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The generalization of the extended Stevens operators to higher ranks and spins, and a systematic review of the tables of the tensor operators and their matrix elements

C Rudowicz[1] **and C Y Chung**

Department of Physics and Materials Science, City University of Hong Kong, 83 Tat Chee Avenue, Kowloon, Hong Kong SAR, People's Republic of China

E-mail: apceslaw@cityu.edu.hk (C Rudowicz)

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Abstract
Spherical (S) and tesseral (T) tensor operators (TOs) have been extensively used in, for example, EMR and optical spectroscopy of transition ions. To enable a systematic review of the published tables of the operators and their matrix elements (MEs) we have generated the relevant tables by computer, using *Mathematica* programs. Our review reveals several misprints/errors in the major sources of TTOs—the conventional Stevens operators (CSOs—components $q \geqslant 0$) and the extended ones (ESOs—all q) for rank $k = 2, 4$, and 6—as well as of some STOs with $k \leqslant 8$. The implications of using incorrect operators and/or MEs for the reliability of EMR-related programs and interpretation of experimental data are discussed. Studies of high-spin complexes like Mn_{12} ($S = 10$) and Fe_{19} ($S = 33/2$) require operator and ME listings up to $k = 2S$, which are not presently available. Using the algorithms developed recently by Ryabov, the generalized ESOs and their MEs for arbitrary rank k and spin S are generated by computer, using *Mathematica*. The extended tables enable simulation of the energy levels for arbitrary spin systems and symmetry cases. Tables are provided for the ESOs not available in the literature, with odd $k = 3, 5$, and 7 for completeness; however, for the newly generalized ESOs with the most useful even rank $k = 8, 10$, and 12 only, in view of the large listings sizes. General source codes for the generation of the ESO listings and their ME tables are available from the authors.

[1] Author to whom any correspondence should be addressed.

1. Introduction

Electron magnetic resonance (EMR), including, for example, EPR, ESR, and ENDOR (see, e.g. Pilbrow 1990, Mabbs and Collison 1992, Weil *et al* 1994), and optical spectroscopy (OS) (see, e.g. Newman and Ng 2000, Mulak and Gajek 2000) as well as related studies, for example Mössbauer spectroscopy and/or magnetism, of paramagnetic centres require appropriate Hamiltonians (see, e.g., Stevens 1997). The tensor operators of the (effective) spin (**S**) and orbital (**L**) or total (**J**) angular momenta play an important role as a starting point for construction of the generalized spin Hamiltonians (SH), including the zero-field splitting (ZFS) and higher-order electronic Zeeman terms used in EMR, as well as the crystal field (CF) Hamiltonians used in OS (see, e.g. Rudowicz 1987a, 1988, Rudowicz and Misra 2001). Subsequent calculations of the energy levels enable simulation, analysis, and fitting of EMR (or optical) spectra of isolated paramagnetic ions in crystals and exchanged coupled complexes.

Various conventional and operator notations have been used in the EMR area, as reviewed by Rudowicz (1987a), (1988). The existing abundance of operator and ZFS parameter notations has resulted in considerable confusion, which hampers direct comparison of data from different researchers (see, e.g., Rudowicz and Misra 2001, Rudowicz and Sung 2001, Rudowicz 2002). Apart from the early notations using explicitly the angular momentum operators, two classes of the tensor operators (TOs) are used in the literature: (i) spherical (STOs) and (ii) tesseral (TTOs), which are the operator equivalents to the spherical and tesseral harmonics, respectively (see, e.g. Kibler 1980, Rudowicz 1987a, 1988). The major operators belonging to the TTO category are the conventional Stevens operators (CSOs), which include only the components $q \geqslant 0$ (Stevens 1952), and more recently the extended Stevens operators (ESOs), which include all components $-k \leqslant q \leqslant +k$ (Rudowicz 1985a, 1985b). Various types of TTOs and STOs have been reviewed and their conversion factors tabularized (Rudowicz 1987a, 1988, Rudowicz *et al* 1997). Due to the Wigner–Eckart theorem (see, e.g., Mabbs and Collison 1992, Stevens 1997) all STOs differ only by a proportionality constant. The ESOs (CSOs) are by now the most extensively used operators in EMR and the superposition model (Newman and Ng 1989, Rudowicz 1987b) as well as, to a lesser extent, in CF and OS studies, and magnetism (Rudowicz 1987a, 1988, Rudowicz and Misra 2001, Rudowicz and Sung 2001, Rudowicz 2002).

The main rationale for this work is to facilitate EMR-related calculations and simulations by using computer algebra and thus to provide efficient tools for studies of low symmetry and high spin systems. This requires generalization of the existing operators to higher ranks k and including all components q $(-k \leqslant q \leqslant +k)$. Efficient usage of any type of operators requires the knowledge of their matrix elements (MEs). However, such calculations by hand are a cumbersome and error-prone task, and the difficulties increase with increasing rank k and lowering symmetry. The ZFS (CF) Hamiltonians for the lowest triclinic symmetry involve all components q for a given admissible rank $k \leqslant 2S$ ($2L$ or $2J$). Therefore explicit and well-tested ME tables or general expressions, which can be programmed into a computer, are indispensable. The developers of the EMR-related computer programs used in experimental studies rely directly or indirectly on the ME tables for the CSOs (ESOs) available in the literature. Needless to say, such usage of the incorrect MEs from source tables may adversely affect subsequent calculations and interpretation of experimental results. Although the accuracy of such tables is crucial, it appears that since Hutchings (1965) listed some misprints and errors occurring in the earlier published tables, no further check-ups have been carried out. Hence, we also carry out a systematic check-up of the pertinent tables using our *Mathematica* programs and computer-generated tables.

Due to historical development of the Stevens operators from the conventional ($q \geqslant 0$) ones (Stevens 1952) to the extended ($-k \leqslant q \leqslant +k$) ones (Rudowicz 1985a, 1985b, 1987a, 1988), these operators have some drawbacks. Their construction has not been based on a general formula and they are not normalized (Rudowicz 1985a, 1985b, 1987a, 1988). This is unlike the situation for the well-defined and normalized STOs (Rudowicz 1985a, 1985b, 1987a, 1988) originating from the classical papers by Racah (1942a, 1942b, 1942c) and subsequently developed within the angular momentum theory (see, e.g., Silver 1976). While the transformation properties for the STOs have been worked out based on the Wigner rotation matrices (see, e.g., Buckmaster *et al* 1972, Silver 1976), those for the ESOs have been worked out much later utilizing the explicit expressions for the STOs (Buckmaster *et al* 1972) for $k = 2$–6 (Rudowicz 1985a, 1985b; see also Tennant *et al* 2000). Compact ME expressions exist for the STOs (see, e.g. Smith and Thornley 1966). Explicit listings are generally available for the most useful even ranks $k = 2, 4$, and 6 for the ESOs and STOs (for references, see Rudowicz 1985a, 1985b, 1987a, 1988, Rudowicz and Misra 2001), but for the odd ranks $k = 3$, 5, and 7 for the STOs only, while the ESO and STO listings for rank $k = 8$ have until recently been available in unpublished reports (for references, see section 4).

The available listings for $k \leqslant 6$ are sufficient for mononuclear paramagnetic complexes, since the highest spin is $S = 7/2$, e.g. for Gd^{3+}. However, the discovery more than a decade ago of the high-spin complexes, e.g. Mn_{12} and Fe_8 with the total spin $S = 10$, which appear to exhibit macroscopic quantum tunnelling, and Fe_{19} with $S = 33/2$ (for references, see, e.g. Chung 2003), has prompted demand for the higher-rank operators up to $k = 2S$. Hence it is of importance to develop efficient means for generalization of the existing tables of the ES and ST operators as well as their MEs to arbitrary rank k and spin S. The extended tables could be used to simulate the energy levels for arbitrary spin systems and symmetry cases. This may enable a better understanding of the properties of the high-spin Mn_{12} and Fe_8 complexes.

The organization of the paper is as follows. In section 2 we outline the computational methods and present the findings of a systematic review of the published ME tables for the CSOs ($q \geqslant 0$). This survey reveals several misprints and/or errors in the major source tables for the CSOs for the rank $k = 2$, 4, and 6, which have a bearing on the derived MEs for the ESOs ($-k \leqslant q \leqslant +k$). Implications of these findings for the reliability of the available EMR-related computer programs are also discussed. In section 3 we consider the generalization in question using the algebraic algorithms developed by Ryabov (1999) based on the relationships between the STOs and TTOs. Using the conversion factors between the ESOs and various TTOs, we have generated explicit tables of both ES and ST operators as well as their MEs by computer, using *Mathematica*. Various misprints and inconsistencies in the available listings of the CSOs or ESOs and several types of the STOs of various ranks revealed by our survey are outlined in section 4. For the benefit of practitioners who need explicit forms, the computer generated tables are provided for completeness in appendix B.1 for the ESOs with odd $k = 3$, 5, and 7 not available in the literature, including all components ($-k \leqslant q \leqslant +k$) necessary for low symmetry. In appendix B.2 the listings of the newly generalized ESOs are provided beyond the usual listings for $k = 2$, 4, and 6 available in the literature. However, in view of the large sizes, the listings are limited to the most useful even ranks $k = 8$, 10, and 12 and $q \geqslant 0$ only, whereas rules for obtaining the negative components are provided. General source codes for the generation of the ESOs and their ME tables for arbitrary high rank and spin are available from the authors.

2. Tables of the matrix elements of the conventional and extended Stevens operators

A number of computer programs for simulation and interpretation of experimental EMR spectra have been worked on in various groups; to name a few, Nettar (1984), Mabbs and Collison

(1992), McGavin *et al* (1993), Mombourquette *et al* (1995), Wang and Hanson (1995), and Stoll (2003a). The developers of such programs as well as EMR practitioners rely directly or indirectly on the major source listings of the CSOs (ESOs) and their ME tables available in the literature: Abragam and Bleaney (1970, 1973, 1986), Altshuler and Kozyrev (1972, 1974)—referred to later as A/B(E1), A/B(R), A/B(E2), A/K(R), and A/K(E), respectively. Explicit partial listings of the CSOs by Orbach (1961) and those of the ESOs by Newman and Urban (1975) were also often referred to. Hutchings (1965) has listed some misprints and errors occurring in the earlier published ME tables for the CSOs, whereas independently Buckmaster (1962) and Birgeneau (1967) have listed the MEs of several selected STO components in the form later used in A/B(E1) and in numerical form, respectively. Lindgård (1975), Lindgård and Danielsen (1974), Danielsen (1973), Danielsen and Lindgård (1972) have discussed the interrelationships between the Racah and Stevens operators and provided their explicit listings for some ranks (including $k = 8$) and components. Pilbrow (1990) has provided the ME tables for components of the spin operators S_i $(i = x, y, z)$ and their second-order combinations for $S = 1/2$ to 3. Since the latter tables are of limited usefulness nowadays, no attempt has been made to develop a special computer program needed for generating similar tables for comparison.

