The general harmonic-oscillator brackets: compact expression, symmetries, sums and Fortran code

G.P. Kamuntavičius\textsuperscript{a}, R.K. Kalinauskas\textsuperscript{b}, B.R. Barrett\textsuperscript{c}, S. Mickevičius\textsuperscript{a}, and D. Germanas\textsuperscript{a}

\textsuperscript{a}Vytautas Magnus University, Kaunas LT-3000 Lithuania
\textsuperscript{b}Institute of Physics, Vilnius LT-2600 Lithuania
\textsuperscript{c}Department of Physics, University of Arizona, Tucson, Arizona 85721

We present a very simple expression and a Fortran code for the fast and precise calculation of three-dimensional harmonic-oscillator transformation brackets. The complete system of symmetries for the brackets along with analytical expressions for sums, containing products of two and three brackets, is given.

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1 Introduction

A basis of harmonic-oscillator functions has proven to be extremely useful and efficient in describing compact quantum systems, such as nucleons in atomic nuclei and quarks in hadrons. The traditional applications, such as the nuclear shell-model, however, are based on a model Hamiltonian with individual one-particle variables. Hence, the corresponding model wave functions, which are dependent on one-particle coordinates, are not translationally invariant and cannot represent the wave function of such a system in proper way because the center of mass (c.m.) of a free nucleus (or a free hadron) must be described by an exponential function, corresponding to a freely-moving point mass. This need not to be a problem in the case when the expression for the realistic wave function in an harmonic-oscillator basis is known. In fact, having this expression, at least two possibilities exist to find a solution of the
problem of translational invariance of the wave function. The first approach is based on constructing the superpositions of shell-model states which possess a fixed state for the c.m. of the system, see [1]. Utilizing a basis of this kind, we do not need to worry about the c.m. state because all operators for observables are translationally invariant so that the final result is independent of this state. The second possibility is based on a direct construction of the many-fermion wave function, which is independent of the c.m. coordinate, see [2], [3], [4]. In this case, the harmonic-oscillator basis set, in terms of intrinsic (Jacobi) coordinates, is necessary. By a set of Jacobi coordinates for a system of \(N\) particles, we mean the \(N - 1\) independent vectors that each represents the displacement of the c.m. of two different subsystems. For \(N > 2\), there exists more than one set of Jacobi coordinates that can be assigned to an \(N\)-particle system. The different possible sets of Jacobi coordinates can be identified by use of a Jacobi tree (see, for example, [5]) and are related to each other by orthogonal transformations. In general, when the transformation from one set of Jacobi coordinates to another is performed, one obtains an expansion for the wave function containing an infinite number of terms. Only the set of harmonic-oscillator functions can be chosen in such a manner that the transformation from one set of Jacobi coordinates to another results in a corresponding expansion with a finite number of terms. In any of the above mentioned approaches, the essential feature is the Talmi-Moshinsky transformation [6], [7], [8] and corresponding harmonic-oscillator brackets (HOBs). Historically, the first application of this procedure was transformation of the product of two harmonic-oscillator functions from single-particle coordinates to relative motion and c.m. coordinates, a reduction that has proven to be very useful for the evaluation of two-body matrix elements. Because the HOBs are constantly employed in various model calculations of nuclear and hadrons structure, it is desirable to have a simple and efficient method for calculating them. Many papers have been devoted to the study of the Talmi-Moshinsky transformation and brackets, and various methods for the calculation of these brackets and several explicit expressions for them are described in the literature (see [9] and references therein, [10] and references therein). In this paper we present a complete system of symmetries for these brackets, a very simple expression for the HOBs based on the result of [10], new expressions for the sums of products of HOBs and a computer code, written in Fortran, which calculates the HOBs quickly and precisely.
First, let us consider the HOBs, defined in the following way:

\[ |e_1 l_1 (r_1), e_2 l_2 (r_2) : \Lambda \lambda \rangle = \sum_{E_l, e_l} \langle E_l, e_l : \Lambda \mid e_1 l_1, e_2 l_2 : \Lambda \rangle_d |E_l (R), e_l (r) : \Lambda \lambda \rangle, \]

(1)

or, in other words:

\[ \langle E_l, e_l : \Lambda \mid e_1 l_1, e_2 l_2 : \Lambda \rangle_d = \frac{1}{2\Lambda + 1} \sum_{\lambda} \int dR dr \langle E_l (R), e_l (r) : \Lambda \lambda \mid e_1 l_1 (r_1), e_2 l_2 (r_2) : \Lambda \lambda \rangle. \]

