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Angular momentum projection integrals for coherent states

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Abstract. Angular momentum projection integrals arising from the coherent state representation of bosonic spectrum generating algebras are evaluated using analytical and algebraic methods. For the vibron model of diatomic molecules, a closed expression is derived by direct integration. For the general case, the integral is evaluated as a 1/N expansion by exploiting the symmetries of the underlying boson system and making use of computer algebra.

1. Introduction

Algebraic methods have become important tools in nuclear and molecular structure physics [1]. The interacting boson model (IBM) of collective nuclei [2] and the vibron model of molecules [3] are two examples of bosonic spectrum generating algebras (SGA) widely used in the analysis of experimental data. Though algebraic methods are computationally superior to solving differential equations, they tend to be abstract, lacking an immediate physical picture often associated with the solutions of Schrödinger-like equations. This shortcoming has been overcome with the introduction of coherent (intrinsic) states which conferred a geometric picture to the algebraic models [2-4]. The intrinsic states have also been used in deriving various matrix elements (ME) of interest in the IBM [2]. However, because the rotational symmetry is broken in the intrinsic frame, these can only provide a rough estimate for the ME. In order to obtain more accurate results, one has to restore the rotational invariance by performing angular momentum projection. This program has been carried out in the IBM [5] and was shown to lead to a 1/N expansion for all ME where N denotes the number of bosons in the system. Since variation after projection (with a complete set of states) is equivalent to solving the Schrödinger equation, this approach has the potential of providing analytical solutions for bosonic SGA to any desired level of accuracy (in powers of 1/N).

A vital ingredient in the 1/N calculations is the evaluation of angular momentum projection integrals. These are presently available, in closed form, only in the dynamical symmetry limits of certain SGA, e.g. SU(3) in the IBM and O(4) in the vibron model. For general cases, a Gaussian approximation was employed in the initial papers [5], which limited the accuracy of the expansion to the first layer (see below for the definition of layers). Recently, the projection integrals were evaluated to the order $1/N^2$ using the Laplace method [6]. Although this method can be used, in principle, to calculate the higher orders in the 1/N expansion, it has not been pursued as the algebraic manipulations required are tedious.

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Also the Laplace method requires a separate calculation for each SGA which misses the common thread among such integrals. The level of accuracy needed to describe either the high-spin states in nuclei or the rotation-vibration spectra in molecules is such that one has to evaluate energy expressions up to the order $1/N^6$ (or to the third layer). Clearly, this is beyond hand calculation using asymptotic expansion methods. What is needed is either an exact evaluation of the integrals or an iterative method which can be adapted to machine calculation. In this paper, we show that the projection integral can be evaluated in closed form for the simplest bosonic SGA, namely the U(4) algebra of the vibron model. For general evaluation of the projection integrals, we propose an algebraic method based on the symmetries of the boson system (as opposed to the direct integration methods), which can easily be extended to the higher layers using the MATHEMATICA software [7].

2. Review of 1/N expansion method

We consider a set of boson creation and annihilation operators $\{b_{lm}^{\dagger}, b_{lm}\}$ which describe a variety of quantum systems depending on the values of *l*. For example, l = 0, 2 (sd IBM) describes quadrupole collectivity in nuclei. By adding l = 4 or l = 1, 3 bosons, the sd IBM can be extended to include hexadecapole or octupole excitations. The system with l = 0, 1 bosons is known as the vibron model [3], and describes the molecular rotationvibration spectra. Each boson system has an algebra $U(n), n = \sum_{i} (2l_i + 1)$ associated with it, which, through the use of group theoretical techniques, provides analytical solutions at certain dynamical symmetry limits. The 1/N expansion method, which is based on the angular momentum projected mean field theory, extrapolates between these limits, providing analytical solutions for intermediate cases which are usually more realistic.