Our studies of high-spin complexes (Chung and Rudowicz 2000, Sung *et al* 2000, Chung 2003) have prompted us to develop tools for simulations and interpretation of EMR spectra based on the *Mathematica* programming language, which also provides algebraic and graphic capabilities. By using a computer program for algebraic manipulations, human or typographical errors could be avoided. Note that other programs involving computations of the MEs of spin operators have some limitations; for example, the *Mathematica* program of Siu (1994) used the built-in matrices for $k = 2$ and 4 and S limited to $S \leqslant 5/2$, whereas the *Fortran*-based *EPR.FOR* (McGavin *et al* 1993) and *EPR-NMR* (Mombourquette *et al* 1995) programs have some internal (size of the arrays) and external (see below) restrictions on the values of k and S. The latter two programs internally generate the MEs from those for the lowest rank $k = 1$ using explicit forms of the higher-rank operators and prescriptions given, for example, by Buckmaster *et al* (1972). Hence, special care must be taken to ensure the correctness of such involved computations.

Initially we have designed two *Mathematica* programs for ME computations: (i) *MatrixElements* for the ESOs $O_k^q(\mathbf{S})$, and (ii) *MEGenerator* for various major STOs (Chung 2003). These programs utilize internally the Buckmaster (1962) and Smith and Thornley (1966), i.e. BST operators $O_q^{(k)}$ (Rudowicz 1987a, 1988), and incorporate the general ME expression for $O_q^{(k)}$ in the basis of the angular momentum eigenstates $|j, m\rangle$ (Smith and Thornley 1966):

$$\langle j, m'|O_q^{(k)}|j, m\rangle = (-1)^{j-m'} \begin{pmatrix} j & k & j \\ -m' & q & m \end{pmatrix} \langle j||O^k||j\rangle, \tag{1}$$

where the reduced matrix element is given by

$$\langle j||O^k||j\rangle = \frac{1}{2^k}\left\{\frac{(2j+k+1)!}{(2j-k)!}\right\}^{1/2}. \tag{2}$$

The $3j$-symbols $\left(\begin{smallmatrix} j & k & j \\ -m' & q & m \end{smallmatrix}\right)$ can be either calculated from the algebraic expressions (see, e.g., Buckmaster *et al* 1972, Silver 1976) or taken from tables (see, e.g. Heine 1993, Silver 1976), both of which are limited to certain cases. Fortunately, the $3j$- (and $6j$-) symbols are provided as built-in *Mathematica* functions. The triangular rule limits the non-zero MEs of the STOs and TTOs, and hence of the required ZFS (CF) terms, to the ranks $k \leqslant 2j$. This rule is employed in our *Mathematica* programs to avoid computing the MEs that are zero by default. The programs start computations only if the indices m and m' comply with the rule $m' = q + m$; otherwise zero ME values are directly returned. When considering a specific system, the generic symbol j in equations (1) and (2) shall be replaced by, for example, a 'spin' quantum number, for an orbital singlet ground state of a paramagnetic ion with an *effective* spin $\tilde{S}$ or an exchange-coupled system with a *total* spin S_T or a *fictitious* spin S', whereas an orbital quantum number L or J is used for the multiplet ${}^{2S+1}$L ($3d^n$) or ${}^{2S+1}L_J$ ($4f^n$), respectively (Rudowicz 1987a, 1988, Rudowicz and Misra 2001). For simplicity, in the text and appendices we use the symbol S, J, or j for any 'spin' depending on the context.

In order to verify that equations (1) and (2) represent correctly the MEs of the BST operators, we have cross-checked them with the general ME expressions for the Koster and Statz (1959) and Buckmaster *et al* (1972), i.e. KS/BCS operators T_{kq} (Rudowicz 1987a, 1988). This yields the same general conversion relation: $O_q^{(k)} = \alpha_k T_{kq}$, where $\alpha_k = \sqrt{(2k)!/(2^k k!k!)}$, as given by Rudowicz (1987a, 1988). The explicit multiplication factors required for the conversions dealt with in the programs *MatrixElements* and *MEGenerator* were taken from Rudowicz (1987a, 1988; see, also, Rudowicz *et al* 1997). These programs yield the MEs of the ESOs and major STOs for arbitrary values of S. The program *MatrixElements* was applied to generate the ME tables for the ESOs $O_k^q(\mathbf{S})$ for $k = 2, 4$, and 6 and $S = 1/2$ to 10 (Chung 2003). In principle both programs could be extended for an arbitrary rank k and any positive integer or half-integer spin S. The major obstacle was the lack of the interconversion relations between the BST operators or other STOs and the ESOs, since no explicit definitions of the ESOs have until recently existed for $k > 6$ (see section 3).

The computer-generated ME listings for the ESOs for $k = 2, 4$, and 6 (Chung 2003) were used to survey the major ME source tables (A/B(E1), A/B(R), A/B(E2), A/K(R), A/K(E)). Our survey reveals several misprints or errors in the MEs for the CSOs ($q \geqslant 0$) listed in appendix A, which have a bearing on the derived data for the ESOs ($-k \leqslant q \leqslant +k$). Note that the recent listing by Misra (1999b) (M99) is mostly reproduced from A/K(E) and carries over the original misprints/errors with a few corrections as per A/B(E2) listings (see appendix A). A similar survey for the STOs is discussed in section 4. In appendix A we adopt the ME notation used in A/K(E), i.e. rank $k = n$, component $q = m$, and we list only the MEs of the type $\langle M|O_n^m|M-m\rangle$, whereas the other half of the MEs can obtained from the relation

$$\langle M|O_n^m|M-m\rangle = (-1)^{m+n}\langle -M|O_n^m|-M+m\rangle = \langle M-m|O_n^m|M\rangle. \qquad (3)$$

For example, the ME entries $\langle 5||3\rangle$ for the operator O_6^2 ($j = 6$) refer to $\langle +5||+3\rangle$ and $\langle -5||-3\rangle$. Ryabov (1999) mentioned the existence of some errors in the earlier listings of the Stevens operators and their ME tabulations; however, no errors were explicitly provided. The listing provided to us by Ryabov (2001), including altogether nine ME errors and one error in the scaling factors, enables a double-check of both sets of results—excluding the latter errors 15 more cases (not counting the same errors in difference sources) are listed in appendix A.

Some additional points relevant for users of the CSO/ESO listings and ME tables in question are worth noting. In the A/K(E) tables (reproduced in M99),

(i) in some cases all MEs for a given S are zero, yet a non-zero common factor F is provided, e.g. 1/2, 1; this inconsistency may be misleading;

(ii) for O_4^4 ($S = 3/2$) and O_6^4 ($S = 5/2$) no MEs are given; however, common factors $F = 12$ and 60 are provided, respectively; note that the triangular rule excludes these cases since $k > 2S$, hence these entries are meaningless;

(iii) some ME entries appear unnecessarily—either they do not exist or are not necessary for the lower spin systems, e.g. the operator O_6^0, which is actually needed only for $S \geqslant 3$, since all MEs are zero for $S < 3$.

The correctness of the ME tables, and to a lesser extent of the operator listings, may bear crucially on the accuracy of the EMR-related computer programs based on such data. Since the error in sign of the MEs of O_2^0 for $S = 1$ and $3/2$ occurs only in A/K(R) and A/K(E), the impact of these misprints may be rather limited; nevertheless, some expressions for the various derived quantities and possibly the signs of ZFS parameters for such spin systems may be incorrect in the literature, especially in older Russian works. The errors in ME values for various operators O_6^q might have affected the corresponding expressions and hence the resulting ZFS parameters for the systems with spin $S = j$ listed in appendix A. A thorough recheck of all pertinent source codes would be required to assess the implications of any errors involved. The feasibility of a large-scale verification of the existing EMR-related computer programs hinges upon concerted efforts and international collaboration of developers of various computer programs. The framework for such collaboration has been proposed by Rudowicz (2003a, 2003b). At the present stage we can offer some specific comments regarding two programs. The list of the ESOs included in the current version of the program *EasySpin* (Stoll 2003a) has been corrected subsequent to the communication between the author (CZR) and Stoll (2003b). However, the MEs used in this program still need to be verified pending the comparison with appendix A.

During our initial attempts to apply the program *EPR-NMR* (Mombourquette *et al* 1995) for higher spin values, we have encountered problems in generating reasonable energy levels (Galeev and Rudowicz 1999). This has prompted us to extract the MEs of the Stevens operator O_2^0 from the output file of the program *EPR-NMR* for the integer spin $S = 1$–8. The outcomes of our testing can be summarized as follows:

(i) for $S < 5$ the extracted MEs were exactly half of the MEs for O_2^0 (ES) obtained from our program *MatrixElements*, which are identical with those given by A/B(E), where the maximum listed spin is $S = 8$;
(ii) for $S = 5$ the same results, i.e. '(1/2) rule', were obtained except for $\langle 5|O_2^0|5\rangle$, for which the extracted value is 20, which is less more than half of the value for O_2^0 (ES), i.e. 45;
(iii) for $S \geqslant 6$ several extracted MEs differ in an erratic way from the values of half of the MEs for O_2^0 (ES), e.g. three MEs with the highest M_S (starting from $M_S = S$) do not conform to the '(1/2) rule' for $S = 6$, whereas there are five for $S = 7$, and seven for $S = 8$; and
(iv) for $S \geqslant 6$ some unexpected non-diagonal MEs start to appear, e.g. for $S = 6$: $\langle \mp 6|O_2^0|\pm 5\rangle$ and $\langle \mp 5|O_2^0| \pm 6\rangle$.

The program *EPR-NMR* (Mombourquette *et al* 1995) employs two separate subroutines to calculate MEs internally: first the MEs of the spin operators (S_+, S_-, S_z) are established and then they are utilized to obtain the MEs of the Stevens operators from the explicit forms of the STOs in terms of (S_+, S_-, S_z) listed in the unpublished tables of Buckmaster and Dering (1967) discussed in section 4. The most probable reasons for the discrepancies revealed by our tests may be an incorrect representation of the STOs and/or expressions for their MEs for higher spin in the source code as well as the conversion factors used internally within the program *EPR-NMR*. These problems were discussed in private communications between the author (CZR) and Tennant (1999), who has also mentioned several other technical problems and/or mistakes in the higher-order spin terms encountered during his work with the program *EPR-NMR* (version 6.0). Some of these problems may have been solved/corrected in the later versions of the program. It seems that the program *EPR-NMR* has never been used for practical applications for spin systems with $S > 5/2$.