(2)

Here \( d \) is a nonnegative real number (see Eq. (7)). The two-particle wave functions with bound momenta are defined as:

\[ |e_1 l_1 (r_1), e_2 l_2 (r_2) : \Lambda \lambda \rangle \equiv \{ \phi_{e_1 l_1} (r_1) \otimes \phi_{e_2 l_2} (r_2) \}_\Lambda \lambda \]

(3)

\[ = \sum_{m_1 m_2} \langle l_1 m_1, l_2 m_2 : \Lambda \lambda \mid \phi_{e_1 l_1 m_1} (r_1) \phi_{e_2 l_2 m_2} (r_2) \rangle \]

\[ \phi_{e l m} (r) = (-1)^n \left[ \frac{2 (n!)}{\Gamma (n + l + 3/2)} \right]^{1/2} \exp \left( -r^2 / 2 \right) r^l L_n^{(l+1/2)} \left( r^2 \right) Y_{lm} (r/r), \]

(4)

where the corresponding dimensionless eigenvalue equals \((e + 3/2)\), \( n = (e - l) / 2 = 0, 1, 2, ..., \). We prefer the quantum number \( e = 2n + l \), rather than \( n \), due to conservation of the total oscillator energy on both sides of the bracket:

\[ e_1 + e_2 = E + e. \]

(5)

Obviously, this relation gives the requirement for the angular momenta:

\[ (-1)^{l_1 + l_2} = (-1)^{L + l}. \]

(6)

Let us next define the transformation of variables present in the expression for the brackets in the following way:

\[ \begin{pmatrix} R \\ r \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} \\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}} \end{pmatrix} \begin{pmatrix} r_1 \\ r_2 \end{pmatrix}; \quad \begin{pmatrix} r_1 \\ r_2 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} \\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}} \end{pmatrix}^{-1} \begin{pmatrix} R \\ r \end{pmatrix}. \]

(7)
We prefer the above order for the variables and the coupling of the angular momenta because this produces an orthogonal and, at the same time, symmetric transformation matrix, hence, giving higher symmetry to the brackets:

\[ \langle EL, el : \Lambda | e_{1l_1}, e_{2l_2} : \Lambda \rangle_d = \langle e_{1l_1}, e_{2l_2} : \Lambda | EL, el : \Lambda \rangle_d. \]  

(8)

Any orthogonal matrix of second order can be represented in form (7). If problems arise, the matrix can be easily rewritten in this form. The complete solution of this problem is as follows: In general, the matrix in (7) has the form

\[
\begin{pmatrix}
\sin \theta & \cos \theta \\
\cos \theta & -\sin \theta 
\end{pmatrix}
\]

and possesses the required distribution of signs, i.e.,

\[
(+ +) \quad \text{only in the case } 0 \leq \theta \leq \pi/2. \quad \text{When } \pi/2 \leq \theta \leq \pi, \text{ the signs change so that the matrix looks like } (+-), \text{ but by an elementary transformation of variables, namely } R \rightarrow -r \text{ and } r \rightarrow R, \text{ we can transform it to the previous form, i.e., only one minus sign in the lower right corner. If } \pi \leq \theta \leq 3\pi/2, \text{ distribution of signs is } (- -) \text{ and the necessary transformation of variables is } R \rightarrow -R \text{ and } r \rightarrow -r. \text{ The last case, when } 3\pi/2 \leq \theta \leq 2\pi, \text{ gives the matrix } (+ +); \text{ the correcting transformation is now } R \rightarrow r \text{ and } r \rightarrow -R. \text{ When the transformation is given by a nonsymmetric orthogonal matrix, the HOBs must, in general, be written in the form}
\]

\[
\langle EL, el : \Lambda | e_{1l_1}, e_{2l_2} : \Lambda \rangle_d = \delta_{e_{1l_1}, e'_{1l'_1}} \delta_{e_{2l_2}, e'_{2l'_2}}. \]  

(9)

which clearly demonstrates the correspondence between quantum numbers and variables. Some authors define these brackets without referencing this correspondence; in such a case, one must be careful, when employing some of their symmetries.

