_0''}(a', b')$ are severely restricted; e.g. if $|\Gamma_{\sigma}\alpha_{\sigma}\rangle$ and $|\Gamma_{\sigma'}\alpha_{\sigma'}\rangle$ are both shell model states of a 2s1d shell nucleus, then both a' and b', and consequently $N''-q+a$, $b-q$, $N''+a$, b in eq. (31d), are restricted by a', $b' \leqslant 4$. Finally, the ingredients for the evaluation of eq. (31) are: (i) SU(3) Racah and $9-\Gamma$

coefficients which are readily available through the codes of ref. [21]), (ii) the κ matrix elements which can be evaluated by powerful simple approximation formulae [15,16]) or exactly by the techniques of refs. [9,13,14]), and (iii) a set of simple expansion coefficients $c_{q^n}^{\Gamma}(\Gamma)$. These are tabulated for $N \leq 10$ in appendix A. Despite the severe limits on a', b', and the very limited range of the possible values for q, $\bar{q}$, it might appear that the total number of terms in the summations of eq. (31) is quite large. For most of the simpler symplectic excitations, of greatest interest in the actual applications to physical problems, however, most of the multiplicity labels, ρ, are unnecessary, and most of the $n\rho$ sums disappear since most of the κ matrices are 1-dimensional. The total number of terms needed for the evaluation of eq. (31) may thus be quite small, and a straightforward method has been established for the evaluation of two-body interaction matrix elements connecting states of arbitrary excitations in a $Sp(6, R) \supset U(3)$ basis. In sect. 4 it will be shown that a slight modification of the reduction formula can also be used to evaluate the interaction matrix element connecting symplectic excitations and states of the microscopic cluster model.

4. Cluster model-symplectic interaction matrix elements

The normalized states of the microscopic cluster model for a nucleus made up of fragments of mass numbers f and $A-f$ are defined in an SU(3)-coupled basis by

$$|[\Gamma_c \times (Q0)]\Gamma_{\omega'}\alpha_{\omega'}\rangle = [\sigma(\Gamma_c Q; \Gamma_{\omega'})]^{-1/2}\{|\mathfrak{A}[[\phi^{\Gamma_f} \times \phi^{\Gamma_{A-f}}]^{\Gamma_c\rho_c} \times \chi(\boldsymbol{R})^{(Q0)}]^{\Gamma_{\omega'}}_{\alpha_{\omega'}}\rangle\}\,, \quad (33)$$

where the antisymmetrization operator, $\mathfrak{A}$, handles antisymmetrization between clusters. The properly antisymmetrized internal wave functions, ϕ, of the two fragments are assumed to be lowest possible Pauli-allowed states of the fragments. The relative motion function, χ, is an oscillator function in the (dimensionless) relative distance vector $\boldsymbol{R}$ between the two fragments. As before, Γ_c is shorthand for $(\lambda_c\mu_c)$, etc. The normalization constant is given in terms of $\sigma(\Gamma_c Q; \Gamma_{\omega'})$, the diagonal overlap matrix element between the states in { } brackets. These will often by abbreviated by $|\mathfrak{A}[\phi^{\Gamma_c} \times \chi^{(Q0)}]^{\Gamma_{\omega'}}_{\alpha_{\omega'}}\rangle$.

In refs. [6,7]) it was shown that simple cluster model states of this type often have large overlaps with the lowest symplectic excitations, (with $N=2$), and the same total number of oscillator excitations and overall SU(3) symmetry Γ_ω. However, for most binary cluster systems such overlaps decrease rapidly with increasing symplectic excitation, $N \geq 4$, showing the complementary character of the two types of wave functions [7]).

The techniques used in sect. 3 can be used to evaluate the SU(3) reduced matrix element of a two-body interaction between a cluster state of the type expressed in eq. (33) and a symplectic state of arbitrary excitation, $\langle\mathfrak{A}[\phi^{\Gamma_c} \times \chi^{(Q0)}]^{\Gamma_{\omega'}}_{\alpha_{\omega'}}\| V^{\Gamma_0} \| \Gamma_\sigma \Gamma_n \rho \Gamma_\omega\rangle_{\rho_0}$. The method again involves a process of commuting the symplectic raising polynomial to the left of V^{Γ_0} by means of the expansion (20) and

its inverse (24). Complications due to the presence of the antisymmetrizer, $\mathfrak{A}$, are now avoided since the totally symmetric operators, such as $P^{\Gamma_n}_{\alpha_n}(A^\dagger)$ or $P^{\bar{\Gamma}}_{\bar{\alpha}}(A^\dagger)$, commute with $\mathfrak{A}$ and can thus act directly on a cluster model state $[\phi^{\Gamma_c}\times\chi^{(Q0)}]^{\Gamma_{\omega'}}_{\alpha_{\omega'}}$ antisymmetrized only in the first f and the last $(A-f)$ nucleons. When acting to the left on such a cluster model state a polynomial in the $A^\dagger$ can now be expanded in terms of a new set of Jacobi variables appropriate to the cluster decomposition $f+(A-f)$,

$$A^\dagger_{\alpha_{ij}}=\sqrt{2}\,P^{(20)}_{\alpha_{ij}}(\boldsymbol{b}^\dagger_{\text{rel.}})+\sum_{s'=2}^{A-1} b^\dagger_{s'i}b^\dagger_{s'j}\,, \tag{34}$$

where $\boldsymbol{b}^\dagger_{\text{rel.}}$ is an oscillator creation operator in the relative motion variable $\boldsymbol{R}$ and the $\boldsymbol{b}^\dagger_{s'}$ with $s'=2,\ldots A-1$, involve the $A-2$ internal degrees of freedom of the fragments f and $(A-f)$. Since the internal functions correspond to the lowest possible Pauli-allowed states of the two fragments $|\mathfrak{A}b_{s'}[\phi^{\Gamma_c}\times\chi^{(Q0)}]^{\Gamma_{\omega'}}_{\alpha_{\omega'}}\rangle=0$ for all s' corresponding to fragment internal degrees of freedom. [7]) In an expansion of $P^{\Gamma_n}_{\alpha_n}(A^\dagger)$ or $P^{\bar{\Gamma}}_{\bar{\alpha}}(A^\dagger)$ in the analogue of eq. (25) only the leading term, (completely independent of $\boldsymbol{b}^\dagger_{s'}$), survives; and in the analogue of eq. (20) only the leading term in the expansion is needed, e.g.,

$$P^{\Gamma_n}_{\alpha_n}(A^\dagger)=\delta_{\Gamma_n,(N0)}\left[\frac{N!}{(\frac{1}{2}N)!2^{N/2}}\right]^{1/2}P^{\Gamma_n}_{\alpha_n}(\boldsymbol{b}^\dagger_{\text{rel.}})+\cdots. \tag{35}$$