An important property of a bosonic SGA describing a finite spectrum is that the number of bosons, N, in the system is conserved. Thus, the ground state of a boson system can be written as a projective coherent state (or a condensate of intrinsic bosons) as

$$|N, \boldsymbol{x}\rangle = (N!)^{-1/2} (b^{\dagger})^N |0\rangle \qquad b^{\dagger} = \sum_{lm} x_{lm} b_{lm}^{\dagger}$$
(1)

where x_{lm} are the (normalized) boson mean fields which are associated with the shape variables of the system, and hence provide a connection with the geometry and a physical picture for the SGA. As a trial state, equation (1) is complete and gives the exact ground energy when varied after projection (VAP). A simplifying feature of collective nuclei is that they are axially symmetric to a good approximation (this is, of course, exact for diatomic molecules). As this assumption makes the calculations much more tractable, we will consider in the following boson systems with axial symmetry. For such systems, K, the projection to the symmetry axis is a good quantum number, and the intrinsic boson operators can be labelled by K, i.e. $b_K^{\dagger} = \sum_l x_{lK} b_{lK}^{\dagger}$. For the ground state which has K = 0, this amounts to suppressing the m sum in equation (1). Other bands are obtained from the ground band by acting with the orthogonal intrinsic boson operators, for example, the one-phonon bands are given by $|\phi_K\rangle = b_K^{\dagger} |N-1, x\rangle$. For convenience, we will suppress the zero subscripts from now on, e.g. $x_{l0} \equiv x_l$, $b_0^{\dagger} \equiv b^{\dagger}$.

The fundamental quantity in the 1/N expansion is the projected norm integral for the ground band, $\mathcal{N}_g(N, L)$, as all the other matrix elements can be evaluated through algebraic manipulations of it. The norm with angular momentum projection is given by [5]

$$\mathcal{N}_{g}(N,L) = \langle N, \boldsymbol{x} | P_{00}^{L} | N, \boldsymbol{x} \rangle$$

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$$= \frac{2L+1}{2} \int_0^{\pi} d\beta \, \sin\beta d_{00}^L(\beta) \left[\sum_l x_l^2 d_{00}^l(\beta) \right]^N \tag{2}$$

where P_{00}^L is the projection operator and d_{00}^L denote Wigner *d* matrices [8]. Evaluation of this integral in closed form in the vibron model, and as a 1/N expansion in general, will be discussed in the following sections. Here we give its generic form as a 1/N expansion [5] to facilitate the discussion of layers

$$\mathcal{N}_{g}(N,L) = \frac{2(2L+1)}{aN} \sum_{n=0}^{\infty} \frac{(-1)^{n}}{n!(aN)^{n}} \sum_{m=0}^{n} \alpha_{nm} \bar{L}^{m}$$

$$= \frac{2(2L+1)}{aN} \left[1 - \frac{1}{aN} (\bar{L} + \alpha_{10}) + \frac{1}{2(aN)^{2}} (\bar{L}^{2} + \alpha_{21} \bar{L} + \alpha_{20}) - \frac{1}{6(aN)^{3}} (\bar{L}^{3} + \alpha_{32} \bar{L}^{2} + \alpha_{31} \bar{L} + \alpha_{30}) + \cdots \right]$$
(3)

where the bar denotes the angular momentum eigenvalues, $\bar{L} \equiv L(L+1)$ and

$$a = \sum_{l} \bar{l}x_{l}^{2} \tag{4}$$

is ubiquitous to the angular momentum projection and represents the 'average angular momentum squared' carried by a single boson. The coefficients α_{nm} in equation (3) are functions of the mean fields x_l and hence are specific to a given SGA. The expanded form of the norm is given to illustrate the concept of layers in the 1/N expansion. As a general terminology, the coefficients $\alpha_{nn} \equiv 1$ in the first column are called 'first layer', α_{nn-1} in the second column 'second layer', et

A general boson Hamiltonian with one- and two-body terms can be written as

$$H = \sum_{l} \varepsilon_{l} \hat{n}_{l} + \sum_{k=0}^{2t_{max}} \kappa_{k} T^{(k)} \cdot T^{(k)}$$

$$\hat{n}_{l} = \sum_{m} b_{lm}^{\dagger} b_{lm} \qquad T^{(k)} = \sum_{jl} t_{kjl} [b_{j}^{\dagger} \tilde{b}_{l}]^{(k)}$$
(5)

where brackets denote the tensor coupling of the boson operators, $\tilde{b}_{lm} = (-1)^m b_{l-m}$, and \hat{n}_l and $T^{(k)}$ are the boson number and multipole operators, respectively. The parameters in the model are the single boson energies ε_l , the multipole strengths κ_k , and the coefficients t_{kjl} . For consistency, the same multipole operators are used in the calculation of electromagnetic transition rates.