The HOBs, defined as above, are the real entries of an orthogonal matrix. Consequently, they obey usual orthogonality conditions:

\[
\sum_{EL,el} \langle e_{1l_1}, e_{2l_2} : \Lambda | EL, el : \Lambda \rangle_d \langle EL, el : \Lambda | e'_{1l'_1}, e'_{2l'_2} : \Lambda \rangle_d = \delta_{e_{1l_1}, e'_{1l'_1}} \delta_{e_{2l_2}, e'_{2l'_2}}. \]  

(10)
\[
\sum_{e_{1l_1},e_{2l_2}} \langle EL, el : \Lambda | e_{1l_1}, e_{2l_2} : \Lambda \rangle_d \langle e_{1l_1}, e_{2l_2} : \Lambda | E'L', e'l' : \Lambda \rangle_d = \delta_{EL,E'L'} \delta_{el,e'l'}.
\]

(11)

Here and below we apply the compact expressions for the Kronecker deltas, e.g., \( \delta_{EL,E'L'} \equiv \delta_E \delta_{L,L'} \). The symmetry properties of the coefficients are:

\[
\langle e_{1l_1}, e_{2l_2} : \Lambda | EL, el : \Lambda \rangle_d = \langle EL, el : \Lambda | e_{1l_1}, e_{2l_2} : \Lambda \rangle_d \quad (12)
\]

\[
(-1)^{L+l_2} \langle e_{2l_2}, e_{1l_1} : \Lambda | el, EL : \Lambda \rangle_d \quad (13)
\]

\[
(-1)^{\Lambda - L} \langle e_{2l_2}, e_{1l_1} : \Lambda | EL, el : \Lambda \rangle_{1/d} \quad (14)
\]

\[
(-1)^{\Lambda - l_1} \langle e_{1l_1}, e_{2l_2} : \Lambda | el, EL : \Lambda \rangle_{1/d} \quad (15)
\]

The symmetry defined in (12) follows from the definition of the coefficients and the requirement for the angular momenta (6); it is already given in (8). The next symmetry, (13), is not so trivial. It can be derived using the fact that the same transformation matrix connects not only the original, but also the transformed variables:

\[
\begin{pmatrix}
-r \\
R
\end{pmatrix}
= \begin{pmatrix}
\sqrt{\frac{1}{1+d}} & \sqrt{\frac{1}{1+d}} \\
\sqrt{\frac{d}{1+d}} & -\sqrt{\frac{d}{1+d}}
\end{pmatrix}
\begin{pmatrix}
r_2 \\
-r_1
\end{pmatrix}
\]

(16)

Using this condition for corresponding wave functions, one immediately obtains the symmetry relation (13). The symmetries (14) and (15) are even more complicated. The first one, (14), is based on observation that

\[
\begin{pmatrix}
R \\
-r
\end{pmatrix}
= \begin{pmatrix}
\sqrt{\frac{1}{1+d}} & \sqrt{\frac{d}{1+d}} \\
\sqrt{\frac{d}{1+d}} & -\sqrt{\frac{1}{1+d}}
\end{pmatrix}
\begin{pmatrix}
r_2 \\
r_1
\end{pmatrix}
\]

(17)

where the transformation matrix corresponds to the parameter value \(1/d\) instead of the original value \(d\). Let us illustrate the derivation of the symmetry in this case. The expression for the brackets can be represented in the form:

\[
\langle e_{1l_1}, e_{2l_2} : \Lambda | EL, el : \Lambda \rangle_d \\
= \frac{1}{2\Lambda + 1} \sum_\Lambda \langle e_{1l_1} (r_1) , e_{2l_2} (r_2) : \Lambda \lambda | EL (R) , el (r) : \Lambda \lambda \rangle \\
= \frac{1}{2\Lambda + 1} \sum_\Lambda \int d r_1 d r_2 \{ \phi_{e_{1l_1}} (r_1) \otimes \phi_{e_{2l_2}} (r_2) \}^{+} \{ \phi_{EL} (R) \otimes \phi_{el} (r) \}_{\Lambda \lambda}.
\]

(18)

Now it is enough to reorder the variables according to both sides of (17). To do this, the following simple, well-known expressions are necessary:

\[
\phi_{elm} (-r) = (-1)^l \phi_{elm} (r)
\]

(19)
and
\[ \{ \phi_{e_1 l_1}(r_1) \otimes \phi_{e_2 l_2}(r_2) \}_\Lambda = (-1)^{l_1+l_2-\Lambda} \{ \phi_{e_2 l_2}(r_2) \otimes \phi_{e_1 l_1}(r_1) \}_\Lambda. \] (20)