3. Generalization of the extended Stevens operators to higher ranks and spins

Hoffmann (1990) considered generalization of Stevens' operator-equivalent method in application to the Racah STOs using the computer program *REDUCE*. He provided only a relation between the "*usual Stevens' operators*" and the newly defined operator equivalents. Independently and more recently Ryabov (1999) worked out general algorithms for generation of the Racah STOs and the ESOs, and also provided explicit formulae for the interconversions of these operators and their MEs. Ryabov's (1999) algorithms are more suitable for practical purposes, e.g. programming on a computer. Interestingly, a recent SCI (Science Citation Index) search for citations of the two papers reveals that neither Hoffmann's nor Ryabov's method has been utilized for practical applications as yet. Using Ryabov (1999) algorithms, we have extended the range of applicability of the ME programs for the ESOs (Chung 2003) to any rank and spin.

The algebraic forms of the ESOs, i.e. the '*Stevens operator equivalents*' defined by Ryabov (1999) in terms of the angular momentum operators $J_\pm$ and J_z, are:

$$O_k^q(c) = \frac{\alpha}{2F_{k,q}} \sum_{m=0}^{k-q} a(k,q;m)[J_+^q + (-1)^{k-q-m} J_-^q] J_z^m \qquad (q = 0, 1, 2, \ldots, k) \tag{4}$$

$$O_k^q(s) = \frac{\alpha}{2\mathrm{i}F_{k,q}} \sum_{m=0}^{k-q} a(k,q;m)[J_+^q - (-1)^{k-q-m} J_-^q] J_z^m \qquad (q = 1, 2, \ldots, k). \tag{5}$$

Ryabov (1999) introduced the factors $\alpha = 1$ for all q if k is an odd integer and $\alpha = 1$ or $1/2$ for even and odd q, respectively, if k is even. The coefficient $F_{k,q}$ is the largest common factor for all $a(k,q;m)$ defined as

$$\begin{aligned} a(k, q-1; m) = {} & (2q+m-1)a(k,q;m-1) + \left[q(q-1) - \frac{m(m+1)}{2}\right] a(k,q;m) \\ & + \sum_{n=1}^{k-q-m} (-1)^n \left[\binom{m+n}{m} J(J+1) - \binom{m+n}{m-1} - \binom{m+n}{m-2}\right] \\ & \times a(k,q;m+n) \end{aligned} \tag{6}$$

with $a(k,k;0) = 1$. Equations (4) and (5) imply a specific normalization and hence yield specific conversion factors between the ESOs and other operators. The components $O_k^q(c)$ and $O_k^q(s)$ correspond to the ESOs with positive q (including $q = 0$) and negative q, respectively (Rudowicz 1985a, 1985b). The *Mathematica* program *GenESOsME* for generating explicitly the ESOs $O_k^q(\mathbf{J})$ of arbitrary rank computes first all coefficients $a(k,q;m)$ and then $F_{k,q}$. Note that Ryabov (1999) algorithms generate the ESOs in the asymmetric form. However, in the literature the symmetric (anticommutator) form has been used exclusively for the CSOs (A/B(E1), A/B(R), A/B(E2); A/K(R), A/K(E); M99), and most commonly for the STOs, for which also the asymmetric form has occasionally been used (see section 4).

The program *GenESOsME* enables generation of the ESOs of higher ranks, beyond those available in the literature, as well as extension of the *MatrixElements* program (Chung 2003) to compute the MEs of the ESOs for arbitrary rank and spin. The explicit ESO listings and their ME tables may be used in conjunction with the all-purpose simulation and fitting program *SIM* developed by Weihe (2004; see also, Glerup and Weihe 1991, Jacobsen *et al* 1993). Such programs require an external supply of the MEs, which once tabulated can be built into the relevant subroutines, thus saving computing time. For the benefit of practitioners who need explicit forms, some computer-generated ESO listings are provided in the appendices. In appendix B.1 for completeness we provide the ESOs with odd $k = 3, 5$, and 7, including all components ($-k \leqslant q \leqslant +k$) necessary for low symmetry, which are not available in the literature. Note that conversion factors for $k = 3$ and 5 are also listed (Rudowicz 1987a, 1988, Rudowicz *et al* 1997). In appendix B.2 we provide the listings of the newly generalized ESOs beyond the usual listings for $k = 2, 4$, and 6 available in the literature. However, in view of the large size, the listings are limited to the most useful even ranks $k = 8$, 10, and 12 only. General *Mathematica* source codes for the generation of the ESOs and their ME tables for arbitrary high rank and spin are available from the authors upon request.

4. Listings of the tesseral and spherical tensor operators, and various conversion factors

In order to verify the correctness of our new programs for generation of the ESO and STO listings as well as the ME tables, first our *Mathematica* outputs have been tested utilizing several examples given by Ryabov (1999, 2001). Second, we have cross-checked the outputs against various listings available in the literature. Especially useful are the source tables for the various STOs, which extend to rank 8. Our *Mathematica* outputs have been fully compared with the available asymmetric forms of the STOs, but only randomly checked against the existing symmetric listings of the CSOs and STOs. The latter procedure required manual conversions of our outputs to the anticommutator form using the basic relations $J_+J_z = J_zJ_+ - J_+$ and $J_-J_z = J_zJ_- + J_-$. Positive results of such tests provide conclusive evidence that both our program *GenESOsME* and Ryabov's (1999) equations are correct. As required by equations (4) and (5), the program outputs show proper symmetry, i.e. the components $O_k^q(s) = O_k^{-q}$ can be obtained from $O_k^q(c) = O_k^{+q}$ by multiplying O_k^{+q} by the factor $(-i)$ and changing to negative the sign at the J_-^q terms (denoted Jm^q in appendices B.1 and B.2). A by-product of these tests is the identification of several errors and inconsistencies in the listings surveyed, which are outlined below.

Comparison of the Racah STOs for $k = 0$–8 and $q = +k$ to $-k$ in the symmetric form in Lindgård and Danielsen (1974) with those in Danielsen (1973) and Danielsen and Lindgård (1972) shows that they are nearly identical. The definitions of the Racah and Stevens operators have also been provided in Lindgård (1975), and explicit listings of the Stevens operators $O_k^q(c)$ in the symmetric form for $k = 2, 4, 6, 8$ and even q only in Danielsen and Lindgård (1972) and Danielsen (1973). Checking against our *Mathematica* outputs the listings of the Racah STOs in these tables randomly (i.e. for $k = 2, q = 1; k = 4, q = 2, 3; k = 6, q = 4, 5; k = 7, q = 4, 6; k = 8, q = 0, 2, 4, 6, 8$), whereas those of the Stevens operators fully, and also against other published listings for $k = 2, 4, 6$ (i.e. A/B(E2), A/K(E)), reveals the misprints listed in appendices C.1 and C.2, respectively. The unpublished tables of Buckmaster and Dering (1967), which nevertheless have been extensively utilized by various authors over the years (see section 2), comprise the KS/BCS (Rudowicz 1987a, 1988) operators for $k = 0$–7 and $q = +k$ to $-k$ given in both the symmetric and asymmetric form. The symmetric form of these tables has been randomly checked as in the case of the equivalent tables in Danielsen and Lindgård (1972), Danielsen (1973), and Lindgård and Danielsen (1974), and the misprints identified are listed in appendix C.3.1. The misprints identified in our comprehensive check of Buckmaster and Dering (1967) tables in the asymmetric form are listed in appendix C.3.2. Several misprints identified in the listing of Racah operators for $k = 0$–6 in table 2 of Tuszynski (1990), which was referred to in Buckmaster *et al* (1972), are listed in appendix C.4. An independent check of the original table 1 (for $k = 0$–7) in Buckmaster *et al* (1972) reveals no misprints. A cross-check of Buckmaster *et al* (1972) and Tuszynski (1990) operator listings suggests that the inconsistencies in the latter are genuine misprints. Assuming that these misprints were not carried over to the subsequent numerical ME calculations, it may be expected that the ME tables of Tuszynski (1990) given in numerical form may be correct. However, we have not attempted to verify the correctness of these ME tables, since in view of the little use of these tables for any practical purpose, the amount of effort involved would not be justified.

Ryabov (1999) has mentioned without providing explicit examples that the list of operator equivalents in Misra *et al* (1996) contains a number of errors. Comparison of the latter list and that in M99 with our computer-generated explicit ESO forms reveals identical misprints as communicated to us by Ryabov (2001). It turns out that Misra *et al* (1996) and M99 reproduced the original A/K(R) [A/K(E)] operators $O_n^{\pm m}$ re-labelling them as $\hat{Y}_n^{\pm m}$ (**S**), so with some misprints, which are listed for completeness in appendix C.5. Note that these are the combinations of the operators $O_n^{\pm m}$ defined by A/K(R) [A/K(E)] (*alias* $\hat{Y}_n^{\pm m}$ in Misra *et al* 1996 and M99), which yield the actual ESOs (see, e.g., A/K(E), Rudowicz 1987a, 1988). The notation $\hat{Y}_n^{\pm m}$ (Misra *et al* 1996, M99) instead of the original one $O_n^{\pm m}$ (A/K(R), A/K(E)) is superfluous and may be misleading since the spherical harmonics are customarily denoted $Y_n^{\pm m}$. Also the ME listings (see appendix A—note that the MEs of O_2^0 appear correctly in M99, possibly taken from A/B(E1) or A/B(E2)) and some pertinent ME relations were reproduced by Misra *et al* (1996) and M99 from the original source A/K(E). Ryabov (2001) has pointed out to us two other inconsistencies:

(i) the original A/K(E) definition '$O_n^m = (O_n^{+m} + O_n^{-m})/2$', where the LHS represents the ESOs with positive m, is missing in Misra *et al* (1996) and M99; and
(ii) in the last formula on p 45 of Misra *et al* (1996) the RHS should read '$\pm\mathrm{i}\langle M|O_n^m|M \pm m\rangle$' (it is correct in M99).

Additionally, Rudowicz (2000) discussed various drawbacks of the reviews (Misra *et al* 1996, Misra 1999a, 1999b, 1999c, 1999d), which concern the usage of a variety of symbols, correlated neither mutually nor with the existing ESO notation (Rudowicz 1985a, 1985b, 1987a, 1988), as well as the confusion between the properties of the TTOs and STOs, and inappropriate nomenclature. Usage of separate symbols for the negative ESO components O_k^q ($q < 0$), e.g. Ω_n^m (Misra *et al* 1996, Misra 1999b) or R_n^m (Misra 1999d), and C_n^m for the associated ZFS parameters, which follows the early notation of A/K(R) and A/K(E), is no longer justified in view of the consistent notation introduced by Newman and Urban (1975) and Rudowicz (1985a, 1985b, 1987a, 1988).