The reduced matrix element of $P^{(N0)}(\boldsymbol{b}^+_{\text{rel}})$ in a basis of relative motion functions $\chi^{(Q0)}(\boldsymbol{R})$ follows from the analogue of eq. (19) and leads to the reduced matrix element in the SU(3) coupled cluster model basis through

$$\begin{aligned}
&(P^{\Gamma_n}_{\alpha_n}(A^\dagger))^\dagger|\mathfrak{A}[\phi^{\Gamma_c}\times\chi^{(Q0)}]^{\Gamma_{\omega'}}_{\alpha_{\omega'}}\rangle\\
&\quad=(-1)^{\sigma(\Gamma_n,\alpha_n)}P^{\bar{\Gamma}}_{\bar{\alpha}_n}(A)|\mathfrak{A}[\phi^{\Gamma_c}\times\chi^{(Q0)}]^{\Gamma_{\omega'}}_{\alpha_{\omega'}}\rangle\\
&\quad=\delta_{\Gamma_n(N0)}\left[\frac{Q!}{(Q-N)!(\frac{1}{2}N)!2^{N/2}}\right]^{1/2}\\
&\qquad\times\sum_{\Gamma_{\omega''}\alpha_{\omega''}}\langle\Gamma_{\omega''}\alpha_{\omega''}(N0)\alpha_n|\Gamma_{\omega'}\alpha_{\omega'}\rangle\\
&\qquad\times U(\Gamma_c(Q-N,0)\Gamma_{\omega'}(N0);\,\Gamma_{\omega''}(Q0))\times|\mathfrak{A}[\phi^{\Gamma_c}\times\chi^{(Q-N,0)}]^{\Gamma_{\omega''}}_{\alpha_{\omega''}}\rangle\,.
\end{aligned} \tag{36}$$

This equation, a generalization of eq. (23) of ref. [7]), is very useful to calculate the overlap of the states between the cluster and the symplectic models. With this relation, the methods of sect. 3 then lead to the reduced matrix element between a normalized cluster state of the type (33) and a symplectic state of arbitrary excitation,

$$
\begin{aligned}
&\langle[\Gamma_c\times(Q0)]\Gamma_{\omega'}\|V^{\Gamma_0}\|\Gamma_\sigma\Gamma_{n_1}\rho_1\Gamma_\omega\rangle_{\rho_0}\\
&\quad=\sum_{n\rho}(\kappa^{-1}(\Gamma_\sigma,\Gamma_\omega))_{n_1\rho_1,n\rho}\Bigg\{\delta_{\Gamma_n,(N0)}\sum_{\Gamma_{\omega''}\rho_0'}\left[\frac{\sigma(\Gamma_cQ-N;\Gamma_{\omega''})}{\sigma(\Gamma_cQ;\Gamma_{\omega'})}\right]^{1/2}\\
&\qquad\times\left[\frac{Q!}{(Q-N)!(\frac{1}{2}N)!2^{N/2}}\right]^{1/2}\langle[\Gamma_c\times(Q-N,0)]\Gamma_{\omega''}\|V^{\Gamma_0}\|\Gamma_\sigma\rangle_{\rho_0'}(-1)^{\Gamma_{\omega''}-\Gamma_{\omega'}}\\
&\qquad\times U(\Gamma_c(Q-N,0)\Gamma_{\omega'}(N0);\Gamma_{\omega''}(Q0))\\
&\qquad\times U((N0)\Gamma_\sigma\Gamma_{\omega'}\Gamma_0;\Gamma_{\omega-}\rho_0;\Gamma_{\omega''}\rho_{0-}')\\
&\qquad+\sum_{q=2}^{N}\sum_{\Gamma}c_q^{\Gamma_n}(\Gamma)\sum_{\bar q=0}^{N-q}c_{\bar q}^{\Gamma}((N-q-\bar q,0))(-1)^{\bar q/2}\\
&\qquad\times\sum_{\Gamma_{\omega''}}\sum_{\Gamma_0'\rho_0'}\sum_{ab}(-1)^{\Gamma_{\omega''}-\Gamma_{\omega'}}\left[\frac{\sigma(\Gamma_c(Q-N+q+\bar q);\Gamma_{\omega''})}{\sigma(\Gamma_cQ;\Gamma_{\omega'})}\right]^{1/2}\\
&\qquad\times\left[\frac{Q!}{(Q-N+q+\bar q)![\frac{1}{2}(N-q-\bar q)]!2^{(N-q-\bar q)/2}}\right]^{1/2}\\
&\qquad\times\left[\frac{\mathrm{d}(\Gamma_0')\,\mathrm{d}(\Gamma_n)}{\mathrm{d}(\Gamma_0)\,\mathrm{d}((N-q-\bar q,0))}\right]^{1/2}\langle[\Gamma_c\times(Q-N+q+\bar q,0)]\Gamma_{\omega''}\|\mathcal{U}^{\Gamma_0'}(b,a)\|\Gamma_\sigma\rangle_{\rho_0'}\\
&\qquad\times U(\Gamma_c(Q-N+q+\bar q,0)\Gamma_{\omega'}(N-q-\bar q,0);\Gamma_{\omega''}(Q0))\\
&\qquad\times\sum_{\Gamma_{q+\bar q}\bar\rho_0}(-1)^{\Gamma_{q+\bar q}}U((N-q-\bar q,0)(\bar q0)\Gamma_n(q0);\Gamma\Gamma_{q+\bar q})\\
&\qquad\times\begin{bmatrix}\Gamma_n & \tilde\Gamma_{q+\bar q} & (N-q-\bar q,0) & -\\ \Gamma_\sigma & \Gamma_0' & \Gamma_{\omega''} & \rho_0'\\ \Gamma_\omega & \Gamma_0 & \Gamma_{\omega'} & \rho_0\\ \rho & \bar\rho_0 & - & \end{bmatrix}F(\Gamma_0q\bar q;\Gamma_0'\Gamma_{q+\bar q}\bar\rho_0;ab)\quad,
\end{aligned}
\tag{37}
$$

where the function, F, is given by eq. (31a). Note also that for large values of N, corresponding to a Pauli-forbidden value of $Q-N$, the first term disappears by virtue of the overlap $\sigma(\Gamma_c, Q-N;\Gamma_{\omega''})$. In the first term also the reduced matrix element of V^{Γ_0} can be related to reduced matrix elements of unit operators of type $\mathcal{U}^{\Gamma_0}(b,a)$ by the analogue of eq. (31c), (see eq. (29b)).

The relation (37) is again a reduction formula which expresses the matrix element between a cluster model state and a Sp(6, R) state of arbitrary excitation N in terms of much simpler matrix elements. These simpler matrix elements connect the cluster model state to a symplectic bandhead state via the unit operators $\mathcal{U}^{\Gamma_0}(b,a)$. Since the symplectic bandhead state is a simple shell model state which, with a proper normalization factor, can in general also be expressed as a cluster model state with a minimum Pauli-allowed relative motion excitation Q, the cluster-symplectic matrix element has been reduced to one of simple cluster type. The next section will illustrate how such starting matrix elements are evaluated.

