J. Phys. A: Math. Gen. 18 (1985) L1003-L1008. Printed in Great Britain

LETTER TO THE EDITOR

An approximation formula for the κ-matrix elements of the symplectic algebra Sp(6, R)

K T Hecht†

Physics Department, University of Michigan, Ann Arbor, MI 48109, USA

Received 4 September 1985

Abstract. A simple approximation formula, valid to the high degree of accuracy of the Toronto approximation, is given for both the off-diagonal and diagonal matrix elements of the κ matrices which transform the bosonic realisations of the symplectic algebra into an orthonormal basis for a unitary irreducible representation of Sp(6, R).

In the past few years the mathematics of the non-compact symplectic groups Sp(2d, R) has been fully developed through the use of a generalised coherent state theory (Rowe *et al* 1984, Rowe 1984, Deenen and Quesne 1982, 1984, 1985, Kramer *et al* 1983) or through the use of boson realisations of the symplectic algebras (Moshinsky *et al* 1984, Moshinsky 1985, Castaños *et al* 1985a, b) which have led to very explicit constructions for the discrete infinite-dimensional unitary irreducible representations of Sp(2d, R). The case of Sp(6, R) is of particular interest since Sp(6, R) has emerged as the appropriate dynamical group for a many-body theory of nuclear collective motion (Rosensteel and Rowe 1977, 1980). Since Sp(6, R) is also the dynamical group for the three-dimensional harmonic oscillator, symplectic symmetry has also established a powerful link between the nuclear shell model and the collective model and has led to the possibility of fully microscopic calculations of nuclear collective phenomena (for a review, see Rowe 1985). Despite the powerful mathematical advances the applications have been somewhat limited. In this connection the work of the Toronto group is particularly relevant. It has been shown that a very simple analytical formula for the matrix elements of the Sp(6, R) generators, which is exact for all states of an irreducible representation which are multiplicity free with respect to the U(3) subgroup, is also a remarkably good approximation formula, in general, for the Sp(6, R) irreducible representations of actual interest in deformed nuclei (Rowe *et al* 1984).

For detailed applications to nuclear spectroscopy a similar approximation formula would be useful for the matrix elements of the κ matrices which are central for the Sp(2d, R) state construction. These are the matrices which transform the states of the associated boson algebras from a mere labelling scheme into an orthonormal basis for a unitary representation of Sp(6, R). Very recently it has been shown that the operator κ^2 can be evaluated from a coherent state generating kernel for which a closed analytic expression can be given (Castaños *et al* 1985, Kramer 1985, Quesne 1985). To obtain the needed matrix elements of κ^2 it is necessary to expand this kernel in the appropriate basis polynomials of the associated Bargmann space of complex variables. Although

† Supported in part by the US National Science Foundation.

specific results have been given for Sp(4, R) (Castaños *et al* 1985, Moshinsky *et al* 1985), results for the general states of Sp(6, R) irreducible representations can be expected to be complicated and final analytical expressions can be given only in terms of formulae involving a number of summations. Although exact values of κ^2 matrix elements can be evaluated either by these elegant new techniques or the older numerical methods of solving recursion relations, the process is somewhat complicated. Moreover, the needed matrix elements are those of κ. Their evaluation, in the general case, requires a further process of square root taking involving prior diagonalisation of the κ^2 matrices. It is the purpose of this letter to show that the powerful Toronto approximation formula can be extended for a direct evaluation of the matrix elements of κ, both off-diagonal and diagonal. The high degree of accuracy of this approximation transcends the requirements of nuclear spectroscopy and should thus facilitate the practical applications.