Other aspects arising from our survey are briefly summarized below. Ozier (1974) has independently provided the STOs, of the type KS/BCS (Rudowicz 1987a, 1988), for $k = 8$ and $q = 0, \pm4, \pm5, \pm6, \pm7$, and ±8. The general form of these operators agrees with our results. Marshall *et al* (1988) have provided listing of the '*Racah polynomial operators*' and the coefficients $B(k, q; j)$ appearing in their MEs. Independent verification of the correctness of this listing requires developing another computer program to generate such explicit forms. In view of the limited usefulness of such listings we have not attempted such work. Various aspects of the analysis of EPR spectra using '*tesseral tensor angular momentum operators*' by Buckmaster and Chatterjee (1998) have been critically commented on by Rudowicz (2003c). Here we note only that clear definitions of the operator notations and crucial notions used in the EMR area are important in order to avoid misunderstanding and incorrect results. In this regard it may be useful to consult the recent reviews on

(i) the spin Hamiltonian formalisms (Rudowicz and Misra 2001);
(ii) the interrelations between the CF and ZFS quantities, which are often confused (Rudowicz and Sung 2001); and

(iii) the major intricacies awaiting unwary EMR spectroscopists (Rudowicz 2002), as well as
(iv) a note on the incorrect orthorhombic ZFS parameter relations (Rudowicz 2000).

The TTOs of the type classified by Rudowicz (1987a, 1988) as the normalized combinations of spherical tensor (NCST) operators have several advantages over the ESOs and have been promoted by McGavin *et al* (1990) and Tennant *et al* (2000), but with rather limited success (Rudowicz and Misra 2001). The NCSTOs are simply related to the normalized Stevens (NS) operators (for references, see Rudowicz 1985a, 1985b, 1987a, 1988) and at the same time are linear combinations of the STOs. McGavin *et al* (1990) have defined their NCSTOs in terms of the KS/BCS operators discussed in section 2 (see the classification by Rudowicz 1987a, 1988). They also provided the conversion factors A_l^m (or A_k^q) relating the ESOs denoted as $\bar{O}_l^m$ and the '*tesseral combinations of spherical-tensor operators*', i.e. the NCSTOs, in their table 1 for rank $l(k) = 0$–8. Using the conversion factors between the ES and KS/BCS operators (Rudowicz 1987a, 1988) obtained from our new *Mathematica* program based on Ryabov (1999) algorithms we have generated independently table 1 of McGavin *et al* (1990) and found the same results. This test also proves the correctness of our general computer code.

Interestingly, in spite of the well-defined operators existing in the literature as discussed above, some authors provide 'independent-like' explicit listings of some operator components they need, e.g. for rank $k = 2$ or 4. However, in the case when regrettably no references to the well-established definitions are provided, such practices (see, e.g., Shimokoshi and Ohi 1990, Barra *et al* 1998, Lipiński 1999, Allard and Härd 2001, Mossin *et al* 2001, Misra *et al* 2003, Sessoli and Gatteschi 2003) only add up to the widespread confusion concerning operator and parameter notations (Rudowicz 1987a, 1988, Rudowicz and Misra 2001, Rudowicz and Sung 2001). In view of the above survey, an updated comprehensive review of the intricacies and interrelations between various notations used in the EMR and related areas covering the post-1987 period would be timely and is now in progress.

5. Summary

We hope that the generalization of the ESOs to higher ranks k and arbitrary spin S carried out here will boost the application of the ES and other related operators to high-spin complexes like Mn_{12} and Fe_{10} with spin $S = 10$ or Fe_{19} with spin $S = 33/2$ at least for the magnetic field parallel to the z-axis of the generalized ESOs. For general arbitrary magnetic field, the transformation expressions for the generalized ESOs (Rudowicz 1985a, 1985b) as well as those for the STOs (Buckmaster 1964, 1966, Weiler and Wylie 1965, Tennant *et al* 2000) need to be extended to higher ranks. The corrections to the existing operator and matrix elements tables as well as the pertinent clarifications presented here may reduce the confusion and enhance the reliability of the computer programs and the subsequent data analysis.

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Appendix A.

See table opposite.

Table A.1. Corrections to various matrix elements of the Stevens operators listed in the respective sources. (Note: The first figure in the matrix element entries stands for the scaling factor; e.g., $30 \times (44\sqrt{273})$ means that 30 is the scaling factor.)

							Present work		
							Scaling factors		
Operator	ME	A/K(R)	A/K(E)	Misra	A/B(E1) (E2)	A/B(R)	Extracted		Multiplied
O_2^0									
$j = 1$	$\langle 1\|\|1\rangle$	$1 \times (-1)^{a,e}$	$1 \times (-1)^{a}$	$1 \times (+1)$	$1 \times (+1)$	$1 \times (+1)$	$1 \times (+1)$	=	+1
$j = 3/2$	$\langle 3/2\|\|3/2\rangle$	$3 \times (-1)^{a,e}$	$3 \times (-1)^{a}$	$3 \times (+1)$	$3 \times (+1)$	$3 \times (+1)$	$3 \times (+1)$	=	+3
O_4^4									
$j = 7$	$\langle 4\|\|0\rangle$	$12 \times (5\sqrt{162})^{a}$	$12 \times (5\sqrt{162})^{a}$	$12 \times (5\sqrt{162})^{a}$	$12 \times (5\sqrt{462})$	$12 \times (5\sqrt{462})$	$12 \times (5\sqrt{462})$	=	$60\sqrt{462}$
O_6^1									
$j = 8$	$\langle 8\|\|7\rangle$	$115 \times (1092)^{b}$	$115 \times (1092)^{b}$	$115 \times (1092)^{b}$	NA[d]	NA[d]	$15 \times (12012)$	=	180 180
	$\langle 7\|\|6\rangle$	$115 \times (-91\sqrt{30})^{b}$	$115 \times (-91\sqrt{30})^{b}$	$115 \times (-91\sqrt{30})^{b}$	NA[d]	NA[d]	$15 \times (-1001\sqrt{30})$	=	$-15\,015\sqrt{30}$
	$\langle 6\|\|5\rangle$	$115 \times (-143\sqrt{42})^{b}$	$115 \times (-143\sqrt{42})^{b}$	$115 \times (-143\sqrt{42})^{b}$	NA[d]	NA[d]	$15 \times (-1573\sqrt{42})$	=	$-23\,595\sqrt{42}$
	$\langle 5\|\|4\rangle$	$115 \times (-126\sqrt{13})^{b}$	$115 \times (-126\sqrt{13})^{b}$	$115 \times (-126\sqrt{13})^{b}$	NA[d]	NA[d]	$15 \times (-1386\sqrt{13})$	=	$-20\,790\sqrt{13}$
	$\langle 4\|\|3\rangle$	$115 \times (70\sqrt{15})^{b}$	$115 \times (70\sqrt{15})^{b}$	$115 \times (70\sqrt{15})^{b}$	NA[d]	NA[d]	$15 \times (770\sqrt{15})$	=	$11\,550\sqrt{15}$
	$\langle 3\|\|2\rangle$	$115 \times (91\sqrt{66})^{b}$	$115 \times (91\sqrt{66})^{b}$	$115 \times (91\sqrt{66})^{b}$	NA[d]	NA[d]	$15 \times (1001\sqrt{66})$	=	$15\,015\sqrt{66}$
	$\langle 2\|\|1\rangle$	$115 \times (87\sqrt{70})^{b}$	$115 \times (87\sqrt{70})^{b}$	$115 \times (87\sqrt{70})^{b}$	NA[d]	NA[d]	$15 \times (957\sqrt{70})$	=	$14\,355\sqrt{70}$
	$\langle 1\|\|0\rangle$	$115 \times (210\sqrt{2})^{b}$	$115 \times (210\sqrt{2})^{b}$	$115 \times (210\sqrt{2})^{b}$	NA[d]	NA[d]	$15 \times (2310\sqrt{2})$	=	$34\,650\sqrt{2}$
$j = 9/2$	$\langle 5/2\|\|3/2\rangle$	$120 \times (-2\sqrt{21})^{b}$	$120 \times (-2\sqrt{21})^{b}$	$120 \times (-2\sqrt{21})^{b}$	NA[d]	NA[d]	$120 \times (2\sqrt{21})$	=	$240\sqrt{21}$
$j = 15/2$	$\langle 5/2\|\|3/2\rangle$	$330 \times (60\sqrt{15})^{b}$	$330 \times (60\sqrt{15})^{b}$	$330 \times (60\sqrt{15})^{b}$	NA[d]	NA[d]	$330 \times (70\sqrt{15})$	=	$23\,100\sqrt{15}$
O_6^2									
$j = 4$	$\langle 4\|\|2\rangle$	$30 \times (27\sqrt{7})^{a}$	$30 \times (27\sqrt{7})^{a}$	$30 \times (27\sqrt{7})^{a}$	$30 \times (24\sqrt{7})$	$30 \times (24\sqrt{7})$	$30 \times (24\sqrt{7})$	=	$720\sqrt{7}$
$j = 5$	$\langle 1\|\|-1\rangle$	$120 \times (28)^{a,e}$	$120 \times (28)^{a}$	$120 \times (84)$	$120 \times (84)$	$120 \times (84)$	$120 \times (84)$	=	10 080
	$\langle 5\|\|3\rangle$	$120 \times (-42\sqrt{5})^{a,e}$	$120 \times (-42\sqrt{5})^{a}$	$120 \times (-42\sqrt{5})^{a}$	$120 \times (42\sqrt{5})$	$120 \times (42\sqrt{5})$	$120 \times (42\sqrt{5})$	=	$5040\sqrt{5}$
$j = 6$	$\langle 5\|\|3\rangle$	$72 \times (-14\sqrt{165})$	$72 \times (-14\sqrt{165})$	$72 \times (-14\sqrt{165})$	$72 \times (-14\sqrt{165})$	$72 \times (-14\sqrt{65})^{a,e}$	$72 \times (-14\sqrt{165})$	=	$-1008\sqrt{165}$

Table A.1. (Continued.)