5. Matrix elements of SU(3) unit tensor operators

The reduced matrix element of the unit operator $\mathcal{U}^{\Gamma_0}_{\alpha_0}(b, a)$ between a cluster state and the symplectic bandhead state

$$\langle [\Gamma_c \times (Q0)]\Gamma_{\omega'} \| \sum_{i<j} \mathcal{U}^{\Gamma_0}(b, a)_{ij} \| \Gamma_\sigma \rangle_{\rho_0}, \tag{38}$$

can be derived from a generating function

$$f_{\alpha_0;\alpha_c\alpha_\sigma}(\boldsymbol{K}) = \langle \mathfrak{A}\{[\phi^{\Gamma_f} \times \phi^{\Gamma_{A-f}}]^{\Gamma_c}_{\alpha_c} A(\boldsymbol{K}, \boldsymbol{R})^*\} | \sum_{i<j} \mathcal{U}^{\Gamma_0}_{\alpha_0}(b, a)_{ij} | \phi^{\Gamma_\sigma}_{\alpha_\sigma} \rangle, \tag{39}$$

where the symplectic bandhead state is an A-particle state with the same characteristics as the f and $(A-f)$ internal functions ϕ^{Γ_f}, $f^{\Gamma_{A-f}}$. In this generating function

$$\begin{aligned} A(\boldsymbol{K}, \boldsymbol{R}) &= \pi^{-3/4} \exp\left[-\tfrac{1}{2}\boldsymbol{K}\cdot\boldsymbol{K} + \sqrt{2}\,\boldsymbol{K}\cdot\boldsymbol{R} - \tfrac{1}{2}\boldsymbol{R}\cdot\boldsymbol{R}\right] \\ &= \sum_{Q\alpha_Q} P^{(Q0)}_{\alpha_Q}(\boldsymbol{K}) \chi^{(Q0)}_{\alpha_Q}(\boldsymbol{R})^*, \end{aligned} \tag{40}$$

is the kernel function which generates the Bargmann transform in the space of the single 3-dimensional variable $\boldsymbol{R}$ (see e.g., ref. [8]). By including the cm motion degree of freedom and converting the matrix element of eq. (39) to one involving integrations over all A variables it is possible to convert the generating function to the standard Brink form [28]) extensively used in cluster model calculations. In this form the f and $(A-f)$-particle functions are converted to shell model-like wave functions, (denoted by ψ), which are centered at $[2A/(A-f)]^{1/2}\boldsymbol{K}$ and at the origin, respectively, e.g.

$$\psi^{\Gamma_f}_{\alpha_f}\left(\left[\frac{2A}{A-f}\right]^{1/2}\boldsymbol{K}\right) = \phi^{\Gamma_f}_{\alpha_f}\pi^{-3/4}\exp\left[-\frac{1}{2}\left(\boldsymbol{X}_f - \left[\frac{2A}{A-f}\right]^{1/2}\boldsymbol{K}\right)^2\right], \tag{41}$$

where $\boldsymbol{X}_f = (\boldsymbol{r}_1 + \boldsymbol{r}_2 + \cdots + \boldsymbol{r}_f)/\sqrt{f}$, and the dimensionless single particle $\boldsymbol{r}_i$ are physical $\boldsymbol{r}_i$ divided by the oscillator length parameter $[\hbar/m\omega]^{1/2}$. The corresponding functions $\psi^{\Gamma_{A-f}}$, and similarly ψ^{Γ_σ}, are to be centered at the origin. This leads to the generating function

$$\begin{aligned} f_{\alpha_0;\alpha_c\alpha_\sigma}(\boldsymbol{K}) = \exp&\left[\frac{A}{2(A-f)}(\boldsymbol{K}\cdot\boldsymbol{K})\right] \\ &\times \left\langle \mathfrak{A}[\phi^{\Gamma_f} \times \phi^{\Gamma_{A-f}}]^{\Gamma_c}_{\alpha_c}\left(\pi^{-3/4}\exp\left[-\frac{1}{2}\left(\boldsymbol{X}_f - \left[\frac{2A}{A-f}\right]^{1/2}\boldsymbol{K}\right)^2\right]\right)^* \right. \\ &\left. \times \pi^{-3/4}\exp\left[-\tfrac{1}{2}(\boldsymbol{X}_{A-f}\cdot\boldsymbol{X}_{A-f})\right] \middle| \sum_{i<j} \mathcal{U}^{\Gamma_0}_{\alpha_0}(b, a)_{ij} | \psi^{\Gamma_\sigma}_{\alpha_\sigma}(0) \right\rangle. \end{aligned} \tag{42}$$

For many simple cluster systems the ψ^{Γ_f}, $\psi^{\Gamma_{A-f}}$, and ψ^{Γ_σ}, can be expanded in terms of simple Slater determinants. It is then possible to extract the K-dependence of the generating function by reducing eq. (42) to a sum over a few basic two-body matrix elements (see, e.g., eq. (10) of ref. [28])).

It may be useful to illustrate with a very specific simple example, and we choose for this purpose the $\alpha+\alpha$ cluster decomposition of ^{8}Be. In this case $\Gamma_\sigma=(40)$, and we make the choice $\alpha_\sigma=\mathrm{SU(3)}$ highest weight state in a cartesian intrinsic basis where all four p-shell nucleons in ^{8}Be carry one oscillator quantum in the z direction. For the $\alpha+\alpha$ cluster we have $\Gamma_c=(00)$, and hence $\alpha_c=000$. A straightforward application of the techniques of ref. [28]) then gives

$$\begin{aligned}
f_{\alpha_0,\alpha_c\alpha_\sigma}(\boldsymbol{K}) = (P_z)^2\{&(X_d+X_e)\langle\psi_1\psi_1|\mathcal{U}|\phi_2\phi_2\rangle\\
&+[((-1)^a+(-1)^b)X_d+(1+(-1)^{a+b})X_e]\langle\psi_1\psi_2|\mathcal{U}|\phi_1\phi_2\rangle P_z\\
&-[(1+(-1)^b)X_d+(1+(-1)^b)X_e]\langle\psi_1\psi_2|\mathcal{U}|\phi_2\phi_2\rangle\\
&+(X_d+X_e)\langle\psi_2\psi_2|\mathcal{U}|\phi_1\phi_1\rangle(P_z)^2\\
&-[(1+(-1)^a)X_d+(1+(-1)^a)X_e]\langle\psi_2\psi_2|\mathcal{U}|\phi_1\phi_2\rangle P_z\\
&+(X_d+X_e)\langle\psi_2\psi_2|\mathcal{U}|\phi_2\phi_2\rangle\}\,,
\end{aligned}\tag{43}$$

where the coefficients X_d and X_e of the direct and exchange matrix elements are given through eq. (9) of ref. [28]). Since $\mathcal{U}$ is a unit tensor operator, $\mathcal{U}^{\Gamma_0}_{\alpha_0}(b,a)_{12}$, with specific a and b, the symmetry properties of this operator under $\boldsymbol{r}_1\leftrightarrow\boldsymbol{r}_2$ have been used to reduce the number of terms in the expansion. The single particle wave functions in the ket side are harmonic oscillator functions centered at the origin

$$\phi_1=\phi_{0s}\,,\qquad \phi_2=\phi_z\,,$$

while those in the bra side are given by

$$\psi_1=A(\gamma\boldsymbol{K},\boldsymbol{r})^*\qquad\text{with }\gamma=\left[\frac{8}{4\cdot4}\right]^{1/2},\qquad \psi_2=\phi_{0s}\,.$$