The states of the Sp(6, R) $\supset$ U(3) basis are labelled 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 the raising polynomial, and Γ_ω the U(3) symmetry of the final state. It will be convenient to use the general shorthand label, Γ, for a U(3) or SU(3) representation label, and α for a convenient set of U(3) subgroup labels. Otherwise the notation follows that of Rowe *et al.* Thus

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

where $(\lambda\mu)$ are Elliott SU(3) labels (Elliott 1958) and the N's give the number of squares in the U(3) Young tableaux. The familiar realisation of the symplectic 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, $\boldsymbol{C}$, which can be expressed in terms of oscillator creation and annihilation operators $(b^\dagger_{si}, b_{si})$; with $A^\dagger_{ij} = \Sigma_s b^\dagger_{si} b^\dagger_{sj}$, $A_{ij} = \Sigma_s b_{si} b_{sj}$, and $C_{ij} = \frac{1}{2}\Sigma_s (b^\dagger_{si} b_{sj} + b_{sj} b^\dagger_{si})$, where $i, j = 1, 2, 3$. In the nuclear applications the s variables stand for a convenient set of Jacobi relative motion variables with $s = 1, \ldots, A-1$, where A = nucleon number. The Sp(6, R) state construction proceeds via the states

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

where the square bracket denotes SU(3) coupling, and the multiplicity quantum number ρ which distinguishes multiple occurrences 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 raising polynomials can be given by the expansions

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

with

$$x^{\Gamma_n}(\Gamma_{n'}) = N^{-1}(n \| a^\dagger \| n'), \tag{4}$$

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

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

where the boson SU(3)-reduced matrix elements are given, e.g., by equation (12) of Rowe *et al* and have the property $\Sigma_{n'}(n\|a^\dagger\|n')^2 = N$.

The non-orthonormal states $|\Omega(\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\alpha_\omega)\rangle$ lead to the overlap matrix which is the matrix κ^2 (Le Blanc and Rowe 1985), central for the Sp(6, R) state construction,

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

where κ^2 is diagonal in Γ_σ and Γ_ω and independent of U(3) subgroup labels α_ω, with rows and columns labelled by Γ_n and ρ. For actual calculations it is also useful to define normalised states

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

with overlap matrices

$$\langle\bar{\Psi}(\Gamma_\sigma\Gamma_{n'}\rho'\Gamma_\omega)\alpha_\omega|\bar{\Psi}(\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\alpha_\omega)\rangle = (M(\Gamma_\sigma,\Gamma_\omega))_{n'\rho',n\rho}, \tag{8}$$

with diagonal elements of unity, $M_{aa} = 1$. Off-diagonal matrix elements M_{ab}, $a \neq b$, are of order $(3/2\sigma)$, the parameter of smallness of the Toronto approximation formula (Rowe 1984), with $\sigma = \lambda_\sigma + 2\mu_\sigma + 3(\sigma_3 + 1/2(A-1))$ (cf equation (1)). Although small, these off-diagonal matrix elements are by no means negligible to the high degree of accuracy of the Toronto approximation.

Finally, the states $|\Psi\rangle$ of (2) are related to the orthonormal basis states of the unitary irreducible representation of Sp(6, R) (Le Blanc and Rowe 1985) by

$$|\Psi(\Gamma_\sigma\Gamma_{n_i}\rho_i\Gamma_\omega\alpha_\omega)\rangle = \sum_j (\kappa(\Gamma_\sigma,\Gamma_\omega))_{n_i\rho_i,n_j\rho_j}|\Gamma_\sigma\Gamma_{n_j}\rho_j\Gamma_\omega\alpha_\omega\rangle, \tag{9}$$

where $|\Gamma_\sigma\Gamma_{n_j}\rho_j\Gamma_\omega\alpha_\omega\rangle$, 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. It is in this orthonormal basis that the SU(3) reduced matrix elements of the raising generators are given by the simple Toronto approximation formula

$$\begin{aligned}\langle\Gamma_\sigma\Gamma_{n'}\rho'\Gamma_{\omega'}\|A^\dagger\|\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\rangle \simeq{}& [\Omega(\sigma n'\omega') - \Omega(\sigma n\omega)]^{1/2}(n'\|a^\dagger\|n)\\ &\times(-1)^{\Gamma_\omega - \Gamma_{\omega'}}U((20)\Gamma_n\Gamma_\omega\Gamma_\sigma;\Gamma_{n'-}\rho';\Gamma_\omega\rho_-).\end{aligned} \tag{10a}$$