Once the norm of an intrinsic state $|\phi_K\rangle$ is known, the ME of any operator can be evaluated in a straightforward manner using boson calculus and angular momentum algebra techniques [5]. Here we quote the results for the expectation values of the number and multipole operators in the ground band [5], which will be used in section 4 in an algebraic calculation of the coefficients α_{nm} :

$$\langle \hat{n}_{l} \rangle_{L} = \frac{Nx_{l}^{2}}{F(N,L)} \sum_{I} \langle L0l00|I0 \rangle^{2} F(N-1,I)$$

$$\langle T^{(k)} \cdot T^{(k)} \rangle_{L} = \frac{2k+1}{F(N,L)} \left\{ N \sum_{jl} \frac{(t_{kjl}x_{l})^{2}}{2l+1} \sum_{I} \langle L0l00|I0 \rangle^{2} F(N-1,I) + N(N-1) \sum_{jlj'l'J} t_{kjl} t_{kj'l'} x_{j} x_{l} x_{j'} x_{l'} \langle j0j'0|J0 \rangle \langle l0l'0|J0 \rangle$$

$$\times \left\{ \begin{array}{c} j & j' & J \\ l' & l & k \end{array} \right\} \sum_{I} \langle L0J0|I0 \rangle^{2} F(N-2,I) \right\}$$

$$(6)$$

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where we have introduced $\mathcal{N}_g(N, L) = (2/a)(2L+1)F(N, L)$ to simplify the expressions. The various angular momentum sums involving the Clebsch-Gordon coefficients and the 6-*j* symbols in equation (6) can be evaluated using the techniques described in [5]. It is clear from equation (6) that knowledge of the norm integral is both necessary and sufficient for an accurate evaluation of the ME. Rather than discussing individual MEs, which is not the main concern of this paper, we concentrate on the general form of the ensuing 1/N expansion as this will provide the motivation for the algebraic technique to be used in section 4. Using the generic form of the normalization (3), one obtains for the expectation value of a k-body operator \hat{O} :

$$\langle \hat{O} \rangle_{L} = N^{k} \sum_{n,m} \frac{O_{nm}}{(aN)^{m}} \left(\frac{\bar{L}}{a^{2}N^{2}} \right)^{n}$$

$$= N^{k} \left\{ O_{00} + \frac{O_{01}}{aN} + \frac{O_{02}}{(aN)^{2}} + \frac{O_{03}}{(aN)^{3}} + \cdots \right.$$

$$+ \frac{\bar{L}}{a^{2}N^{2}} \left(O_{10} + \frac{O_{11}}{aN} + \frac{O_{12}}{(aN)^{2}} + \cdots \right) + \left(\frac{\bar{L}}{a^{2}N^{2}} \right)^{2} \left(O_{20} + \frac{O_{21}}{aN} + \cdots \right)$$

$$+ \left(\frac{\bar{L}}{a^{2}N^{2}} \right)^{3} (O_{30} + \cdots) + \cdots \right\}.$$

$$(7)$$

The expansion coefficients O_{nm} in equation (7) involve, besides the Hamiltonian parameters and α_{nm} , various quadratic forms of the mean fields x_{lm} corresponding to the single-boson ME of \hat{O} and its moments. Again, the expanded form is given to facilitate the illustration of layers in the 1/N expansion. Notice that the *i* coefficients O_{nm} in the *i*th column have n+m=i-1 constant, and are referred as the layer 'i-1'. The leading term in equation (7) is independent of the angular momentum projection and forms the zeroth layer. The N and \overline{L} dependence of the *i*th layer is the same as the *i*th power of the first layer. Thus one can consider the double expansion N and \overline{L} as a single expansion in layers. The connection between the layers in the normalization (3) and the ME (7) is that in order to calculate the ME up to the *i*th layer, one needs to know the coefficients α_{nm} up to that layer (to order $1/N^{2i}$). This is very useful in higher-order calculations as it restricts the number of terms in the expansion, cutting down the amount of algebra. To make this point clear, we note that the terms in equation (7) is complete to the third layer whereas a complete calculation to order $1/N^6$ would require six more terms belonging to the fourth, fifth and sixth layers. As will be seen in section 4, the complexity of the coefficients O_{nm} increases exponentially with layers, and each of the extra terms would lead to expressions pages long. From a practical point of view, such accuracy is never required, and hence the use of layers is a more sensible approach than a complete calculation to a given order in 1/N.