The total number of oscillator quanta in the bra side of equation (38) cannot be less than those in the ket side in the matrix elements of actual interest in the present application. The last two terms can therefore be eliminated from eq. (43) since the number of oscillator quanta in the bra side of the 2-particle matrix elements again cannot be less than those in the ket side. Effectively, the sum in eq. (43) is thus reduced to the first four terms. By using the expansion of eq. (40) for the orbital ψ_1 in eq. (43) the 2-particle matrix elements can be reduced to standard (single center) shell model form, e.g.

$$\langle\psi_1\psi_2|\mathcal{U}^{\Gamma_0}_{\alpha_0}(b,a)|\phi_1\phi_2\rangle=\sum_{q\alpha_q}P^{(q0)}_{\alpha_q}(\gamma\boldsymbol{K})\langle\phi^{(q0)}_{\alpha_q}(\boldsymbol{r}_1)\phi_{0s}(\boldsymbol{r}_2)|\mathcal{U}^{\Gamma_0}_{\alpha_0}(b,a)|\phi_{0s}(\boldsymbol{r}_1)\phi_z(\boldsymbol{r}_2)\rangle\tag{44}$$

In eq. (43) P_z is a shorthand notation for $P^{(10)}_{200}(\gamma\boldsymbol{K})$, where the SU(3) subgroup label is given in terms of Elliott $\mathrm{SU(2)\times U(1)}$ labels, $\alpha=\varepsilon\Lambda M$. To extract the K-dependent factors from eq. (43) it is still necessary to combine such terms as

$$P_z^2P^{(q0)}_{\alpha_q}(\gamma\boldsymbol{K})P_z=(P^{(10)}_{200}(\gamma\boldsymbol{K}))^3P^{(q0)}_{\alpha_q}(\gamma\boldsymbol{K})\,.$$

The combination of such products is carried out below, see eqs. (48) and (49). The single center 2-particle matrix elements of eq. (44)

$$\begin{aligned}\langle\phi_{\alpha_1'}^{(q_1'0)}(\boldsymbol{r}_1)\phi_{\alpha_2'}^{(q_2'0)}(\boldsymbol{r}_2)|\mathcal{U}_{\alpha_0}^{\Gamma_0}(b,a)|\phi_{\alpha_1}^{(q_1 0)}(\boldsymbol{r}_1)\phi_{\alpha_2}^{(q_2 0)}(\boldsymbol{r}_2)\rangle \\ = \sum_{(\lambda\mu)\alpha}\sum_{(\lambda'\mu')\alpha'}\sum_{\rho_0}\langle(q_1'(0)\alpha_1'(q_2'0)\alpha_2'|(\lambda'\mu')\alpha'\rangle \\ \times\langle(q_1 0)\alpha_1(q_2 0)\alpha_2|(\lambda\mu)\alpha\rangle\langle(\lambda\mu)\alpha(\lambda_0\mu_0)\alpha_0|(\lambda'\mu')\alpha'\rangle_{\rho_0} \\ \times\langle[\phi^{(q_1'0)}(\boldsymbol{r}_1)\times\phi^{(q_2'0)}(\boldsymbol{r}_2)]^{(\lambda'\mu')}\|\mathcal{U}^{(\lambda_0\mu_0)}(b,a)\|[\phi^{(q_1 0)}(\boldsymbol{r}_1)\times\phi^{(q_2 0)}(\boldsymbol{r}_2)]^{(\lambda\mu)}\rangle_{\rho_0}\end{aligned} \tag{45}$$

are easy to evaluate since the reduced matrix elemehs can be expressed in terms of SU(2) d-functions through

$$\begin{aligned}\langle[\phi^{(q_1'0)}(\boldsymbol{r}_1)\times\phi^{(q_2'0)}(\boldsymbol{r}_2)]^{(\lambda'\mu')}\|\mathcal{U}^{(\lambda_0\mu_0)}(b,a)\|[\phi_{(\boldsymbol{r}_1)}^{(q_1 0)}\times\phi^{(q_2 0)}(\boldsymbol{r}_2)]^{(\lambda\mu)}\rangle_{\rho_0} \\ = \delta_{q_1+q_2-a,q_1'+q_2'-b}\, d^{\lambda/2}_{(q_1-q_2)/2,a-(q_1+q_2)/2}(\tfrac{1}{2}\pi)\, d^{\lambda'/2}_{(q_1'-q_2')/2,b-(q_1'+q_2')/2}(\tfrac{1}{2}\pi) \\ \times(-1)^{a+b+\lambda+\mu+\lambda'+\mu'}U((q_1+q_2-a,0)(a0)(\lambda'\mu')(\lambda_0\mu_0);(\lambda\mu)_-\rho_0;(b0)_{--})\,.\end{aligned} \tag{46}$$

The key to the evaluation of the reduced matrix elements (38) through the generating function involves the expansion of $f_{\alpha_0;\alpha_c\alpha_\sigma}(\boldsymbol{K})$ in the form (42) in terms of K-space polynomials $P_{\alpha_Q}^{(Q0)}(\boldsymbol{K})$. From the expansion of form (39), on the other hand, $f_{\alpha_0;\alpha_c\alpha_\sigma}(\boldsymbol{K})$ can be related to the needed reduced matrix elements. With simple SU(3) coupling

$$\begin{aligned}f_{\alpha_0;\alpha_c\alpha_\sigma}(\boldsymbol{K}) = \sum_{Q\alpha_Q}P_{\alpha_Q}^{(Q0)}(\boldsymbol{K})\sum_{\Gamma_{\omega'}\rho_0}\Bigg(\sum_{\alpha_{\omega'}}\langle\Gamma_c\alpha_c(Q0)\alpha_Q|\Gamma_{\omega'}\alpha_{\omega'}\rangle\langle\Gamma_\sigma\alpha_\sigma\Gamma_0\alpha_0|\Gamma_{\omega'}\alpha_{\omega'}\rangle_{\rho_0}\Bigg) \\ \times\langle\mathfrak{A}[[\phi^{\Gamma_f}\times\phi^{\Gamma_{A-f}}]^{\Gamma_c}\times\chi^{(Q0)}(\boldsymbol{R})]^{\Gamma_{\omega'}}\|\sum_{i<j}\mathcal{U}^{\Gamma_0}(b,a)_{ij}\|\phi^{\Gamma_\sigma}\rangle_{\rho_0}\,.\end{aligned} \tag{47}$$

The calculation of $f_{\alpha_0;\alpha_c\alpha_\sigma}(\boldsymbol{K})$ is simplified by a convenient choice of the subgroup labels α_c, α_σ, as already illustrated by the simple example of eq. (43). In general, α_c and α_σ corresponding to SU(3) highest weight labels in a cartesian intrinsic or SU(2)×U(1) basis are most economical in actual calculations. For such a fixed α_c, α_σ it is in general still necessary to vary α_0 in order to get a sufficient number of equations for the determination of the reduced matrix elements of $\mathcal{U}^{\Gamma_0}$ from a comparison of the coefficients of $P_{\alpha_Q}^{(Q0)}(\boldsymbol{K})$.