Applying these expressions, the right-hand side of (18) can be rewritten as
\[
\langle e_1 l_1, e_2 l_2 : \Lambda | EL, el : \Lambda \rangle_d
\]
\[ = (-1)^{l_1+l_2-\Lambda+l} \frac{1}{2\Lambda+1} \sum \int d r_1 d r_2 \{ \phi_{e_2 l_2}(r_2) \otimes \phi_{e_1 l_1}(r_1) \}_\Lambda \{ \phi_{EL}(R) \otimes \phi_{el}(-r) \}_\Lambda \]
\[ = (-1)^{L-L+\Lambda} \langle e_2 l_2, e_1 l_1 : \Lambda | EL, el : \Lambda \rangle_{1/d}. \] (21)

The last symmetry, (15), follows from the transformation
\[
\begin{pmatrix}
  r \\
  R
\end{pmatrix} = \begin{pmatrix}
  \sqrt{\frac{1}{1+d}} & \sqrt{\frac{d}{1+d}} \\
  \sqrt{\frac{d}{1+d}} & -\sqrt{\frac{1}{1+d}}
\end{pmatrix} \begin{pmatrix}
  r_1 \\
  -r_2
\end{pmatrix}. \] (22)

The self-consistence of the transformations and, hence, the symmetries can be checked by applying two transformations, say (14) and (15), for the same bracket. The result yields an identity, as expected:
\[
\langle e_1 l_1, e_2 l_2 : \Lambda | EL, el : \Lambda \rangle_d
\]
\[ = (-1)^{A-L} \langle e_2 l_2, e_1 l_1 : \Lambda | EL, el : \Lambda \rangle_{1/d}
\]
\[ = (-1)^{A-L} (-1)^{A-l_2} \langle e_2 l_2, e_1 l_1 : \Lambda | el, EL : \Lambda \rangle_d
\]
\[ = \langle e_1 l_1, e_2 l_2 : \Lambda | EL, el : \Lambda \rangle_d. \] (23)

Hence, our definition of brackets is based on an assumption that variables in brackets are arranged in a fixed way, and the corresponding transformation matrix is given as in (7):
\[
\langle R, r | r_1, r_2 \rangle_d = \begin{pmatrix}
  \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} \\
  \frac{1}{\sqrt{1+d}} & -\sqrt{\frac{d}{1+d}}
\end{pmatrix}. \] (24)

3 Compact expression

The HOBs have been considered previously by a number of authors; however, these results were quite complicated and led to expressions, whose structures are not transparent. In our opinion, the simplest known expression for the general oscillator bracket is the one derived by B.Buck and A.C.Merchant in
Ref. [10]:

\[
\langle EL, el : \Lambda | e_1 l_1, e_2 l_2 : \Lambda \rangle_d
\]

\[
= i^{-(l_1 + l_2 + L + \ell) / 2} \times 2^{-(l_1 + l_2 + L + \ell) / 4}
\]

\[
\times \sqrt{(n_1)! (n_2)! (N)! (n)! [2 (n_1 + l_1) + 1]!! [2 (n_2 + l_2) + 1]!! [2 (N + L) + 1]!! [2 (n + l) + 1]!!}
\]

\[
\times \sum_{abcdl_0l_0l_0l_0} (-1)^{l_a + l_b + l_c} \frac{[2l_a + 1] (2l_b + 1) (2l_c + 1) (2l_d + 1)}{a!b!c!d! [2(a + l_a) + 1]!! [2(b + l_b) + 1]!! [2(c + l_c) + 1]!! [2(d + l_d) + 1]!!}
\]

\[
\times \left\{ \begin{array}{c} l_a \ b \ l_1 \\
 l_c \ d \ l_2 \\
 L \ l \ \Lambda 
\end{array} \right\} \left( \begin{array}{c} l_a l_b l_1 \\
 l_c l_d l_2 \\
 L l \ \Lambda 
\end{array} \right) \langle l_a0l_00 L0 \rangle \langle l_b0l_00 l0 \rangle \langle l_a0l_00 l10 \rangle \langle l_c0l_00 l20 \rangle ,
\]

(25)

where \( N = (E - L) / 2 \), \( n = (e - l) / 2 \), \( n_1 = (e_1 - l_1) / 2 \), and \( n_2 = (e_2 - l_2) / 2 \). This expression for the HOBs is derived using harmonic-oscillator wave functions without the phase multiplier \((-1)^n\) present in our Eq. (4). The introduction of this modification results in a slightly different phase in the expression for HOBs. This phase equals \((-1)^{N+n+n_1+n_2} \equiv (-1)^{(L+l-l_1-l_2)/2} \).