The U coefficient is an SU(3) Racah coefficient (Hecht 1965), readily available through the computer code of Akiyama and Draayer (1973a, b). The phase factor $(-1)^\Gamma$ is an abbreviation for $(-1)^{\lambda+\mu}$. The eigenvalues $\Omega(\sigma n\omega)$ are given by (13) of Rowe *et al*. For ready calculation it is convenient to put the difference in the form

$$\begin{aligned}&[\Omega(\sigma n'\omega') - \Omega(\sigma n\omega)]\\ &\quad= [\tfrac{1}{2}(\Delta\omega_1^2 + \Delta\omega_2^2 + \Delta\omega_3^2) + (\lambda_\omega + \mu_\omega - 1)\Delta\omega_1 + (\mu_\omega - 2)\Delta\omega_2\\ &\qquad - 3\Delta\omega_3 + 2\omega_3 + (A-1) + \chi(\boldsymbol{n})],\end{aligned}$$

with

$$\chi(\boldsymbol{n}) = \begin{cases} -n_1 \\ -n_2 + 1 \\ -n_3 + 2 \end{cases} \quad \text{for} \begin{cases} \Delta n_1 = 2 \\ \Delta n_2 = 2 \\ \Delta n_3 = 2 \end{cases} \tag{10b}$$

and where $\Delta\psi_i = \omega_i' - \omega_i$, $\Delta n_i = n_i' - n_i$, $\lambda_\omega = \omega_1 - \omega_2$, $\mu_\omega = \omega_2 - \omega_3$.

Using the orthonormality of the states $|\Gamma_\sigma \Gamma_{n_i} \rho_i \Gamma_\omega \alpha_\omega\rangle$ (9) leads to

$$
\begin{aligned}
&(\kappa(\Gamma_\sigma, \Gamma_\omega))_{n_i\rho_i, n_j\rho_j} \\
&\quad = \langle \Gamma_\sigma \Gamma_{n_j} \rho_j \Gamma_\omega \alpha_\omega | \Psi(\Gamma_\sigma \Gamma_{n_i} \rho_i \Gamma_\omega \alpha_\omega)\rangle \\
&\quad = \sum_{\Gamma_{n''}} x^{\Gamma_{n_i}}(\Gamma_{n''}) \sum_{\Gamma_{\omega''}\rho''} U((20)\Gamma_{n''}\Gamma_\omega\Gamma_\sigma; \Gamma_{n_i}\rho_i; \Gamma_{\omega''}\rho''_-) \\
&\qquad \times \langle \Gamma_\sigma \Gamma_{n_j} \rho_j \Gamma_\omega \| A^{\dagger(20)} \| \Psi(\Gamma_\sigma \Gamma_{n''} \rho'' \Gamma_{\omega''})\rangle (-1)^{\Gamma_\omega - \Gamma_{\omega''}}, \qquad (11)
\end{aligned}
$$

where (2) and (3) were substituted into the right-hand side, and the standard definition of the SU(3) reduced matrix element required a change in the order of the SU(3) coupling $[(20) \times \Gamma_{\omega''}]^{\Gamma_\omega}$. Using the transformation (9) for the state $|\Psi(\Gamma_\sigma \Gamma_{n''} \rho'' \Gamma_{\omega''})\rangle$ with $N'' = N - 2$ and the basic approximation formula, (10), leads to the final approximation formula for the transformation coefficients, κ,

$$
\begin{aligned}
&(\kappa(\Gamma_\sigma, \Gamma_\omega))_{n_i\rho_i, n_j\rho_j} \\
&\quad \simeq \sum_{\Gamma_{n''}} \sum_{\Gamma_{\omega''}\rho''} \sum_{\Gamma_{n'''}\rho'''} \frac{1}{N} (n_i \| a^\dagger \| n'')(n_j \| a^\dagger \| n''') \\
&\qquad \times [\Omega(\sigma n_j \omega) - \Omega(\sigma n''' \omega'')]^{1/2} (\kappa(\Gamma_\sigma, \Gamma_{\omega''})_{n''\rho'', n'''\rho'''} \\
&\qquad \times U((20)\Gamma_{n''}\Gamma_\omega\Gamma_\sigma; \Gamma_{n_i}\rho_i; \Gamma_{\omega''}\rho''_-) U((20)\Gamma_{n'''}\Gamma_\omega\Gamma_\sigma; \Gamma_{n_j}\rho_j; \omega_{n''}\rho'''_-). \qquad (12)
\end{aligned}
$$