The expansion of $f_{\alpha_0;\alpha_c\alpha_\sigma}(\boldsymbol{K})$, in the form (42), in terms of the polynomials $P_{\alpha_Q}^{(Q0)}(\boldsymbol{K})$ is best carried out in a cartesian basis. In this basis

$$K_x^{n_1}K_y^{n_2}K_z^{n_3} = [n_1!\,n_2!\,n_3!]^{1/2}P_{\varepsilon\Lambda M}^{(Q0)}(\boldsymbol{K})\,, \tag{48a}$$

where Elliott SU(2)×U(1) labels ε, Λ, M are related to the n_i by

$$\begin{aligned}\varepsilon = 2n_3 - n_1 - n_2\,, \qquad \Lambda = \tfrac{1}{2}(n_1+n_2)\,, \qquad M = \tfrac{1}{2}(n_1-n_2)\,, \\ Q = n_1+n_2+n_3 = \tfrac{1}{2}\varepsilon + 3\Lambda\,.\end{aligned} \tag{48b}$$

In this cartesian basis the analogue of eq. (19) becomes

$$P^{(Q_1 0)}_{\varepsilon_1 \Lambda_1 M_1}(\boldsymbol{K}) P^{(Q_2 0)}_{\varepsilon_2 \Lambda_2 M_2}(\boldsymbol{K}) = \left[\binom{\Lambda_1 + M_1 + \Lambda_2 + M_2}{\Lambda_1 + M_1} \binom{\Lambda_1 - M_1 + \Lambda_2 - M_2}{\Lambda_1 - M_1} \binom{\Lambda_1 + \frac{1}{2}\varepsilon_1 + \Lambda_2 + \frac{1}{2}\varepsilon_2}{\Lambda_1 + \frac{1}{2}\varepsilon_1} \right]^{1/2} \times P^{(Q_1+Q_2,0)}_{\varepsilon_1+\varepsilon_2, \Lambda_1+\Lambda_2, M_1+M_2}(\boldsymbol{K}) , \tag{49a}$$

leading to

$$(P^{(Q0)}_{\varepsilon \Lambda M}(\boldsymbol{K}))^a = \left[\frac{(a\Lambda + aM)!(a\Lambda - aM)!(a\Lambda + \frac{1}{2}a\varepsilon)!}{[(\Lambda + M)!(\Lambda - M)!(\Lambda + \frac{1}{2}\varepsilon)!]^a} \right]^{1/2} P^{(aQ,0)}_{a\varepsilon, a\Lambda, aM}(\boldsymbol{K}) . \tag{49b}$$

Tables 1-3 are included to show some examples of the starting matrix elements of the type given by eq. (38). The examples chosen are some of the simplest α-cluster nuclei. Note that the cluster functions are normalized functions as defined through eq. (33). Note also that reduced matrix elements of $\sum_{i<j} \mathcal{U}^{(\lambda_0\mu_0)}(b, a)_{ij} P_{xij}$, where P_x is the space exchange operator, follow from those in the tables by multiplying the entries in the tables by $(-1)^a$. The tables show the rapid falloff of these starting matrix elements as Q increases appreciably beyond the minimum Pauli-allowed value. Matrix elements with Q = minimum Pauli-allowed values have also been checked by standard shell model techniques [27]). These are also the bandhead-bandhead starting matrix elements needed for the calculation of more general symplectic-symplectic matrix elements by the method of sect. 3.

TABLE 1

Cluster-symplectic starting matrix elements for $\alpha + \alpha / {}^8\mathrm{Be}(40)$

Q	$(\lambda_0\mu_0)$	$\left\langle [(00)\times(Q0)](Q0) \Vert \sum_{i<j} \mathcal{U}^{(\lambda_0\mu_0)}(b, a)_{ij} \Vert \phi^{(40)}({}^8\mathrm{Be}) \right\rangle$		
		$a=0$	$a=1$	$a=2$
4	(00)	15	10	3
	(11)		$\frac{5}{2}\sqrt{7}$	$3\sqrt{\frac{7}{10}}$
	(22)			$2\sqrt{\frac{7}{10}}$
6	(20)	$\frac{3}{2}\sqrt{3}$	5	$\frac{3}{2}\sqrt{\frac{1}{2}}$
	(31)		$\frac{5}{2}\sqrt{\frac{3}{2}}$	$\frac{9}{4}\sqrt{\frac{1}{7}}$
	(42)			$\frac{3}{8}\sqrt{\frac{15}{7}}$
8	(40)	$\frac{1}{2}\sqrt{\frac{15}{2}}$	$5\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{8}}$
	(51)		$\frac{5}{8}\sqrt{\frac{11}{3}}$	$\frac{1}{12}\sqrt{11}$
	(62)			$\frac{1}{6}\sqrt{\frac{11}{10}}$
10	(60)	$\frac{3}{4}\sqrt{\frac{21}{34}}$	$\frac{5}{2}\sqrt{\frac{3}{34}}$	$\frac{3}{8}\sqrt{\frac{3}{34}}$
	(71)		$\frac{1}{8}\sqrt{\frac{195}{17}}$	$\frac{3}{16}\sqrt{\frac{39}{187}}$
	(82)			$\frac{1}{16}\sqrt{\frac{273}{374}}$

$b = Q - 4 + a$.

$\alpha + \alpha$ cluster states are the normalized states of eq. (33).

TABLE 2

Cluster-symplectic starting matrix elements for $\alpha + {}^{12}\mathrm{C}/{}^{16}\mathrm{O}(00)$

Q	$(\lambda_0\mu_0)$	$\left\langle [04)\times(Q0)]^{(\lambda_0\mu_0)} \| \sum_{i<j} \mathcal{U}^{(\lambda_0\mu_0)}(b,a)_{ij} \| \phi^{(00)}({}^{16}\mathrm{O}) \right\rangle$		
		$a=0$	$a=1$	$a=2$
4	(00)	42	60	18
6	(20)	5.809475	11.180340	2.371708
	(31)		1.067391	0.296464
	(42)			−0.530330
8	(40)	1.931389	2.879145	0.498682
	(51)		−0.181076	−0.041818
	(62)			−0.178820
10	(60)	0.503420	0.634250	0.095138
	(71)		−0.112409	−0.022736
	(82)			−0.048120

$b = Q - 4 + a$.

$\alpha + {}^{12}\mathrm{C}$ cluster states are the normalized states of eq. (33).