							Present work		
							Scaling factors		
Operator	ME	A/K(R)	A/K(E)	Misra	A/B(E1) (E2)	A/B(R)	Extracted		Multiplied
O_6^3									
$j = 7$	$\langle 4\|\|1\rangle$	$90 \times (-70\sqrt{35})$[a]	$90 \times (-70\sqrt{35})$[a]	$90 \times (-70\sqrt{33})$	$90 \times (-70\sqrt{33})$	$90 \times (-70\sqrt{33})$	$90 \times (-70\sqrt{33})$	=	$-6300\sqrt{33}$
O_6^4									
$j = 3$	$\langle 2\|\|-2\rangle$	$60 \times (-6)$	$60 \times (-6)$	$60 \times (+6)$[a]	$60 \times (-6)$	$60 \times (-6)$	$60 \times (-6)$	=	-360
$j = 7$	$\langle 4\|\|0\rangle$	$60 \times (-6\sqrt{4211})$[b,e]	$60 \times (-6\sqrt{4211})$[b]	$60 \times (-6\sqrt{4211})$[b]	$60 \times (-6\sqrt{462})$	$60 \times (-6\sqrt{462})$	$60 \times (-6\sqrt{462})$	=	$-360\sqrt{462}$
	$\langle 5\|\|1\rangle$	$60 \times (143\sqrt{33})$[a,e]	$60 \times (143\sqrt{33})$[a]	$60 \times (143\sqrt{33})$[a]	$60 \times (147\sqrt{33})$	$60 \times (147\sqrt{33})$	$60 \times (147\sqrt{33})$	=	$8820\sqrt{33}$
$j = 7/2$	$\langle 7/2\|\|-1/2\rangle$	$60 \times (3\sqrt{55})$[a,e]	$60 \times (3\sqrt{55})$[a]	$60 \times (3\sqrt{55})$[a]	$60 \times (3\sqrt{35})$	$60 \times (3\sqrt{35})$	$60 \times (3\sqrt{35})$	=	$180\sqrt{35}$
$j = 9/2$	$\langle 9/2\|\|1/2\rangle$	$60\sqrt{7} \times (3\sqrt{2})$[a]	$60\sqrt{7} \times (3\sqrt{2})$[a]	$60\sqrt{7} \times (3\sqrt{2})$[a]	$60\sqrt{7} \times (30\sqrt{2})$	$60\sqrt{7} \times (30\sqrt{2})$	$60\sqrt{7} \times (30\sqrt{2})$	=	$1800\sqrt{14}$
O_6^5									
$j = 8$	$\langle 8\|\|3\rangle$	$30 \times (44\sqrt{273})$	$30 \times (44\sqrt{273})$	$30 \times (41\sqrt{273})$[a]	NA[d]	NA[d]	$30 \times (44\sqrt{273})$	=	$1320\sqrt{273}$
O_4^0									
$j = 3$	Scaling factor	$F = 60$	$F = 60$	$F = 60$	$F = 60$	$F = 20$[b,e]			
O_4^3									
$j = 11/2$	Scaling factor	$F = 12$[c]	$F = 12$[c]	$F = 12\sqrt{5}$[c]	NA[d]	NA[d]			

[a] Apparent misprint.
[b] Error.
[c] Difference in presentation only, no error.
[d] NA = not applicable since data for this operator are not given in this source.
[e] Errors found by Ryabov (private communication, 2001).

Appendix B.

B.1. Listing of the explicit form for the ES operators with $k = 3, 5, 7$ and for both positive and negative values of q

Note: $Jp = J_+$; $Jm = J_-$; and $X = J(J+1)$

$$O[3,3] = \tfrac{1}{2}(Jm^3 + Jp^3)$$
$$O[3,-3] = \tfrac{1}{2}\mathbf{i}(Jm^3 - Jp^3)$$
$$O[3,2] = \tfrac{1}{2}(Jm^2(-1+Jz) + Jp^2(1+Jz))$$
$$O[3,-2] = -\tfrac{1}{2}\mathbf{i}(-Jm^2(-1+Jz) + Jp^2(1+Jz))$$
$$O[3,1] = \tfrac{1}{2}(5(-Jm+Jp)Jz + 5(Jm+Jp)Jz^2 - (Jm+Jp)(-2+X))$$
$$O[3,-1] = -\tfrac{1}{2}\mathbf{i}(5(Jm+Jp)Jz + 5(-Jm+Jp)Jz^2 + (Jm-Jp)(-2+X))$$
$$O[3,0] = Jz + 5Jz^3 - 3JzX$$
$$O[5,5] = \tfrac{1}{2}(Jm^5 + Jp^5)$$
$$O[5,-5] = \tfrac{1}{2}\mathbf{i}(Jm^5 - Jp^5)$$
$$O[5,4] = \tfrac{1}{2}(Jm^4(-2+Jz) + Jp^4(2+Jz))$$
$$O[5,-4] = -\tfrac{1}{2}\mathbf{i}(-Jm^4(-2+Jz) + Jp^4(2+Jz))$$
$$O[5,3] = \tfrac{1}{2}(27(-Jm^3+Jp^3)Jz + 9(Jm^3+Jp^3)Jz^2 - (Jm^3+Jp^3)(-24+X))$$
$$O[5,-3] = -\tfrac{1}{2}\mathbf{i}(Jp^3(24+27Jz+9Jz^2-X) + Jm^3(-24+27Jz-9Jz^2+X))$$
$$O[5,2] = \tfrac{1}{2}(Jm^2(-1+Jz)(6-6Jz+3Jz^2-X) + Jp^2(1+Jz)(6+6Jz+3Jz^2-X))$$
$$O[5,-2] = -\tfrac{1}{2}\mathbf{i}(-Jm^2(-1+Jz)(6-6Jz+3Jz^2-X) \\ + Jp^2(1+Jz)(6+6Jz+3Jz^2-X))$$
$$O[5,1] = \tfrac{1}{2}(42(-Jm+Jp)Jz^3 + 21(Jm+Jp)Jz^4 + 14(Jm-Jp)Jz(-3+X) \\ - 7(Jm+Jp)Jz^2(-9+2X) + (Jm+Jp)(12-8X+X^2))$$
$$O[5,-1] = -\tfrac{1}{2}\mathbf{i}(42(Jm+Jp)Jz^3 + 21(-Jm+Jp)Jz^4 - 14(Jm+Jp)Jz(-3+X) \\ + 7(Jm-Jp)Jz^2(-9+2X) + (-Jm+Jp)(12-8X+X^2))$$
$$O[5,0] = Jz(12 + 63Jz^4 - 50X + 15X^2 - 35Jz^2(-3+2X))$$
$$O[7,7] = \tfrac{1}{2}(Jm^7 + Jp^7)$$
$$O[7,-7] = \tfrac{1}{2}\mathbf{i}(Jm^7 - Jp^7)$$
$$O[7,6] = \tfrac{1}{2}(Jm^6(-3+Jz) + Jp^6(3+Jz))$$
$$O[7,-6] = -\tfrac{1}{2}\mathbf{i}(-Jm^6(-3+Jz) + Jp^6(3+Jz))$$
$$O[7,5] = \tfrac{1}{2}(65(-Jm^5+Jp^5)Jz + 13(Jm^5+Jp^5)Jz^2 - (Jm^5+Jp^5)(-90+X))$$
$$O[7,-5] = -\tfrac{1}{2}\mathbf{i}(Jp^5(90+65Jz+13Jz^2-X) + Jm^5(-90+65Jz-13Jz^2+X))$$
$$O[7,4] = \tfrac{1}{2}(Jm^4(-2+Jz)(75-52Jz+13Jz^2-3X) \\ + Jp^4(2+Jz)(75+52Jz+13Jz^2-3X))$$
$$O[7,-4] = -\tfrac{1}{2}\mathbf{i}(-Jm^4(-2+Jz)(75-52Jz+13Jz^2-3X) \\ + Jp^4(2+Jz)(75+52Jz+13Jz^2-3X))$$

$$O[7,3] = \tfrac{1}{2}(858(-Jm^3 + Jp^3)Jz^3 + 143(Jm^3 + Jp^3)Jz^4 + 66(Jm^3 - Jp^3)Jz(-49 + 3X) - 11(Jm^3 + Jp^3)Jz^2(-215 + 6X) + 3(Jm^3 + Jp^3)(600 - 62X + X^2))$$

$$O[7,-3] = -\tfrac{1}{2}\mathbf{i}(858(Jm^3 + Jp^3)Jz^3 + 143(-Jm^3 + Jp^3)Jz^4 - 66(Jm^3 + Jp^3)Jz(-49 + 3X) + 11(Jm^3 - Jp^3)Jz^2(-215 + 6X) + 3(-Jm^3 + Jp^3)(600 - 62X + X^2))$$

$$O[7,2] = \tfrac{1}{2}(715(-Jm^2 + Jp^2)Jz^4 + 143(Jm^2 + Jp^2)Jz^5 - 55(Jm^2 + Jp^2)Jz^3(-37 + 2X) + 55(Jm^2 - Jp^2)Jz^2(-59 + 6X) + 15(-Jm^2 + Jp^2)(72 - 18X + X^2) + (Jm^2 + Jp^2)Jz(2862 - 490X + 15X^2))$$

$$O[7,-2] = -\tfrac{1}{2}\mathbf{i}(715(Jm^2 + Jp^2)Jz^4 + 143(-Jm^2 + Jp^2)Jz^5 + 55(Jm^2 - Jp^2)Jz^3(-37 + 2X) - 55(Jm^2 + Jp^2)Jz^2(-59 + 6X) + 15(Jm^2 + Jp^2)(72 - 18X + X^2) + (-Jm^2 + Jp^2)Jz(2862 - 490X + 15X^2))$$

$$O[7,1] = \tfrac{1}{2}(1287(-Jm + Jp)Jz^5 + 429(Jm + Jp)Jz^6 + 495(Jm - Jp)Jz^3(-11 + 2X) - 165(Jm + Jp)Jz^4(-23 + 3X) + 9(-Jm + Jp)Jz(332 - 160X + 15X^2) + 3(Jm + Jp)Jz^2(1832 - 645X + 45X^2) - 5(Jm + Jp)(-144 + 108X - 20X^2 + X^3))$$

$$O[7,-1] = -\tfrac{1}{2}\mathbf{i}(1287(Jm + Jp)Jz^5 + 429(-Jm + Jp)Jz^6 - 495(Jm + Jp)Jz^3(-11 + 2X) + 165(Jm - Jp)Jz^4(-23 + 3X) + 9(Jm + Jp)Jz(332 - 160X + 15X^2) + 3(-Jm + Jp)Jz^2(1832 - 645X + 45X^2) + 5(Jm - Jp)(-144 + 108X - 20X^2 + X^3))$$

$$O[7,0] = Jz(180 + 429Jz^6 - 882X + 385X^2 - 35X^3 - 231Jz^4(-10 + 3X) + 21Jz^2(101 - 105X + 15X^2)).$$

B.2. Listing of the explicit form for the ES operators with $k = 8, 10, 12$ and for positive values of q only