Although the above summation runs over eight indices, the real summation is only over five of them due to three independent constraints. This constrained summation is similar to other, known, modern expressions for the HOBs. Formula (25) is very symmetric, and due to this symmetry, can be rewritten in the following way:

\[
\langle EL, el : \Lambda | e_1 l_1, e_2 l_2 : \Lambda \rangle_d
\]

\[
= d^{(e_1-e)/2} (1 + d)^{-(e_1+e_2)/2} \sum_{e_1 l_1 e_2 l_2} (-d)^{ed} \left\{ \begin{array}{c} l_a \ b \ l_1 \\
 l_c \ d \ l_2 \\
 L \ l \ \Lambda 
\end{array} \right\}
\]

\[
\times G (e_1 l_1; e_1 l_a, e_1 l_b) G (e_2 l_2; e_2 l_c, e_2 l_d) G (EL; e_1 l_a, e_1 l_c) G (el; e_1 l_b, e_1 l_d) ,
\]

(26)

where

\[
G (e_1 l_1; e_1 l_a, e_1 l_b) = \sqrt{[2l_a + 1] (2l_b + 1) \langle l_a0l_00 l_10 \rangle}
\]

\[
\times \left[ \begin{array}{c} e_1 - l_1 \\
 e_1 - l_a; e_b - l_b 
\end{array} \right] \left[ \begin{array}{c} e_1 + l_1 + 1 \\
 e_1 + l_a + 1; e_b + l_b + 1 
\end{array} \right]^{1/2}
\]

(27)
and the coefficients

\[
\begin{pmatrix}
  n_1 \\
  n_a; n_b
\end{pmatrix} = \frac{(n_1)!!}{(n_a)!! (n_b)!!}
\]  

are trinomials defined for the parameter values \( n_1 \geq n_a, n_b \). Moreover, the three parameters of these coefficients are all even or all odd at the same time.

It should be noted that the well-known binomial coefficients can be expanded in trinomials, e.g.,

\[
\binom{n}{k} = \binom{2n}{2k, 2(n-k)}.
\]  

In expression (26) we again have eight summation indices connected in four pairs, \( e_\alpha l_\alpha (\alpha = a, b, c, d) \), with the well-known relation between the oscillator energy and the angular momentum: \( e_\alpha \) is a nonnegative integer and \( l_\alpha = e_\alpha, e_\alpha - 2, ..., 1 \) or 0. The constraints amongst the energies are:

\[
e_a + e_c = E, \quad e_b + e_d = e, \\
e_a + e_b = e_1, \quad e_c + e_d = e_2.
\]  

Due to relation (5), \( (E + e = e_1 + e_2) \), only three of them are independent. The best choice for the independent summation indices is \( e_d \) and the four angular momenta \( l_\alpha (\alpha = a, b, c, d) \).

### 4 Sums of products

The sums of HOBs occur when antisymmetrizing the translationally invariant wave function, i.e., the function of Jacobi and intrinsic (spin, isospin, etc.) variables, because any permutation of one-particle coordinates results in orthogonal transformations of the Jacobian coordinates. These permutations result in different orthogonal transformations; therefore, according to (7), in transformations with different values of the parameters \( d \). The keys to the derivation of the expressions for the sums of products are Eq. (18) and the possibility to represent any orthogonal transformation in the form (24). To illustrate this procedure, let us take two expressions for the HOBs, as given by Eq. (1),

\[
\{ \phi_{EL} (R) \otimes \phi_{el} (r) \}_{\Lambda\Lambda} = \sum_{e_1 l_1, e_2 l_2} \langle EL, el : \Lambda | e_1 l_1, e_2 l_2 : \Lambda \rangle \{ \phi_{e_1 l_1} (r_1) \otimes \phi_{e_2 l_2} (r_2) \}_{\Lambda\Lambda},
\]  