TABLE 3

Cluster-symplectic starting matrix elements for $\alpha + {}^{16}\mathrm{O}/{}^{20}\mathrm{Ne}(80)$

Q	$(\lambda_0\mu_0)$	$\langle [(00)\times(Q0)](Q0) \| \sum_{i<j} \mathcal{U}^{(\lambda_0\mu_0)}(b,a)_{ij} \| \phi^{(80)}({}^{20}\mathrm{Ne}) \rangle$				
		$a=0$	$a=1$	$a=2$	$a=3$	$a=4$
8	(00)	54.75	87.5	33	12.5	2.25
	(11)		11.726039	7.787008	8.291562	1.994412
	(22)			1.189237	3.385016	1.599087
	(33)				0	1.109588
	(44)					0.587139
10	(20)	3.687807	9.124955	4.301545	3.887290	0.680134
	(31)		2.110568	1.465504	2.312011	0.578003
	(42)			−0.293101	0.867004	0.447719
	(53)				0	0.301852
	(64)					0.155876
12	(40)	1.150399	2.400879	1.188127	1.166717	0.192499
	(51)		0	0.230080	0.648176	0.158950
	(62)			−0.219998	0.229819	0.120155
	(73)				0	0.079330
	(84)					0.040227

$b = Q - 8 + a$.

$\alpha + {}^{16}\mathrm{O}$ cluster states are the normalized states of eq. (33).

6. The ^{8}Be system. A simple example

In order to test the new methods of calculating interactions in a mixed cluster model-symplectic basis we choose a very simple example, the ^{8}Be system. It was this simple system in which the physical significance of symplectic excitations was first recognized by Arickx [22]). It has continued to serve as a testing ground for the newer coherent state techniques [23]) which have recently been refined into a powerful tool for symplectic symmetry calculations [9-14]). The $\alpha+\alpha$ system is also one of the most widely studied from the point of view of the microscopic cluster model (for a comprehensive guide to the literature, see ref. [29])). Since ^{8}Be *is* two α particles the pure α-cluster model must be expected to give a good description of this nuclear system. Nevertheless it is interesting to see to what extent a mixed cluster model-symplectic basis improves this description and to what extent a pure symplectic model rivals the pure cluster model.

The basis states of the $\alpha+\alpha$ cluster model are given by

$$[1-2^{2-Q}]^{-1/2}|\mathfrak{A}[[\phi^{(00)}(\alpha)\phi^{(00)}(\alpha)]^{(00)}\times\chi^{(Q0)}(\boldsymbol{R})]^{(QO)}_{LM_L}\rangle\,, \tag{50}$$

with $Q=4,6,\ldots$. The Sp(6, R) band based on the ^{8}Be $(\lambda_\sigma\mu_\sigma)=(40)$ shell model state has a richer spectrum of SU(3) representations. Since our aim is to compare the symplectic and cluster model and to couple the two into a unified framework, we restrict the symplectic basis to those $(\lambda\mu)$-values which are present in the cluster model, (the Sp(2, R) model of ref. [22])). For the stretched $(\lambda_\sigma+N,0)$ states of this model the κ matrices are 1-dimensional leading to the normalized symplectic basis states

$$\left[\frac{13!!}{(N+13)!!}\right]^{1/2}[\boldsymbol{P}^{(N0)}(\boldsymbol{A}^\dagger)\times|\phi^{(40)}(^8\mathrm{Be})\rangle]^{(N+4,0)}_{LM_L}\,, \tag{51}$$

with $N=0,2,4,\ldots$. The normalized cluster state with $Q=4$ is identical to the symplectic bandhead state with $N=0$. A general formula for the overlaps of the symplectic and $\alpha+\alpha$ cluster states has been given for arbitrary $Q=N+4$ in ref. [7]). It is interesting to note that in this simple system this overlap decreases rather slowly with N (from a value of 0.8944 for $N=2$ to 0.6193 for $N=8$). This contrasts with heavier nuclei where the corresponding falloff is much more rapid [7]).

The evaluation of symplectic-symplectic and cluster-symplectic interaction matrix elements has been carried out by the methods of sect. 3-5. The cluster-cluster interaction matrix elements have been evaluated by the methods of ref. [8]). The matrix element of the interaction, V, between states of type (50) can be extracted from the generating function

$$\langle\mathfrak{A}\{[\phi(\alpha)\times\phi(\alpha)]^{(00)}A(\bar{\boldsymbol{K}},\boldsymbol{R})^*\}|V|\mathfrak{A}\{[\phi(\alpha)\times\phi(\alpha)]^{(00)}A(\boldsymbol{K}^*,\boldsymbol{R})\}\rangle\,, \tag{52}$$

by expanding this Bargmann transform of the interaction in terms of oscillator polynomials in the $\bar{\boldsymbol{K}}$ and $\boldsymbol{K}^*$ (cf. eq. (47)). For a gaussian interaction the function (52) is a sum of exponential terms of the form, $\exp[p(\bar{\boldsymbol{K}}\cdot\bar{\boldsymbol{K}})+q(\boldsymbol{K}^*\cdot\boldsymbol{K}^*)+$

$r(\bar{\boldsymbol{K}}\cdot\boldsymbol{K}^*)]$, which can be expanded as, (see ref. [25]))

$$\exp[p(\boldsymbol{K}\cdot\boldsymbol{K})+q(\boldsymbol{K}^*\cdot\boldsymbol{K}^*)+r(\bar{\boldsymbol{K}}\cdot\boldsymbol{K}^*)]$$
$$=\sum_{\bar{Q}QL}\sum_{t=L,L+2,\ldots}^{\min(\bar{Q},Q)}(-1)^L[2L+1]^{1/2}(P_L^{(\bar{Q}0)}(\bar{\boldsymbol{K}})\times P_L^{(0Q)}(\boldsymbol{K}^*))_{lm=00}$$
$$\times\frac{F(t,L)}{[F(\bar{Q},L)F(Q,L)]^{1/2}}\frac{p^{(\bar{Q}-t)/2}q^{(Q-t)/2}r^t}{[\frac{1}{2}(\bar{Q}-t)]![\frac{1}{2}(Q-t)]!}, \tag{53}$$

with

$$F(Q,L)=\frac{[\frac{1}{2}(Q+L)]!}{[\frac{1}{2}(Q-L)]!(Q+L+1)!},$$

and where the round parentheses indicate angular momentum coupling.

The interaction chosen for the present study is the B_1 potential of Brink–Boeker [30]). The oscillator size parameter, b, of the single particle wave function was set equal to 1.53 fm ($\hbar\omega=17.7$ MeV). Table 4 lists the hamiltonian matrix elements for $L=0$

TABLE 4a

Cluster-cluster matrix elements (MeV)

Q' \ Q	4	6	8	10
4	128.4 − 157.7	−25.7 + 0.9	0 + 4.0	0 − 2.8
6		146.1 − 143.5	−36.7 − 3.5	0 + 7.0
8			163.9 − 133.8	−46.2 − 7.8
10				181.6 − 127.2

TABLE 4b

Symplectic-symplectic matrix elements (MeV)

N' \ N	0	2	4	6
0	128.4 − 157.7	−28.7 + 6.5	0 + 4.9	0 − 5.3
2		146.1 − 146.0	−41.4 + 6.6	0 + 7.4
4			163.9 − 137.2	−52.3 + 6.4
6				181.6 − 130.0

TABLE 4c

Cluster-symplectic matrix elements (MeV)