3. Vibron model

In this section, we give an exact evaluation of the norm integral in the vibron model. Substituting $z = \cos \beta$, $d_{00}^L(\beta) = P_L(z)$, and $x_0^2 = 1/(1+r)$, $x_1^2 = r/(1+r)$ for the normalized mean fields, equation (2) can be written as

$$\mathcal{N}_g(N,L) = \frac{2L+1}{2(1+r)^N} \int_{-1}^1 \mathrm{d}z \ P_L(z)(1+rz)^N.$$
(8)

Changing the variables to y = 1 + rz, and using the fact that $P_L(-z) = (-1)^L P_L(z)$, equation (8) can be split into two parts

$$\mathcal{N}_{g}(N,L) = \frac{2L+1}{2r(1+r)^{N}} (\mathcal{I}(r) - (-1)^{L} \mathcal{I}(-r))$$
(9)

where

$$\mathcal{I}(r) = \int_0^{1+r} \mathrm{d}y \, P_L\left(\frac{y-1}{r}\right) y^N. \tag{10}$$

Using the expansion for the Legendre polynomials [9]

$$P_L(x) = \frac{1}{2^L} \sum_{m=0}^{\lfloor L/2 \rfloor} (-1)^m \binom{L}{m} \binom{2L-2m}{L} x^{L-2m}$$
(11)

the y integral in equation (10) becomes standard and is given in terms of the hypergeometric function as [10]

$$\int_{0}^{1+r} dy (y-1)^{L-2m} y^{N} = (-1)^{L-2m} \frac{(1+r)^{N+1}}{N+1} {}_{2}F_{1}(N+1, 2m-L; N+2; 1+r)$$
$$= r^{L-2m} \frac{(1+r)^{N+1}}{N+1} {}_{2}F_{1}\left(1, 2m-L; N+2; \frac{1+r}{r}\right)$$
(12)

where in the last step we have used the identity [11]

$${}_{2}F_{1}(a,b;c;z) = (1-z)^{-b} {}_{2}F_{1}\left(c-a,b;c;\frac{z}{z-1}\right).$$
(13)

Substituting equations (11), (12) in (10), we obtain

$$\mathcal{I}(r) = \frac{(1+r)^{N+1}}{(N+1)2^L} \sum_{m=0}^{\lfloor L/2 \rfloor} (-1)^m \binom{L}{m} \binom{2L-2m}{L} {}_2F_1\left(1, 2m-L; N+2; \frac{1+r}{r}\right).$$
(14)

In order to sum the series in equation (14), we substitute for $_2F_1$ in equation (14):

$${}_{2}F_{1}\left(1,2m-L;N+2;\frac{1+r}{r}\right)$$

$$=1+\sum_{n=1}^{L-2m}\frac{(L-2m)(L-2m-1)\cdots(L-2m-n+1)}{(N+2)(N+3)\cdots(N+n+1)}\left(\frac{1+r}{-r}\right)^{n}.$$
(15)

Since the terms with n > L - 2m are zero, we can extend the upper summation limit in the resulting equation to L, and interchange the sums over m and n. The m summation can now be done easily if one notices from equation (11) that the derivatives of P_L are given by

$$\frac{d^n}{dx^n} P_L(x) \bigg|_{x=1} = \frac{1}{2^L} \sum_{m=0}^{\lfloor L/2 \rfloor} (-1)^m \binom{L}{m} \binom{2L-2m}{L} (L-2m) \times (L-2m-1) \cdots (L-2m-n+1)$$
(16)

which has precisely the form needed. The derivatives of P_L can also be evaluated using the generating function for the Legendre polynomials and are given by [12]

$$\left. \frac{\mathrm{d}^n}{\mathrm{d}x^n} P_L(x) \right|_{x=1} = \frac{(-L)_n (L+1)_n}{n!} \left(\frac{-1}{2}\right)^n \tag{17}$$

where $(a)_n = a(a+1)\cdots(a+n-1)$. Thus, use of equations (15)-(17) in (14) yields

$$\mathcal{I}(r) = \frac{(1+r)^{N+1}}{N+1} \left[1 + \sum_{n=1}^{L} \frac{(-L)_n (L+1)_n}{n! (N+2)_n} \left(\frac{1+r}{2r} \right)^N \right]$$
$$= \frac{(1+r)^{N+1}}{N+1} {}_2F_1 \left(-L, L+1; N+2; \frac{1+r}{2r} \right).$$
(18)