(31)
with different variables and different orthogonal transformations, and multiply them, the left side to the left side and the right side to the right side. Next let us sum over the projection of the angular momentum and integrate over both coordinates to obtain:

$$\frac{1}{2\Lambda + 1} \sum_{\lambda} \int \int dR dr \{ \phi_{EL}(R) \otimes \phi_{el'}(r) \}^+_{\lambda\lambda} \{ \phi_{E'L'}(R') \otimes \phi_{el'''}(r') \}$$

$$= \sum_{e_1l_1, e_2l_2} \langle EL, el : \Lambda | e_1l_1, e_2l_2 : \Lambda \rangle_d \langle E'L', e'l' : \Lambda | e'_1l'_1, e'_2l'_2 : \Lambda \rangle_{d'}$$

$$\times \frac{1}{2\Lambda + 1} \sum_{\lambda} \int \int dr_1 dr_2 \{ \phi_{e_1l_1}(r_1) \otimes \phi_{e_2l_2}(r_2) \}^+_{\lambda\lambda} \{ \phi_{e'_1l'_1}(r'_1) \otimes \phi_{e'_2l'_2}(r'_2) \}_{\lambda\lambda}. \tag{32}$$

Obviously, the variables $R, r$ and $r_1, r_2$ are connected by the orthogonal transformation $\langle R, r | r_1, r_2 \rangle_d$, Eq. (24), and variables $R', r'$ and $r'_1, r'_2$ are connected by another orthogonal transformation $\langle R', r' | r'_1, r'_2 \rangle_{d'}$ of the same structure. In the case when $r_1, r_2$ and $r'_1, r'_2$ are also connected by some orthogonal transformation, say $\langle r_1, r_2 | r'_1, r'_2 \rangle_{d_0}$, both integrals on the left and the right sides of Eq. (32) are expressible as HOBs. Thus, Eq. (32) can be rewritten as

$$\langle EL, el : \Lambda | E'L', e'l' : \Lambda \rangle_D$$

$$= \sum_{e_1l_1, e_2l_2} \langle EL, el : \Lambda | e_1l_1, e_2l_2 : \Lambda \rangle_d \langle e_1l_1, e_2l_2 : \Lambda | e'_1l'_1, e'_2l'_2 : \Lambda \rangle_{d_0}$$

$$\times \langle e'_1l'_1, e'_2l'_2 : \Lambda | E'L', e'l' : \Lambda \rangle_{d'}. \tag{33}$$

The only remaining problem is the definition of the parameter $D$. Having in mind that all transformations of variables are orthogonal and well-defined, we can expand

$$\begin{pmatrix} R \\ r \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} \\ \sqrt{\frac{d}{1+d}} & -\sqrt{\frac{1}{1+d}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{d_0}{1+d_0}} & \sqrt{\frac{1}{1+d_0}} \\ \sqrt{\frac{d_0}{1+d_0}} & -\sqrt{\frac{1}{1+d_0}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{d'}{1+d'}} & \sqrt{\frac{1}{1+d'}} \\ \sqrt{\frac{d'}{1+d'}} & -\sqrt{\frac{1}{1+d'}} \end{pmatrix} \begin{pmatrix} R' \\ r' \end{pmatrix}. \tag{34}$$

Multiplying the above matrices, one obtains the form:

$$\begin{pmatrix} R \\ r \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{D}{1+D}} & \sqrt{\frac{1}{1+D}} \\ \sqrt{\frac{1}{1+D}} & -\sqrt{\frac{D}{1+D}} \end{pmatrix} \begin{pmatrix} R' \\ r' \end{pmatrix}, \tag{35}$$

where

$$\sqrt{D} = \frac{\sqrt{d} + \sqrt{d'}}{1 - \sqrt{dd'} + \sqrt{d_0} \left(1 - \sqrt{d_0d'}\right). \tag{36}$$
and restrictions for values of the parameter $d_0$ are as follows: If $dd' \leq 1$, then
$$\sqrt{d_0} \leq \left(\sqrt{d} + \sqrt{d'}\right) / (1 - \sqrt{dd'})$$; if $dd' \geq 1$, then $\sqrt{d_0} \geq \left(\sqrt{dd'} - 1\right) / (\sqrt{d} + \sqrt{d'})$.