Note: $Jp = J_+$; $Jm = J_-$; $X = J(J+1)$

$$O[8,8] = \tfrac{1}{2}(Jm^8 + Jp^8)$$

$$O[8,7] = \tfrac{1}{4}(Jm^7(-7 + 2Jz) + Jp^7(7 + 2Jz))$$

$$O[8,6] = \tfrac{1}{2}(90(-Jm^6 + Jp^6)Jz + 15(Jm^6 + Jp^6)Jz^2 - (Jm^6 + Jp^6)(-147 + X))$$

$$O[8,5] = \tfrac{1}{4}(Jm^5(-5 + 2Jz)(42 - 25Jz + 5Jz^2 - X) + Jp^5(5 + 2Jz)(42 + 25Jz + 5Jz^2 - X))$$

$$O[8,4] = \tfrac{1}{2}(520(-Jm^4 + Jp^4)Jz^3 + 65(Jm^4 + Jp^4)Jz^4 - 13(Jm^4 + Jp^4)Jz^2(-139 + 2X) + 52(Jm^4 - Jp^4)Jz(-59 + 2X) + (Jm^4 + Jp^4)(2100 - 122X + X^2))$$

$$O[8,3] = \tfrac{1}{4}(Jp^3(3 + 2Jz)(840 + 234Jz^3 + 39Jz^4 - 78Jz(-15 + X) - 106X + 3X^2 - 13Jz^2(-57 + 2X)) + Jm^3(-3 + 2Jz)(840 - 234Jz^3 + 39Jz^4 + 78Jz(-15 + X) - 106X + 3X^2 - 13Jz^2(-57 + 2X)))$$

$$O[8,2] = \frac{1}{2}(858(-Jm^2 + Jp^2)Jz^5 + 143(Jm^2 + Jp^2)Jz^6 - 143(Jm^2 + Jp^2)Jz^4(-22 + X) + 572(Jm^2 - Jp^2)Jz^3(-12 + X) + 11(Jm^2 + Jp^2)Jz^2(853 - 119X + 3X^2) + 22(-Jm^2 + Jp^2)Jz(333 - 67X + 3X^2) - (Jm^2 + Jp^2)(-2520 + 702X - 53X^2 + X^3))$$

$$O[8,1] = \frac{1}{4}(5005(-Jm + Jp)Jz^6 + 1430(Jm + Jp)Jz^7 + 5005(Jm - Jp)Jz^4(-7 + X) - 1001(Jm + Jp)Jz^5(-19 + 2X) + 385(Jm + Jp)Jz^3(131 - 36X + 2X^2) + 385(-Jm + Jp)Jz^2(112 - 41X + 3X^2) + (Jm + Jp)Jz(22\,356 - 12\,488X + 1785X^2 - 70X^3) + 35(Jm - Jp)(-144 + 108X - 20X^2 + X^3))$$

$$O[8,0] = \frac{1}{2}(12\,870Jz^8 - 12\,012Jz^6(-9 + 2X) + 2310Jz^4(81 - 56X + 6X^2) + 70X(-144 + 108X - 20X^2 + X^3) - 12Jz^2(-4566 + 9898X - 3045X^2 + 210X^3))$$

$$O[10,10] = \frac{1}{2}(Jm^{10} + Jp^{10})$$

$$O[10,9] = \frac{1}{4}(Jm^9(-9 + 2Jz) + Jp^9(9 + 2Jz))$$

$$O[10,8] = \frac{1}{2}(Jm^8(324 - 152Jz + 19Jz^2 - X) + Jp^8(324 + 152Jz + 19Jz^2 - X))$$

$$O[10,7] = \frac{1}{4}(Jm^7(-7 + 2Jz)(288 - 133Jz + 19Jz^2 - 3X) + Jp^7(7 + 2Jz)(288 + 133Jz + 19Jz^2 - 3X))$$

$$O[10,6] = \frac{1}{2}(3876(-Jm^6 + Jp^6)Jz^3 + 323(Jm^6 + Jp^6)Jz^4 - 17(Jm^6 + Jp^6)Jz^2(-1127 + 6X) + 102(Jm^6 - Jp^6)Jz(-443 + 6X) + 3(Jm^6 + Jp^6)(14\,112 - 338X + X^2))$$

$$O[10,5] = \frac{1}{4}(8075(-Jm^5 + Jp^5)Jz^4 + 646(Jm^5 + Jp^5)Jz^5 - 340(Jm^5 + Jp^5)Jz^3(-134 + X) + 425(Jm^5 - Jp^5)Jz^2(-329 + 6X) + 15(-Jm^5 + Jp^5)(10\,584 - 500X + 5X^2) + 2(Jm^5 + Jp^5)Jz(114\,627 - 3625X + 15X^2))$$

$$O[10,4] = \frac{1}{2}(3876(-Jm^4 + Jp^4)Jz^5 + 323(Jm^4 + Jp^4)Jz^6 + 2040(Jm^4 - Jp^4)Jz^3(-39 + X) - 85(Jm^4 + Jp^4)Jz^4(-269 + 3X) + 12(-Jm^4 + Jp^4)Jz(16\,792 - 1075X + 15X^2) + (Jm^4 + Jp^4)Jz^2(168\,152 - 7305X + 45X^2) - (Jm^4 + Jp^4)(-105\,840 + 9252X - 218X^2 + X^3))$$

$$O[10,3] = \frac{1}{4}(6783(-Jm^3 + Jp^3)Jz^6 + 646(Jm^3 + Jp^3)Jz^7 + 1785(Jm^3 - Jp^3)Jz^4(-79 + 3X) - 119(Jm^3 + Jp^3)Jz^5(-329 + 6X) + 63(-Jm^3 + Jp^3)Jz^2(8054 - 735X + 15X^2) + 7(Jm^3 + Jp^3)Jz^3(47\,677 - 3000X + 30X^2) + (Jm^3 + Jp^3)Jz(453\,024 - 56\,154X + 1897X^2 - 14X^3) + 21(Jm^3 - Jp^3)(-8640 + 1392X - 68X^2 + X^3))$$

$$O[10,2] = \frac{1}{2}(33\,592(-Jm^2 + Jp^2)Jz^7 + 4199(Jm^2 + Jp^2)Jz^8 - 3094(Jm^2 + Jp^2)Jz^6(-59 + 2X) + 6188(Jm^2 - Jp^2)Jz^5(-101 + 6X) + 91(Jm^2 + Jp^2)Jz^4(16\,601 - 1640X + 30X^2) + 364(-Jm^2 + Jp^2)Jz^3(6877 - 960X + 30X^2)$$

$$- 26(Jm^2 + Jp^2)Jz^2(-106\,074 + 20\,230X - 1057X^2 + 14X^3)$$
$$+ 52(Jm^2 - Jp^2)Jz(-34\,956 + 8694X - 637X^2 + 14X^3)$$
$$+ 7(Jm^2 + Jp^2)(77\,760 - 24\,768X + 2484X^2 - 92X^3 + X^4))$$

$$O[10,1] = \tfrac{1}{4}(37\,791(-Jm + Jp)Jz^8 + 8398(Jm + Jp)Jz^9$$
$$+ 27\,846(Jm - Jp)Jz^6(-21 + 2X) - 5304(Jm + Jp)Jz^7(-41 + 3X)$$
$$+ 546(Jm + Jp)Jz^5(2603 - 474X + 18X^2)$$
$$+ 819(-Jm + Jp)Jz^4(2661 - 620X + 30X^2)$$
$$+ 234(Jm - Jp)Jz^2(-8186 + 3640X - 427X^2 + 14X^3)$$
$$- 52(Jm + Jp)Jz^3(-49\,073 + 17\,073X - 1596X^2 + 42X^3)$$
$$+ 63(-Jm + Jp)(2880 - 2304X + 508X^2 - 40X^3 + X^4)$$
$$+ 6(Jm + Jp)Jz(146\,904 - 90\,504X + 15\,946X^2 - 1022X^3 + 21X^4))$$

$$O[10,0] = 46\,189Jz^{10} - 36\,465Jz^8(-22 + 3X) + 3003Jz^6(1199 - 450X + 30X^2)$$
$$- 715Jz^4(-6248 + 5481X - 966X^2 + 42X^3)$$
$$- 63X(2880 - 2304X + 508X^2 - 40X^3 + X^4)$$
$$+ 33Jz^2(32\,208 - 78\,900X + 29\,680X^2 - 3290X^3 + 105X^4)$$

$$O[12,12] = \tfrac{1}{2}(Jm^{12} + Jp^{12})$$

$$O[12,11] = \tfrac{1}{4}(Jm^{11}(-11 + 2Jz) + Jp^{11}(11 + 2Jz))$$

$$O[12,10] = \tfrac{1}{2}(Jm^{10}(605 - 230Jz + 23Jz^2 - X) + Jp^{10}(605 + 230Jz + 23Jz^2 - X))$$

$$O[12,9] = \tfrac{1}{4}(Jm^9(-9 + 2Jz)(550 - 207Jz + 23Jz^2 - 3X)$$
$$+ Jp^9(9 + 2Jz)(550 + 207Jz + 23Jz^2 - 3X))$$

$$O[12,8] = \tfrac{1}{2}(2576(-Jm^8 + Jp^8)Jz^3 + 161(Jm^8 + Jp^8)Jz^4$$
$$- 7(Jm^8 + Jp^8)Jz^2(-2365 + 6X) + 56(Jm^8 - Jp^8)Jz(-893 + 6X)$$
$$+ (Jm^8 + Jp^8)(59\,400 - 722X + X^2))$$

$$O[12,7] = \tfrac{1}{4}(5635(-Jm^7 + Jp^7)Jz^4 + 322(Jm^7 + Jp^7)Jz^5$$
$$- 140(Jm^7 + Jp^7)Jz^3(-306 + X) + 245(Jm^7 - Jp^7)Jz^2$$
$$(-709 + 6X) + 35(-Jm^7 + Jp^7)(9504 - 218X + X^2)$$
$$+ 2(Jm^7 + Jp^7)Jz(185\,749 - 2805X + 5X^2))$$

$$O[12,6] = \tfrac{1}{2}(55\,062(-Jm^6 + Jp^6)Jz^5 + 3059(Jm^6 + Jp^6)Jz^6$$
$$- 665(Jm^6 + Jp^6)Jz^4(-688 + 3X) + 7980(Jm^6 - Jp^6)Jz^3(-274 + 3X)$$
$$+ 19(Jm^6 + Jp^6)Jz^2(328\,739 - 6315X + 15X^2)$$
$$+ 114(-Jm^6 + Jp^6)Jz(87\,827 - 2535X + 15X^2)$$
$$- 5(Jm^6 + Jp^6)(-1397\,088 + 55\,578X - 575X^2 + X^3))$$