Finally, substituting equation (18) in (9) and noticing from equation (4) that a = 2r/(1+r), we obtain the following closed form expression for the normalization

$$\mathcal{N}_{g}(N,L) = \frac{(2L+1)}{a(N+1)} [{}_{2}F_{1}(-L,L+1;N+2;1/a) - (-1)^{L} (x_{0}^{2} - x_{1}^{2})^{N+1} {}_{2}F_{1}(-L,L+1;N+2;(x_{1}^{2} - x_{0}^{2})/a)].$$
(19)

The second term in equation (19) is specific to mixed-parity boson systems. (For identical parity systems, it is equal to the first term, leading to the factor of 2 in equation (3).) This term vanishes in the O(4) limit of the vibron model $(x_1 = x_0, a = 1)$, and is completely negligible for realistic breakings of the O(4) limit. Therefore, in the following, we have ignored the contributions from the second term to simplify the expressions. To make the connection with equation (3) clear and extract the coefficients α_{nm} in the 1/N expansion, we write $_2F_1$ as

$${}_{2}F_{1}(-L, L+1; N+2; x) = 1 - \frac{\bar{L}}{N+2}x + \frac{\bar{L}(\bar{L}-2)}{2(N+2)(N+3)}x^{2} - \frac{\bar{L}(\bar{L}-2)(\bar{L}-6)}{3!(N+2)(N+3)(N+4)}x^{3} + \cdots.$$
(20)

Inspection of equation (20) shows that the normalization has indeed the form given in equation (3). Below, we tabulate some of the coefficients α_{nm} obtained from the expansion of equations (19), (20):

$$\alpha_{n0} = n!a^{n} \qquad \alpha_{21} = 6a - 2 \qquad \alpha_{32} = 18a - 8 \qquad \alpha_{31} = 6(7a^{2} - 6a + 2)$$

$$\alpha_{43} = 40a - 20 \qquad \alpha_{42} = 4(75a^{2} - 80a + 27) \qquad (21)$$

$$\alpha_{41} = 24(15a^{3} - 25a^{2} + 20a - 6).$$

The second term in equation (19) leads to a similar expansion and, if the need arises, it could easily be included in the final result by modifying α_{nm} .

4. Algebraic evaluation

It is clear from the derivation for the simplest case in the last section that an exact evaluation of the norm integral for other bosonic SGA is not an easy task. In this section, we employ, instead, algebraic techniques to obtain the coefficients α_{nm} in equation (3). The technique is based on the symmetries of the boson system, namely boson number conservation and rotational invariance demands that the expectation values of the number and angular momentum operators must satisfy

$$\left\langle \sum_{l} \hat{n}_{l} \right\rangle_{L} = N \qquad \langle L \cdot L \rangle_{L} = \vec{L}.$$
 (22)

Comparing equation (22) with the general form (7), we see that, for the number operator, all the coefficients O_{nm} should vanish except $O_{00} = 1$. Similarly, for the angular momentum

operator, all should vanish except $O_{10} = a^2$. To illustrate the form of the resulting equations, we give below the ME in equation (22) up to the second layer:

$$\left\{\sum_{l} \hat{n}_{l}\right\}_{L} = N\left\{1 + \frac{a}{(aN)^{2}}(-a + a_{1}/2a - 2\alpha_{10} + \alpha_{21}/2) + \frac{a\bar{L}}{(aN)^{3}}(2/3 + 2a - a_{1}/a - 2\alpha_{10} + 2\alpha_{21} - 2\alpha_{32}/3) + \frac{a\bar{L}^{2}}{(aN)^{4}}(-1/6 - a/2 + a_{1}/4a - \alpha_{10} + 7\alpha_{21}/4 - 4\alpha_{32}/3 + 3\alpha_{43}/8) + \cdots\right\}$$