From this formula the κ matrix elements for a particular value of N can be evaluated directly if the κ matrix elements for states with $N'' = N - 2$ are known. (Note that κ is a unit matrix for the symplectic bandhead state with $N = 0$ and $\Gamma_\omega \equiv \Gamma_\sigma$.) A very straightforward recursive process thus gives an approximate evaluation of the κ matrix elements. If separate evaluations of the normalisation constants $\mathcal{N}$ and the overlaps M_{ab} of (7) and (8) are needed these follow from the above since $\kappa_{ab} = (M^{1/2})_{ab}/\mathcal{N}_a$. To the degree of approximation of (12), $(M^{1/2})_{aa} \simeq 1$, and $(M^{1/2})_{ab} \simeq \frac{1}{2}(M)_{ab}$ with $a \neq b$.

To illustrate the high degree of accuracy of the Toronto approximation for the nuclear applications table 1 shows a few examples in which the exact values are

Table 1. Examples of κ matrices

$\kappa((80),(82))_{\text{Exact}}$		$\kappa((80),(82))_{\text{Approx}}$	
(40)	(02)	(40)	(02)
32.588 68	−0.558 06	32.588 44	−0.559 02
−0.558 06	33.709 87	−0.559 02	33.710 06
$\kappa((80),(10,2))_{\text{Exact}}$		$\kappa((80),(10,2))_{\text{Approx}}$	
(60)	(22)	(60)	(22)
214.448 22	−3.655 45	214.445 53	−3.671 04
−3.655 45	225.340 27	−3.671 04	225.340 86
$\kappa((80),(64))_{\text{Exact}}$		$\kappa((80),(64))_{\text{Approx}}$	
(60)	(22)	(60)	(22)
164.079 59	−1.699 59	164.078 85	−1.706 87
−1.699 59	173.916 97	−1.706 87	173.916 52

$(\lambda_\sigma \mu_\sigma) = (80)$ $\sigma_3 + 1/2(A-1) = 13.5$.

compared with those given by the approximation formula, (12). The examples chosen involve Sp(6, R) excitations of relevance in ^{20}Ne with $\Gamma_\sigma = (\lambda_\sigma \mu_\sigma) = (80)$ and $\sigma_3 + \frac{1}{2}(A-1) = 13.5$; that is, with the smallness parameter $(3/2\sigma) = (1/32.333)$. This is one of the lightest nuclei with strong intrinsic deformation and therefore a high degree of symplectic symmetry. The approximations are even better in heavier deformed nuclei, with larger values of σ. Moreover, the approximation formula, (12), is so simple that explicit analytic expressions can be given for the simpler symplectic excitations of greatest interest in the actual nuclear applications. As an example, with $N = 4$, and $(\lambda_\omega \mu_\omega) = (\lambda_\sigma, \mu_\sigma + 2)$, with $\Gamma_n = (\lambda_n \mu_n) = (40)$ or (02), the off-diagonal matrix eleements of κ are given by

$$
\begin{aligned}
(\kappa(\lambda_\omega \mu_\omega) = (\lambda_\sigma, \mu_\sigma + 2))_{\substack{(40)(02) \\ (02)(40)}} & \\
\simeq \frac{1}{3}\left(\frac{(\lambda_\sigma - 1)(\lambda_\sigma + 3)}{2\lambda_\sigma(\lambda_\sigma + 2)}\right)^{1/2} & \left(\frac{\lambda_\sigma}{(\lambda_\sigma + 1)}[2\sigma_1 + (A-1)]^{1/2}[2\sigma_2 + (A-1)^{-1}_{-4}]^{1/2}\right. \\
+ \left(\frac{(\lambda_\sigma + 2)}{(\lambda_\sigma + 1)}\right. & [2\sigma_2 + (A-1) - 2]^{1/2}[2\sigma_1 + (A-1)^{+1}_{-2}]^{1/2} \\
- 2[\sigma_1 + \sigma_2 + (A-1) - 2]^{1/2} & \left.\left.[\sigma_1 + \sigma_2 + (A-1)^{+1}_{-2}]^{1/2}\right)\right). \qquad (13)
\end{aligned}
$$