$$O[12,5] = \tfrac{1}{4}(15\,295(-Jm^5 + Jp^5)Jz^6 + 874(Jm^5 + Jp^5)Jz^7$$
$$+ 3325(Jm^5 - Jp^5)Jz^4(-205 + 3X) - 133(Jm^5 + Jp^5)Jz^5(-985 + 6X)$$
$$+ 19(Jm^5 + Jp^5)Jz^3(120\,079 - 3020X + 10X^2)$$
$$+ 95(-Jm^5 + Jp^5)Jz^2(51\,056 - 1905X + 15X^2)$$
$$+ (Jm^5 + Jp^5)Jz(6010\,260 - 306\,652X + 4135X^2 - 10X^3)$$
$$+ 5(Jm^5 - Jp^5)(-665\,280 + 44\,076X - 880X^2 + 5X^3))$$

$$\begin{aligned}O[12,4] = \tfrac{1}{2}(&118\,864(-Jm^4+Jp^4)Jz^7+7429(Jm^4+Jp^4)Jz^8\\&-4522(Jm^4+Jp^4)Jz^6(-221+2X)+18\,088(Jm^4-Jp^4)Jz^5(-295+6X)\\&+323(Jm^4+Jp^4)Jz^4(59\,767-2040X+10X^2)\\&+2584(-Jm^4+Jp^4)Jz^3(18\,439-920X+10X^2)\\&-34(Jm^4+Jp^4)Jz^2(-2279\,002+154\,234X-2805X^2+10X^3)\\&+136(Jm^4-Jp^4)Jz(-553\,650+48\,442X-1285X^2+10X^3)\\&+5(Jm^4+Jp^4)(6652\,800-728\,400X+26\,188X^2-340X^3+X^4))\end{aligned}$$

$$\begin{aligned}O[12,3] = \tfrac{1}{4}(&200\,583(-Jm^3+Jp^3)Jz^8+14\,858(Jm^3+Jp^3)Jz^9\\&-7752(Jm^3+Jp^3)Jz^7(-205+3X)+40\,698(Jm^3-Jp^3)Jz^6(-203+6X)\\&+1938(Jm^3+Jp^3)Jz^5(15\,689-762X+6X^2)\\&+2907(-Jm^3+Jp^3)Jz^4(27\,541-1920X+30X^2)\\&-68(Jm^3+Jp^3)Jz^3(-2190\,575+205\,803X-5280X^2+30X^3)\\&+306(Jm^3-Jp^3)Jz^2(-610\,706+73\,962X-2715X^2+30X^3)\\&+45(-Jm^3+Jp^3)(1108\,800-206\,400X+13\,148X^2-340X^3+3X^4)\\&+6(Jm^3+Jp^3)Jz(23\,730\,600-3600\,564X+178\,042X^2-3230X^3+15X^4))\end{aligned}$$

$$\begin{aligned}O[12,2] = \tfrac{1}{2}(&74\,290(-Jm^2+Jp^2)Jz^9+7429(Jm^2+Jp^2)Jz^{10}\\&-4845(Jm^2+Jp^2)Jz^8(-113+3X)+38\,760(Jm^2-Jp^2)Jz^7(-67+3X)\\&+9690(-Jm^2+Jp^2)Jz^5(2501-258X+6X^2)\\&+969(Jm^2+Jp^2)Jz^6(9563-710X+10X^2)\\&-85(Jm^2+Jp^2)Jz^4(-554\,219+77\,439X-3000X^2+30X^3)\\&+340(Jm^2-Jp^2)Jz^3(-193\,637+34\,803X-1860X^2+30X^3)\\&+30(-Jm^2+Jp^2)Jz(1228\,584-346\,356X+32\,182X^2-1190X^3+15X^4)\\&+3(Jm^2+Jp^2)Jz^2(20\,983\,308-4771\,720X+345\,870X^2-9350X^3+75X^4)\\&-3(Jm^2+Jp^2)(-3326\,400+1152\,000X-135\,444X^2\\&+6808X^3-145X^4+X^5))\end{aligned}$$

$$\begin{aligned}O[12,1] = \tfrac{1}{4}(&572\,033(-Jm+Jp)Jz^{10}+104\,006(Jm+Jp)Jz^{11}\\&-124\,355(Jm+Jp)Jz^9(-37+2X)+373\,065(Jm-Jp)Jz^8(-44+3X)\\&+42\,636(Jm+Jp)Jz^7(1383-180X+5X^2)\\&+74\,613(-Jm+Jp)Jz^6(1793-290X+10X^2)\\&-6545(Jm+Jp)Jz^5(-39\,755+9498X-630X^2+12X^3)\\&+6545(Jm-Jp)Jz^4(-53\,702+15\,879X-1290X^2+30X^3)\\&+154(Jm+Jp)Jz^3(2341\,414-937\,880X+113\,055X^2-5100X^3+75X^4)\\&+231(-Jm+Jp)Jz^2(1065\,768-531\,580X+78\,120X^2-4250X^3+75X^4)\\&+231(Jm-Jp)(-86\,400+72\,000X-17\,544X^2+1708X^3-70X^4+X^5)\\&-3(Jm+Jp)Jz(-34\,637\,280+22\,740\,960X-4531\,076X^2\\&+367\,752X^3-12\,705X^4+154X^5))\end{aligned}$$

$$\begin{aligned}O[12,0] = {}&676\,039Jz^{12}-323\,323Jz^{10}(-65+6X)+138\,567Jz^8(1391-330X+15X^2)\\&-17\,017Jz^6(-35\,945+17\,622X-2010X^2+60X^3)\\&+1001Jz^4(606\,164-618\,090X+139\,245X^2-10200X^3+225X^4)\end{aligned}$$

$$+ 231X(-86\,400 + 72\,000X - 17\,544X^2 + 1708X^3 - 70X^4 + X^5)$$
$$- 39Jz^2(-3176\,160 + 8488\,392X - 3601\,048X^2 + 501\,116X^3$$
$$- 26\,565X^4 + 462X^5).$$

Appendix C. Corrections to various operator listings

The original (O) expressions from a given source and the corrected (C) ones are given below. For clarity and easy identification, the nature of a given correction is also provided.

C.1. The listings of the STOs

Table 1 of Danielsen (1973) and Table 1 of Lindgård and Danielsen (1974)

O: $\tilde{O}_{8,0} = \frac{1}{128}[6435J_z^8 - \{12\,012X - 54\,054\}J_z^6 + \{6930X^2 - 64\,680X + 93\,555\}J_z^4$
$- \{1260X^3 - 18\,270X^2 + 59\,388X - 21\,390\}J_z^2$
$+ 35X^4 - 700X^3 + 3780X^2 - 5040X]$

C: $\tilde{O}_{8,0} = \frac{1}{128}[6435J_z^8 - \{12\,012X - 54\,054\}J_z^6 + \{6930X^2 - 64\,680X + 93\,555\}J_z^4$
$- \{1260X^3 - 18\,270X^2 + 59\,388X - 27\,396\}J_z^2$
$+ 35X^4 - 700X^3 + 3780X^2 - 5040X]$

'−21 390' should be replaced by '−27 396'.

Table 1 of Lindgård and Danielsen (1974)

O: $\tilde{O}_{5\pm3} = \mp\sqrt{\frac{35}{256}}\frac{1}{2}\left[\left\{9J_z^2 - Xj\frac{33}{2}\right\}(J^{\pm})^3 + (J^{\pm})^3\{\cdots\}\right],$

C: $\tilde{O}_{5\pm3} = \mp\sqrt{\frac{35}{256}}\frac{1}{2}\left[\left\{9J_z^2 - X - \frac{33}{2}\right\}(J^{\pm})^3 + (J^{\pm})^3\{\cdots\}\right];$

'$Xj\frac{33}{2}$' should be replaced by '$X - \frac{33}{2}$'.

C.2. The listings of the Stevens operators

Table 2 of Danielsen (1973) and Table 6 of Danielsen and Lindgård (1972)

O: $O_8^0 = 6435J_z^8 - \{12\,012X - 54\,054\}J_z^6 + \{6930X^2 - 64\,680X + 93\,555\}J_z^4$
$+ \{-1260X^3 + 18\,270X^2 - 59\,388X + 21\,390\}J_z^2$
$+ 35X^4 - 700X^3 + 3780X^2 - 5040X$

C: $O_8^0 = 6435J_z^8 - \{12\,012X - 54\,054\}J_z^6 + \{6930X^2 - 64\,680X + 93\,555\}J_z^4$
$+ \{-1260X^3 + 18\,270X^2 - 59\,388X + 27\,396\}J_z^2$
$+ 35X^4 - 700X^3 + 3780X^2 - 5040X$

'+21 390' should be replaced by '+27 396'.

C.3. The listings of the STOs

C.3.1. Table 1 in the asymmetric form of Buckmaster and Dering (1967).

O: $T_{4\pm4} = +\frac{1}{2}J_{\pm}^4$, C: $T_{4\pm4} = +\frac{1}{4}J_{\pm}^4$; factor '$+\frac{1}{2}$' should be replaced by '$+\frac{1}{4}$'

O: $T_{4\pm3} = \mp\frac{1}{2}\sqrt{\frac{1}{2}}J_\pm^3\{2J_2 \pm 3\}$, C: $T_{4\pm3} = \mp\frac{1}{2}\sqrt{\frac{1}{2}}J_\pm^3\{2J_z \pm 3\}$;

'$2J_2$' should be replaced by '$2J_z$'

O: $T_{5\pm1} = \mp\frac{1}{4}\sqrt{\frac{5}{21}}J_\pm\{21J_z^4 \pm 42J_z^4 - 7[2J(J+1)+9]J_z^2 \mp 14[J(J+1)-3]J_z + J^2(J+1)^2 - 8J(J+1) + 12\}$

C: $T_{5\pm1} = \mp\frac{1}{4}\sqrt{\frac{5}{21}}J_\pm\{21J_z^4 \pm 42J_z^3 - 7[2J(J+1)-9]J_z^2 \mp 14[J(J+1)-3]J_z + J^2(J+1)^2 - 8J(J+1) + 12\}$

'$\pm 42J_z^4$' should be replaced by '$\pm 42J_z^3$' and '+9' replaced by '−9'

O: $T_{6\pm1} = \mp\frac{1}{4}\sqrt{\frac{1}{22}}\{66J_z^5 \pm 165J_z^4 - 60[J(J+1)-6]J_z^3 \mp 15[6J(J+1)-25]J_z^2 + 2(5J(J+1)^2 - 55J(J+1) + 117)J_2 \mp 5[J^2(J+1)^2 - 8J^2(J+1)^2 + 12]\}$