$$\left\{L \cdot L\right\}_{L} = \left\{(-1 - 2a + a_{1}/a - \alpha_{10} + \alpha_{21}/2) + \bar{L}\left[1 + \frac{1}{aN}(8/3 + 6a - 3a_{1}/a + \alpha_{21} - 2\alpha_{32}/3)\right] + \frac{\bar{L}^{2}}{(aN)^{2}}(-2/3 - 2a + a_{1}/a + \alpha_{10}/2 + \alpha_{21}/4 - 5\alpha_{32}/6 + 3\alpha_{43}/8) + \cdots\right\}$$

$$(23)$$

where $a_n = \sum_l \bar{l}^{n+1} x_l^2$ denotes the higher moments of a in equation (4). There are no firstlayer terms in equation (23) as these conditions are automatically fulfilled by the correct choice of α_{nn} . Each ME in equation (23) leads to three linear equations for the four secondlayer coefficients α_{nn-1} , n = 1-4. Thus, together, the set of six linear equations completely determine these coefficients. We emphasize the recursive form of the equations which makes the solutions trivial to obtain. Extending the calculations in equation (23) to the third layer introduces seven more coefficients ($\alpha_{54}, \alpha_{65}, \alpha_{nn-2}, n = 2-6$) and six more equations into the second-layer set. Of these, two come from the coefficients of \bar{L}^3/N^5 and \bar{L}^4/N^6 , which do not automatically vanish, and involve only the second-layer coefficients. Hence they are used to determine α_{54} , α_{65} . The remaining four equations are obtained from the vanishing of O_{nm} with n + m = 3 and involve the third-layer coefficients α_{nn-2} . In general, the *i*th layer will introduce 3i - 2 coefficients and 3i - 3 equations into the existing system of linear equations for each ME. Hence, together they (over) completely determine the coefficients α_{nm} . Although the proposed method is straightforward, the complexity of calculations increases exponentially with each layer, and a hand calculation beyond the second layer is not feasible. Using the MATHEMATICA software [7], however, the lengthy algebraic manipulations can be performed easily and, in this way, we have determined α_{nm} up to the fourth layer. Here we quote the second- and t' ird-layer coefficients which seem to be sufficient for the purposes of nuclear and molecular SGA:

$$\begin{aligned} \alpha_{10} &= 1 + a - a_1/2a \\ \alpha_{21} &= 4 + 6a - 3a_1/a \\ \alpha_{32} &= 10 + 18a - 9a_1/a \\ \alpha_{43} &= 20 + 40a - 20a_1/a \\ \alpha_{54} &= 35 + 75a - 75a_1/2a \\ \alpha_{65} &= 56 + 126a - 63a_1/a \\ \alpha_{20} &= 2 + 6a + 2a^2 - 3a_1 - 10a_1/3a + 3a_1^2/2a^2 - a_2/3a \end{aligned}$$

$$\alpha_{31} = 18 + 72a + 42a^2 - 54a_1 - 40a_1/a + 45a_1^2/2a^2 - 4a_2/a$$

$$\alpha_{42} = 88 + 400a + 300a^2 - 360a_1 - 220a_1/a + 135a_1^2/a^2 - 20a_2/a$$

$$\alpha_{53} = 308 + 1500a + 1300a^2 - 1500a_1 - 2450a_1/3a + 525a_1^2/a^2 - 200a_2/3a$$

$$\alpha_{64} = 868 + 4410a + 4200a^2 - 4725a_1 - 2380a_1/a + 1575a_1^2/a^2 - 175a_2/a.$$
 (24)

The advantage of the present derivation is that the results are completely general and could be used for any bosonic SGA. In particular, using $a_n = 2^n a$ in equation (24), we recover the vibron model results given in equation (21).

5. Conclusions

Angular momentum projection integrals are essential ingredients in the 1/N expansion calculations. Practical application of this method in either molecular or nuclear physics hinges on accurate evaluation of such integrals to rather high orders. In this paper, we have shown that the normalization integral in the vibron model can be obtained in closed form by direct integration. Generalization of this result to other SGA, however, does not seem to be easy. We have, instead, employed algebraic techniques and calculated the coefficients in the 1/N expansion of the normalization integral for an arbitrary bosonic SGA. The method is easily adapted to computer algebra which allows calculation of the norm integral to any desired level of accuracy without going through the usual algebraic drudgery. Application of the present results to spectra of diatomic molecules and high-spin states in nuclei will be presented elsewhwere.

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