It is clear from this example that the approximation formula, (12), does not preserve the predicted symmetry of the κ matrix. The off-diagonal elements shown for $(\kappa)_{\text{approx}}$ of table 1 are the averages of κ_{ab} and κ_{ba}. The differences between κ_{ab} and κ_{ba} can be used to give a quantitative measure of the accuracy of the approximation formula, (12), in any specific case. For the first entry of table 1 with $(\lambda_\sigma \mu_\sigma) = (80)$, $(\lambda_\omega \mu_\omega) = (82)$, (13) gives

$$\kappa_{(40)(02)} = -0.546\,196, \qquad \kappa_{(02)(40)} = -0.571\,853,$$

so that $\kappa_{\text{average}} = -0.559\,02$. The errors inherent in the approximations of (12) are expected to be of order $1/2(3/2\sigma)^2$ compared with the dominant diagonal matrix elements (cf Rowe 1984). Table 1 shows that actual numbers are well within these limits and the 1 part in 10^4 accuracy actually achieved transcends the usual requirements of nuclear spectroscopy.

References

Akiyama Y and Draayer J P 1973a *Comput. Phys. Commun.* **5** 405

—— 1973b *J. Math. Phys.* **14** 1904

Castaños O, Chacón E, Moshinsky M and Quesne C 1985a *J. Math. Phys.* **26** to be published

Castaños O, Kramer P and Moshinsky M 1985b *J. Phys. A: Math. Gen.* **18** L493

Castaños O, Kramer P, Moshinsky M and Quesne C 1985 to be published

Deenen J and Quesne C 1982 *J. Math. Phys.* **23** 878, 2004

—— 1984a *J. Math. Phys.* **25** 1638, 2354

—— 1984b *J. Phys. A: Math. Gen.* **17** L405

—— 1985 *Preprint, Boson Representations of the Real Symplectic Group and their Application to the Nuclear Collective Model, PTM 84-07*, Université Libre de Bruxelles

Elliott J P 1958 *Proc. R. Soc.* A **245** 128, 562

Hecht K T 1965 *Nucl. Phys.* **62** 1

Kramer P 1985 *Irreducible representations of the Symplectic Group in Hilbert Spaces of Analytic Functions and Associated Dyson and Holstein Primakoff Realisations* to be published
Kramer P, Papadopoulos Z and Schweizer W 1983 *Ann. Phys., NY* **149** 44
Le Blanc R and Rowe D J 1985 *J. Phys. A: Math. Gen.* **18** 1891, 1905
Moshinsky M 1985 *J. Phys. A: Math. Gen.* **18** L1
Moshinsky M, Chacón E and Castaños O 1984 in *Proc. 13th Colloq. on Group Theoretical Methods in Physics* (Singapore: World Scientific)
Quesne C 1985 *Preprints, Coherent States of the Real Symplectic Group in a Complex Analytic Parametrization. I Unitary-Operator Coherent States. II Annihilation-Operator Coherent States, PTM 85-04, PTM 85-05,* Université Libre de Bruxelles
Rowe D J 1984 *J. Math. Phys.* **25** 2662
—— 1985 *Rep. Prog. Phys.* **48** 1419
Rowe D J, Rosensteel G and Carr R 1984 *J. Phys. A: Math. Gen.* **17** L399
Rosensteel G and Rowe D J 1977 *Phys. Rev. Lett.* **38** 10
—— 1980 *Ann. Phys., NY* **126** 343