N \ Q	6	8	10
2	130.7-130.7	−32.8-1.8	0 + 6.0
4	−37.0 + 5.5	129.8 − 109.2	−36.6 − 3.9
6	0 + 6.8	−41.4 + 4.5	127.0 − 92.2

TABLE 5

Comparison of $L=0$ state vectors

$(\lambda 0)$	Pure α-cluster amplitude	Pure Sp(6, R) amplitude	Mixed calc. amplitudes
(40)	0.6154	0.7001	0.6152
(60)	0.5833	0.5806	α 0.5839
			sp 0.0366
(80)	0.4306	0.3505	α 0.4288
			sp 0.0133
(10, 0)	0.2805	0.2069	α 0.2793
			sp 0.0213
(12, 0)	0.1301	0.0842	α 0.1292
			sp 0.0067
	$E_0=-50.94$	$E_0=-46.24$	$E_0=-51.04$ MeV

Comparison of $L=2$ state vectors

$(\lambda 0)$	Pure α-cluster amplitude	Pure Sp(6, R) amplitude	Mixed calc. amplitudes
(40)	0.6094	0.6970	0.6077
(60)	0.5829	0.5811	α 0.5842
			sp 0.0423
(80)	0.4356	0.3552	α 0.4341
			sp 0.0201
(10, 0)	0.2855	0.2069	α 0.2841
			sp 0.0213
(12, 0)	0.1332	0.0865	α 0.1324
			sp 0.0089
	$E_2=-48.10$	$E_2=43.63$	$E_2=-48.20$ MeV

TABLE 6

B(E2) value and α spectroscopic factor comparisons

	Pure α cluster model	Pure Sp(6, R) model	Mixed cluster-Sp(6, R)
B(E2) values [a]			
$2_1^+ \to 0_1^+$	$(6.847)^2$	$(6.422)^2$	$(6.910)^2$
$4_1^+ \to 2_1^+$	$(7.857)^2$	$(7.214)^2$	$(7.971)^2$
S_α 0_1^+	0.8808	0.7199	0.8789
2_1^+	0.8826	0.7193	0.8803
4_1^+	0.8890	0.7173	0.8853

[a] In units of $\frac{15}{16\pi}\left(\frac{e}{2}\frac{\hbar}{m\omega}\right)^2$.

and the lower Q (or N) values. Note that the kinetic energy matrix elements, (limited to ΔQ (or ΔN) ≤ 2), and V matrix elements are listed separately. The similarity between the cluster-cluster and symplectic-symplectic interaction matrix elements are very striking. Table 5 compares the results for the $L=0$ and $L=2$ states of a pure α-cluster model calculation, and a calculation in a mixed α-cluster-symplectic basis, all with SU(3) representations limited to $(\lambda\mu)=(40), (60), \ldots$. For the mixed calculation α designates the α-cluster state, whereas sp designates the component of the (normalized) symplectic state of eq. (51) which is made orthogonal to the α-cluster state of eq. (50). Very similar results are obtained for $L \geq 4$. Table 6 compares some B(E2) values and $\alpha+\alpha$ spectroscopic factors. It is apparent that the mixed α-cluster-symplectic basis leads to only a very small improvement in the ground state energy (in the variational sense) and to only very small changes in the α-cluster wave functions as evidenced by the very small admixtures of the components of the symplectic excitations which lie outside the cluster model basis. It is interesting to note that the pure symplectic model calculation gives a very good account of this system of two α particles. The predicted distribution of core excitations is very similar to that of the α-cluster calculations. The excitation spectra are very similar; e.g., 2^+ and 4^+ excitated states at 2.60 and 9.36 MeV compared with 2.85 and 10.13 MeV for the pure α-model (and 2.84 and 10.07 MeV for the mixed basis). The two models are almost identical in their B(E2) predictions, and although the pure symplectic model predicts somewhat smaller α spectroscopic factors it does give a reasonable account of the $\alpha+\alpha$ character of the simple ^{8}Be system.

7. Summary

A practical method has been developed for the evaluation of matrix elements of a general translationally invariant two-body interaction in a mixed symplectic and microscopic cluster model basis. The method makes use of a reduction formula which expresses (i) a matrix element connecting states of arbitrary excitations N and N' in the same or in different symplectic bands, or (ii) a matrix element between an Nth excitation in a symplectic band and a cluster model state with arbitrary oscillator excitations in its relative motion function, in terms of much simpler matrix elements, see eqs. (31) and (37). These simpler matrix elements are matrix elements of SU(3) unit tensor operators of ordinary shell model or of standard microscopic cluster model type and can therefore be evaluated by the highly developed techniques of these models. The reduction formula is given in complete generality for an arbitrary symplectic excitation. For many of the simpler symplectic excitations, of greatest interest in actual applications, the many possible SU(3) multiplicity labels are unnecessary, and most of the transformation matrices to the new canonical orthonormal Sp(6, R) basis are 1-dimensional, so that the total number of terms

needed for the evaluation of the reduction formula becomes quite small. A few numerical results are given, for some simple nuclei, of the starting matrix elements needed for the reduction formula in order to illustrate the range of these numbers. To establish the new method of calculation a study is made of a very simple system, the ^{8}Be nucleus. Since ^{8}Be is two α-particles, and since the overlap between the $\alpha+\alpha$ cluster functions and the symplectic excitations decreases slowly with the degree of excitation N, it is not surprising that the calculation in a mixed cluster model-symplectic basis leads only to marginally significant improvement in the description of this $\alpha+\alpha$ system. Nevertheless, it is interesting to see that a pure symplectic model calculation also gives a good account of ^{8}Be. In heavier nuclei, however, the overlaps between binary cluster model wave functions and the corresponding symplectic excitations generally fall off rapidly [7]) for $N \geq 4$, even when these overlaps are large for states of $N=2$. In such nuclei a unified treatment merging a cluster model basis with a basis built from several symplectic bands may be required for a satisfactory description of their structure. For ^{16}O, e.g., a basis combining $\alpha + {}^{12}$C cluster model functions with symplectic bands built on $(\lambda_\sigma \mu_\sigma)$'s of at least (00), (42), (84) for positive parity states and (21), (63), and (94) for negative parity states should overcome the deficiencies of earlier studies of this nucleus. The feasibility of such a study has now been demonstrated.

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Appendix A

The expansion coefficients $c_q^{\Gamma_n}(\Gamma)$ of eq. (20) have been calculated by a simple recursive process and are given in table 7. For brevity, terms with $q=0$, given by $c_0^{\Gamma_n}(\Gamma) = \delta_{\Gamma_n,\Gamma}$, are omitted from the table.