The sum in Eq. (34) of the product of three HOBs with different values of the parameter $d$ can be simplified to sums of products of only two HOBs. To do this, the values of the brackets corresponding to the extreme values of the parameter $d$ are necessary, i.e., $d = 0$ or $d \to \infty$. The transformations of variables in these cases are trivial and HOBs can be calculated directly from definition (18), yielding:

$$\langle EL, el : \Lambda | e_1l_1, e_2l_2 : \Lambda \rangle_{d=0} = (-1)^{L+l-\Lambda} \delta_{e_1l_1, e_2l_2} \delta_{e_1l_1, el} \langle EL, el : \Lambda | e_1l_1, e_2l_2 : \Lambda \rangle_{d \to \infty} = (-1)^l \delta_{e_1l_1, EL} \delta_{e_2l_1, el}. \quad (37)$$

Using the HOB with the parameter $d_0 \to \infty$, one obtains the following expressions (the value $d_0 \to \infty$ is consistent only with $dd' \geq 1$):

$$\langle EL, el : \Lambda | E'L', e'l' : \Lambda \rangle \left(\frac{(\sqrt{dd'} - 1)}{(\sqrt{d} + \sqrt{d'})}\right)^2 = \sum_{e_1l_1, e_2l_2} (-1)^{l_2} \langle EL, el : \Lambda | e_1l_1, e_2l_2 : \Lambda \rangle_d \langle e_1l_1, e_2l_2 : \Lambda | E'L', e'l' : \Lambda \rangle_{d'}.$$ \quad (38)

Using the HOB with the parameter $d_0 = 0$ (consistent only with $dd' \leq 1$), one obtains the result:

$$\langle EL, el : \Lambda | E'L', e'l' : \Lambda \rangle \left(\frac{(\sqrt{d} + \sqrt{d'})}{(1 - \sqrt{dd'})}\right)^2 = (-1)^{L'+\Lambda} \sum_{e_1l_1, e_2l_2} (-1)^{l_2} \langle EL, el : \Lambda | e_1l_1, e_2l_2 : \Lambda \rangle_d \langle e_1l_1, e_2l_2 : \Lambda | e'l', E'L' : \Lambda \rangle_{d'}.$$ \quad (39)

These sums appear, when calculating the matrix element of the permutation operator of the particle coordinates in the translationally invariant basis of oscillator functions, see [4]. They are consistent: at $d' = 1/d$ in both cases one can easily obtain the normalization condition for HOBs.

5 Fortran code

Using the above results, we have also developed a Fortran code for the fast and precise calculation of the HOBs in large quantities. Such a computer code is needed because any nuclear calculation, including mentioned above antisymmetrization of a translationally invariant basis, requires large matrices. As one can see from the expression for HOBs, Eqs. (26) - (28), the main elements of these expressions are the Clebsch-Gordan coefficients with zero angular momenta projections, the $9 - j$ symbols and trinomial coefficients. Our code is based on the observation that all group-theoretical expressions...
can be represented as products or sums of products of binomial coefficients. Binomial coefficients are far more acceptable for large calculations than are factorials. For example, to represent $50!$ exactly requires a mantissa with 53 significant numbers. At the same time, the mantissa of the binomial $\binom{50}{25}$ requires only 15 significant numbers, hence it can be stored using real numbers of double precision. Having this in mind, for Clebsch-Gordan coefficients we use the expression:

$$
\langle l_1 0 l_2 0 | 0 \rangle = (-1)^{l_1 + l_2} \left( \frac{2l}{l_1 - l_2 + l} \right) \left( \frac{l_1 + l_2 + l + 1}{2l + 1} \right)^{-1/2} \left( \frac{l}{(l_1 - l_2 + l)/2} \right) \left( \frac{l_1 + l_2 + l}{l} \right). 
$$

For the $9-j$ symbols we first express them in terms of $6-j$ symbols, using the well-known formula:

$$
\begin{pmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \\ k_1 & k_2 & k_3 \end{pmatrix} = \sum_x (-1)^{2x}(2x + 1) \begin{pmatrix} j_1 & j_2 & j_3 \\ l_3 & k_3 & x \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ j_2 & x & k_2 \end{pmatrix} \begin{pmatrix} k_1 & k_2 & k_3 \\ x & j_1 & l_1 \end{pmatrix},
$$

and then utilize the $6-j$ expression in terms of binomials:

$$
\begin{pmatrix} a & b & e \\ d & c & f \end{pmatrix} = \frac{(-1)^{a+d+e+f}}{a+c-f+1} \left( \frac{(a+b+e+1)(c+d+e+1)}{(a+c+f+1)(b+d+f+1)} \right)^{1/2} \times \left( \frac{(a+c+f)}{2a} \frac{(c+d+e)}{2d} \frac{(a+e+b)}{2e} \frac{(2e)}{(a+e-b)} \right)^{1/2} \times \sum_z (-1)^z \frac{z}{(a+c+f)} \frac{(z+c-a)}{(d+f-b-z)} \frac{(b+c+e-f+1+z)}{(c+a+f+1)}.
$$