C: $T_{6\pm1} = \mp\frac{1}{4}\sqrt{\frac{1}{22}}J_\pm\{66J_z^5 \pm 165J_z^4 - 60[J(J+1)-6]J_z^3 \mp 15[6J(J+1)-25]J_z^2 + 2(5J^2(J+1)^2 - 55J(J+1) + 117)J_z \mp 5[J^2(J+1)^2 - 8J^2(J+1)^2 + 12]\}$

'$5J$' should be replaced by '$5J^2$'; 'J_2' by 'J_z', and '$J_\pm$' should appear in front of the RHS

O: $T_{70} = +\frac{1}{8}\sqrt{\frac{1}{143}}\{429J_z^7 - 213[3J(J+1)+10]J_z^5 + 21[15J^2(J+1)^2 - 105J(J+1) + 101]J_z^3 - 35J^3(J+1)^3 + 385J^2(J+1)^2 - 882J(J+1) + 180\}$

C: $T_{70} = +\frac{1}{4}\sqrt{\frac{1}{429}}[429J_z^7 - 231[3J(J+1)-10]J_z^5 + 21[15J^2(J+1)^2 - 105J(J+1) - 101]J_z^3 + (-35J^3(J+1)^3 + 385J^2(J+1)^2 - 882J(J+1) + 180)J_z]$

'$\sqrt{\frac{1}{143}}$' should be replaced by '$\sqrt{\frac{1}{429}}$'; '+10' by '−10' and '$35J^3(J+1)^3 + 385J^2(J+1)^2 - 882J(J+1) + 180$' by '$(-35J^3(J+1)^3 + 385J^2(J+1)^2 - 882J(J+1) + 180)J_z$'

O: $T_{7\pm2} = +\frac{1}{8}\sqrt{\frac{1}{143}}J_\pm\{143J_z^5 \pm 715J_z^4 - 55[2J(J+1)-37]J_z^3 \mp 55[6J(J+1)-59]J_z^2 + [15J^2(J+1)^2 - 490J(J+1) + 2862]J_z + 15[J^2(J+1)^2 - 18J(J+1) + 72]\}$

C: $T_{7\pm2} = +\frac{1}{8}\sqrt{\frac{1}{143}}J_\pm^2\{143J_z^5 \pm 715J_z^4 - 55[2J(J+1)-37]J_z^3 \mp 55[6J(J+1) - 59]J_z^2 + [15J^2(J+1)^2 - 490J(J+1) + 2862]J_z \pm 15[J^2(J+1)^2 - 18J(J+1) + 72]\}$

'$J_\pm$' should be replaced by '$J_\pm^2$' and '+15' by '±15'

O: $T_{7\pm5} = \mp\frac{1}{8}\sqrt{\frac{7}{26}}J_\pm^5\{13J^2 \pm 65J_z - J(J+1) + 90\}$

C: $T_{7\pm5} = \mp\frac{1}{8}\sqrt{\frac{7}{26}}J_\pm^5\{13J_z^2 \pm 65J_z - J(J+1) + 90\}$

'$13J^2$' should be replaced by '$13J_z^2$'.

C.3.2. Table 2 in the symmetric form of Buckmaster and Dering (1967).

O: $T_{4\pm2} = +\frac{1}{4}\sqrt{\frac{1}{7}}[J_\pm^2\{7J_z^2 - J(J+1) - 5\} + \{7J_z^2 - J(J+1) - 5\}J_\pm^2]$

C: $T_{4\pm2} = +\frac{1}{2}\sqrt{\frac{1}{7}}[J_\pm^2\{7J_z^2 - J(J+1) - 5\} + \{7J_z^2 - J(J+1) - 5\}J_\pm^2]$

'$+\frac{1}{4}$' should be replaced by '$+\frac{1}{2}$'

O: $T_{5\pm2} = +\frac{1}{4}\sqrt{\frac{5}{3}}[J_\pm^2\{3J_z^3 - [J(J+1)+6]J_z^2 + 2J^2(J+1)^2 - 2J(J+1) + 3\}$
$+ \{3J_z^3 - [J(J+1)+6]J_z^2 + 2J^2(J+1)^2 - 2J(J+1) + 3\}J_\pm^2]$

C: $T_{5\pm2} = +\frac{1}{4}\sqrt{\frac{5}{3}}[J_\pm^2\{3J_z^3 - [J(J+1)+6]J_z\} + \{3J_z^3 - [J(J+1)+6]J_z +\}J_\pm^2]$

'$[J(J+1)+6]J_z^2$' should be replaced by '$[J(J+1)+6]J_z$' and
'$+ 2J^2(J+1)^2 - 2J(J+1) + 3$' should be deleted

O: $T_{70} = +\frac{1}{4}\sqrt{\frac{1}{143}}[429J_z^7 - 231[3J(J+1)+10]J_z^5 + 21[15J^2(J+1)^2 - 105J(J+1)$
$+ 101]J_z^3 - 35J^3(J+1)^3 + 385J^2(J+1)^2 - 882J(J+1) + 180]$

C: $T_{70} = +\frac{1}{4}\sqrt{\frac{1}{429}}[429J_z^7 - 231[3J(J+1)-10]J_z^5 + 21[15J^2(J+1)^2$
$- 105J(J+1) - 101]J_z^3 + (-35J^3(J+1)^3$
$+ 385J^2(J+1)^2 - 882J(J+1) + 180)J_z]$

'$\sqrt{\frac{1}{143}}$' should be replaced by '$\sqrt{\frac{1}{429}}$'; '+10' by '−10'; '$35J^3(J+1)^3$
$+ 385J^2(J+1)^2 - 882J(J+1) + 180$' by '$(-35J^3(J+1)^3$
$+ 385J^2(J+1)^2 - 882J(J+1) + 180)J_z$'.

C.4. Table 2 in Tuszynski (1990)

O: $T_{\pm2}^3(J) = +\frac{1}{2}(\frac{3}{1})^{1/2}J_\pm^3\{J_z \pm 1\}$ $\quad$ $C: T_{\pm2}^3(J) = +\frac{1}{2}(\frac{3}{1})^{1/2}J_\pm^2\{J_z \pm 1\}$;

'$J_\pm^3$' should be replaced by '$J_\pm^2$'

O: $T_{\pm2}^6 T_{6\pm2}(J) = +\frac{1}{8}(\frac{5}{11})^{1/2}J_\pm^2\{3J_z^4 \pm 132J_z^2 + 3[91 - 6J(J+1)]J_z^2$
$\pm 6[47 - 6J(J + (J+1)] + [120 - 26J(J+1) + J^2(J+1)^2]\}$

C: $T_{\pm2}^6(J) = +\frac{1}{8}(\frac{5}{11})^{1/2}J_\pm^2\{33J_z^4 \pm 132J_z^3 + 3[91 - 6J(J+1)]J_z^2$
$\pm 6[47 - 6J(J+1)]J_z + [120 - 26J(J+1) + J^2(J+1)^2]\}$

'$T_{\pm2}^6 T_{6\pm2}(J)$' should be replaced by '$T_{\pm2}^6(J)$'; '$3J_z^4$' by '$33J_z^4$';
'$\pm 6[47 - 6J(J + (J+1)]$' by '$\pm 6[47 - 6J(J+1)]J_z$'

O: $T_{\pm1}^6(J) = \pm\frac{1}{4}(\frac{1}{22})^{1/2}J_\pm\{66J_z^4 \pm 165J_z^4 + 60[6 - J(J+1)]J_z^3 \pm 15[25 - 6J(J+1)]J_z^2$
$+ 2[117 - 55J(J+1) + 5J^2(J+1)^2]$
$\pm 5[12 - 8J(J+1) + J^2(J+1)^2]\}$

C: $T^6_{\pm1}(J) = \mp\frac{1}{4}(\frac{1}{22})^{1/2}J_\pm\{66J_z^5 \pm 165J_z^4 + 60[6 - J(J+1)]J_z^3 \pm 15[25 - 6J(J+1)]J_z^2$
$+ 2[117 - 55J(J+1) + 5J^2(J+1)^2]J_z$
$\pm 5[12 - 8J(J+1) + J^2(J+1)^2]\}$
'$\pm\frac{1}{4}(\frac{1}{22})^{1/2}$' should be replaced by '$\mp\frac{1}{4}(\frac{1}{22})^{1/2}$'; '$66J_z^4$' by '$66J_z^5$'; '$2[117 - 55J(J+1) + 5J^2(J+1)^2]$' by '$2[117 - 55J(J+1) + 5J^2(J+1)^2]J_z$'.

C.5. Misra et al (1996) and M99

O: $\hat{Y}_5^{\pm1} = \frac{1}{2}\{[21S_z^4 - 14S(S+1)S_z^2 + S^2(S+1)^2 - S(S-1) + \frac{3}{2}]S_\pm + S_\pm[21S_z^4 - 14S(S+1)S_z^2 + S^2(S+1)^2 - S(S-1) + \frac{3}{2}]\}$

C: $\hat{Y}_5^{\pm1} = \frac{1}{2}\{[21S_z^4 - 14S(S+1)S_z^2 + S^2(S+1)^2 - S(S+1) + \frac{3}{2}]S_\pm + S_\pm[21S_z^4 - 14S(S+1)S_z^2 + S^2(S+1)^2 - S(S+1) + \frac{3}{2}]\}$
term '$-S(S-1)$' should be replaced (twice) by '$-S(S+1)$'

O: $\hat{Y}_5^{\pm2} = \frac{1}{2}\{[3S_z^3 - (S(S+1)+5)S_z]S_\pm^2 + S_\pm^2[3S_z^3 - (S(S+1)+5)S_z]\}$

C: $\hat{Y}_5^{\pm2} = \frac{1}{2}\{[3S_z^3 - (S(S+1)+6)S_z]S_\pm^2 + S_\pm^2[3S_z^3 - (S(S+1)+6)S_z]\}$
factor '5' should be replaced (twice) by '6'

O: $\hat{Y}_6^{\pm1} = \frac{1}{2}\{[35S_z^5 - (30S(S+1) - 15)S_z^3 + (5S^2(S+1)^2 - 10S(S+1) + 12)S_z]S_\pm + S_\pm[35S_z^5 - (30S(S+1) - 15)S_z^3 + (5S^2(S+1)^2 - 10S(S+1) + 12)S_z]\}$

C: $\hat{Y}_6^{\pm1} = \frac{1}{2}\{[33S_z^5 - (30S(S+1) - 15)S_z^3 + (5S^2(S+1)^2 - 10S(S+1) + 12)S_z]S_\pm + S_\pm[33S_z^5 - (30S(S+1) - 15)S_z^3 + (5S^2(S+1)^2 - 10S(S+1) + 12)S_z]\}$
factor '35' should be replaced (twice) by '33'.

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