Appendix B

To evaluate the matrix elements

$$\begin{aligned}\langle \Gamma_{\sigma'} \Gamma_{n'} \rho' \Gamma_{\omega'} \alpha_{\omega'} | [[\boldsymbol{P}^{\bar{\Gamma}}(\boldsymbol{A}^\dagger) \times |\Gamma_{\sigma'} \Gamma_{n''} \rho''' \Gamma_{\omega''}\rangle]^{\Gamma_{\omega'}\bar{\rho}}_{\alpha_{\omega'}} \\ = \sum_{n_2\rho_2} (\kappa^{-1}(\Gamma_{\sigma'}, \Gamma_{\omega''}))_{n''\rho''', n_2\rho_2} \sum_{\Gamma_3\rho\rho_3} U(\bar{\Gamma}\Gamma_{n_2}\Gamma_{\omega'}\Gamma_{\sigma'}; \Gamma_3\rho\rho_3; \Gamma_{\omega''}\rho_2\bar{\rho}) \\ \times [[P^{\bar{\Gamma}}(\boldsymbol{A}^\dagger) \times P^{\Gamma_{n_2}}(\boldsymbol{A}^\dagger)]^{\Gamma_3\rho} \times |\Gamma_{\sigma'}\rangle]^{\Gamma_{\omega'}\rho_3}_{\alpha_{\omega'}}, \end{aligned} \tag{B.1}$$

needed for eq. (31b), it is useful to define the coefficients $B(\Gamma_1\Gamma_2, \Gamma_3\rho)$ through

$$[P^{\Gamma_1}(\boldsymbol{A}^\dagger) \times P^{\Gamma_2}(\boldsymbol{A}^\dagger)]^{\Gamma_3\rho}_{\alpha_3} = B(\Gamma_1\Gamma_2, \Gamma_3\rho) P^{\Gamma_3}_{\alpha_3}(\boldsymbol{A}^\dagger). \tag{B.2}$$

These can be evaluated through a recursion formula

$$\begin{aligned} B(\Gamma_1\Gamma_2, \Gamma_3\rho) = \frac{1}{(\Gamma_1 \| \boldsymbol{a}^\dagger \| \Gamma_1')} \sum_{\Gamma_3'\rho'} (\Gamma_3 \| \boldsymbol{a}^\dagger \| \Gamma_3') \\ \times B(\Gamma_1'\Gamma_2, \Gamma_3'\rho') U((20)\Gamma_1'\Gamma_3\Gamma_2; \Gamma_{1-}\rho; \Gamma_3'\rho'_-). \end{aligned} \tag{B.3}$$

TABLE 7

The transformation coefficients $c_{q^n}^{\Gamma_n}(\Gamma)$

$N=4$	Γ_4	
q Γ	(40)	(02)
4 (00)	$\sqrt{3}$	
2 (20)	$\sqrt{2}$	$\sqrt{2}$

$N=6$	Γ_6		
q Γ	(60)	(22)	(00)
6 (00)	$\sqrt{15}$		
4 (20)	3	2	
2 (40)	$\sqrt{3}$	$\sqrt{\frac{4}{3}}$	
2 (02)		$\sqrt{\frac{5}{3}}$	$\sqrt{3}$

$N=8$	Γ_8			
q Γ	(80)	(42)	(04)	(20)
8 (00)	$\sqrt{105}$			
6 (20)	$2\sqrt{15}$	$3\sqrt{2}$		
4 (40)	$3\sqrt{2}$	2	$2\sqrt{2}$	
4 (02)		$\sqrt{7}$		$\sqrt{5}$
2 (60)	2	$\sqrt{\frac{6}{5}}$		
2 (22)		$\sqrt{\frac{14}{5}}$	2	$\sqrt{\frac{5}{2}}$
2 (00)				$\sqrt{\frac{3}{2}}$

$N=10$	Γ_{10}				
q Γ	(10, 0)	(62)	(24)	(40)	(02)
10 (00)	$3\sqrt{105}$				
8 (20)	$5\sqrt{21}$	$2\sqrt{30}$			
6 (40)	$5\sqrt{6}$	$2\sqrt{6}$	$2\sqrt{6}$		
6 (02)		$3\sqrt{5}$		$\sqrt{21}$	
4 (60)	$\sqrt{30}$	$\sqrt{\frac{24}{5}}$	$\sqrt{\frac{24}{5}}$		
4 (22)		$9\sqrt{\frac{1}{5}}$	$\sqrt{\frac{56}{5}}$	$\sqrt{7}$	$\sqrt{10}$
4 (00)				$\sqrt{6}$	
2 (80)	$\sqrt{5}$	$\sqrt{\frac{8}{7}}$			
2 (42)		$\sqrt{\frac{27}{7}}$	$\sqrt{\frac{8}{3}}$	$\sqrt{\frac{7}{3}}$	
2 (04)			$\sqrt{\frac{7}{3}}$		$\sqrt{\frac{5}{3}}$
2 (20)				$\sqrt{\frac{8}{3}}$	$\sqrt{\frac{10}{3}}$

Note that $c_0^{\Gamma_n}(\Gamma) = \delta_{\Gamma_n,\Gamma}$.

TABLE 8

The coefficients $B(\Gamma_1\Gamma_2, \Gamma_3\rho)$

Γ_1	Γ_2	Γ_3	B
[200]	[200]	[400]	$\sqrt{2}$
		[220]	$\sqrt{2}$
[400]	[200]	[600]	$\sqrt{3}$
		[420]	$\sqrt{\frac{4}{3}}$
[220]	[200]	[420]	$\sqrt{\frac{5}{3}}$
		[222]	$\sqrt{3}$
[600]	[200]	[800]	$\sqrt{4}$
		[620]	$\sqrt{\frac{6}{5}}$
[420]	[200]	[620]	$\sqrt{\frac{14}{5}}$
		[422]	$\sqrt{\frac{5}{2}}$
		[440]	$\sqrt{4}$
[222]	[200]	[422]	$\sqrt{\frac{3}{2}}$
[400]	[400]	[800]	$\sqrt{6}$
		[620]	$\sqrt{\frac{4}{3}}$
		[422]	0
		[440]	$\sqrt{\frac{8}{3}}$
[400]	[220]	[620]	$\sqrt{\frac{7}{3}}$
		[422]	$\sqrt{\frac{5}{3}}$
		[440]	0
[220]	[220]	[422]	$\sqrt{\frac{8}{3}}$
		[440]	$\sqrt{\frac{10}{3}}$

For $N_3 \leq 8$ the label ρ is not needed.

This follows from

$$[[A^{\dagger(20)} \times P^{\Gamma_1'}]^{\Gamma_1} \times P^{\Gamma_2}]^{\Gamma_3}_{\alpha_3} = (\Gamma_1 \| a^\dagger \| \Gamma_1') B(\Gamma_1\Gamma_2, \Gamma_3\rho) P^{\Gamma_3}_{\alpha_3}, \tag{B.4}$$

through eq. (5), and a similar expression following an SU(3) recoupling of the left hand side.

$$[[A^{\dagger(20)} \times P^{\Gamma_1'}]^{\Gamma_1} \times P^{\Gamma_2}]^{\Gamma_3\rho}_{\alpha_3} = \sum_{\Gamma_3'\rho'} U((20)\Gamma_1'\Gamma_3\Gamma_2; \Gamma_1 - \rho; \Gamma_3'\rho'_-)(\Gamma_3 \| a^\dagger \| \Gamma_3') B(\Gamma_1'\Gamma_2, \Gamma_3'\rho') P^{\Gamma_3}_{\alpha_3}. \tag{B.5}$$

The coefficients $B(\Gamma_1\Gamma_2\ \Gamma_3\rho)$ with $N_3 \leq 8$ are given explicitly in table 8.

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