This formula for the $6-j$ symbol is well-balanced because every unit summed over has an equal number of binomials in the numerator and in the denominator. This results in the highest precision for the sum. Our code starts the calculations of the HOBs by filling the arrays of the binomial and trinomial coefficients. For the binomials we use recurrence formulas with corrections taking into account the fact that the binomial coefficients are integer numbers. For the three-dimensional array of trinomials we apply a completely analogous method. When both arrays are filled, the calculation of the HOBs is an
extremely fast and precise operation. In Table 1 we give values of

$$\delta (E_0) = \sum_{E_0} \left| \sum_{e_1 l_1, e_2 l_2} \langle EL, e l : \Lambda | e_1 l_1, e_2 l_2 : \Lambda \rangle_d \langle e_1 l_1, e_2 l_2 : \Lambda | E'L', e'l' : \Lambda \rangle_d - \delta_{EL,E'L'}\delta_{e,l,e'l'} \right|,$$

(43)

which characterize the precision of our calculations. Equation (43) represents the sum of the absolute values of the deviations of the calculated normalization conditions for the HOBs from the exact values given by Eq. (11). The first sum runs over all free parameters of the normalization condition, i.e., $E, L, e, l, E', L', e', l'$ and $\Lambda$, taking all allowed values between 0 and $E_0$. The total number of HOBs calculated for a given value of $E_0$ equals $N(E_0)$. The processor time (in seconds), necessary to perform these calculations on a personal computer, is listed under $T(E_0)$.

Table 1

<table>
<thead>
<tr>
<th>$E_0$</th>
<th>$N(E_0)$</th>
<th>$\delta(E_0)$</th>
<th>$T(E_0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>4,672</td>
<td>$0.2956 \times 10^{-14}$</td>
<td>0.28</td>
</tr>
<tr>
<td>4</td>
<td>32,054</td>
<td>$0.6832 \times 10^{-13}$</td>
<td>1.65</td>
</tr>
<tr>
<td>5</td>
<td>157,648</td>
<td>$0.5028 \times 10^{-12}$</td>
<td>11.9</td>
</tr>
<tr>
<td>6</td>
<td>658,000</td>
<td>$0.2394 \times 10^{-11}$</td>
<td>74.7</td>
</tr>
<tr>
<td>7</td>
<td>2,298,144</td>
<td>$0.7336 \times 10^{-10}$</td>
<td>385</td>
</tr>
<tr>
<td>8</td>
<td>7,165,706</td>
<td>$0.7032 \times 10^{-9}$</td>
<td>1,760</td>
</tr>
<tr>
<td>9</td>
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<td>6,830</td>
</tr>
<tr>
<td>10</td>
<td>51,349,192</td>
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</tr>
<tr>
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<td>122,193,968</td>
<td>$0.2131 \times 10^{-5}$</td>
<td>79,900</td>
</tr>
<tr>
<td>12</td>
<td>273,872,766</td>
<td>$0.3481 \times 10^{-4}$</td>
<td>248,000</td>
</tr>
</tbody>
</table>

As Table 1 clearly demonstrates, our method for calculating the HOBs is fast and universal and, hence, applicable to any calculations using a basis of many-particle harmonic-oscillator functions. Our Fortran code is available for general use and distribution, as described in the Conclusions.

6 Conclusions

Starting with the result of Ref.[10] for the General Harmonic-Oscillator Brackets (HOBs), we have simplified this earlier expression into a more compact and
highly symmetrical relationship, given in Eqs. (26)-(27). Our new result for the HOBs is well-suited for fast and precise numerical calculations of large quantities of HOBs. The numerical procedure is based upon independent calculations of the Clebsch-Gordan coefficients of zero angular momentum projections, the $6-j$ symbols and the $9-j$ symbols using binomial and ”trinomial” coefficients, which are precalculated and stored in appropriate arrays. The Fortran code, which we have written for computing the HOBs, is available for general use and can be obtained from the Vytautas Magnus University, Kaunas Lithuania, web server at http://www.nuclear.physics.vdu.lt/.

References


