Program to calculate coefficients of transformations between three–particle hyperspherical harmonics

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Abstract. A program to calculate the three–particle hyperspherical brackets is presented. Test results are listed and it is seen that the program is well applicable up to very high values of the hypermomentum and orbital momenta. The listed runs show that it is also very fast. Applications of the brackets to calculating interaction matrix elements and constructing hyperspherical bases for identical particles are described. Comparisons are done with the programs published previously.

Keywords: Three–body problem; hyperspherical brackets; Raynal–Revai coefficients

PROGRAM SUMMARY

Program Title: HHBRACKETS
Licensing provisions: GPLv3
Programming language: Fortran-90
Nature of problem:
When solving three–body problems, expansions of hyperspherical harmonics over harmonics similar in form but pertaining to different sets of Jacobi vectors are required. A universal and fast routine that provides the coefficients of such expansions, called hyperspherical brackets or Raynal–Revai coefficients, is needed to researchers in the field. The expansions are used both to calculate interaction matrix elements and construct states (anti)symmetric with respect to particle permutations.

Solution method:
At the hypermomentum that is minimum possible at given Jacobi orbital momenta, hyperspherical brackets are calculated using an explicit expression that includes only few summations. To calculate the brackets at larger hypermomenta, a recursion relation is employed. It perfectly works up to very high hypermomenta. Attention is paid to avoiding difficulties with large quantum numbers.

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I. INTRODUCTION

The first version of the program, named RRCOE, was written by the author in 1987 and first used (though not published) in Refs. 1 and 2 at studying halo nuclei. It was used afterwards by the author and his collaborators, e.g., 3, as well as by other researchers. In the present version, considerable modifications and improvements are done. In particular, the program is made applicable up to very large values of both the hypermomentum and orbital momenta. Hyperspherical harmonics (HH) required in realistic three–nucleon calculations involve such large values. The program is also made faster. Besides, the features of Fortran–77 which at present are considered to be obsolete, are eliminated.

Expansions over HH are an efficient tool to solve three–nucleon problems. At present these problems attract considerable attention in relation to nuclear interactions derived from Effective Field Theory. Three–cluster nuclear systems are also intensively studied via solving three–body problems in the HH approach.

II. HYPERSPHERICAL BRACKETS

The three–particle Jacobi vectors

\[ \xi_1 = \sqrt{\mu_{12}}(r_2 - r_1), \quad \xi_2 = \sqrt{\mu_{12,3}}[r_3 - (m_1 r_1 + m_2 r_2)/(m_1 + m_2)] \]  

are used below. Here \( r_i \) and \( m_i \) are the particle positions and their masses, \( \mu_{12} = m_1 m_2/[(m_1 + m_2)m] \), and \( \mu_{12,3} = (m_1 + m_2)m_3/[(m_1 + m_2 + m_3)m] \) where \( m \) is some reference mass.

In non–relativistic quantum mechanics, motion of the center of mass is separated and three–particle dynamics problems pertain to the space spanned by the \( |\xi_1 \xi_2 \rangle \) states.

The three–particle HH we employ are denoted as \( Y_{KLM}^{l_1 l_2} \). The quantum numbers labeling them are the orbital momenta \( l_1 \) and \( l_2 \) with respect to the \( \xi_1 \) and \( \xi_2 \) vectors, the total orbital momentum \( L \), its projection \( M \), and the hypermomentum \( K \). The orbital momenta allowed at a given \( K \) value are determined by the conditions that \( l_1 + l_2 \leq K \), parity of \( l_1 + l_2 \) is the same as that of \( K \), and \( |l_1 - l_2| \leq L \leq l_1 + l_2 \). The dimension of the space of HH having the same \( K, L, \) and \( M \) values is

\[ N(K, L, M) = (i_1 + 1)(i_2 + 1), \quad i_1 = L - \epsilon, \quad i_2 = (K - L - \epsilon)/2 \]  

where \( \epsilon = 0 \) or \( 1 \) when \( K - L \) is even or odd, respectively.
HH depend on 5 angles parametrizing the 6-dimensional hypersphere $\xi_1^2 + \xi_2^2 = \rho^2 = \text{const.}$ These angles are denoted as $\{\Omega\}$. One has $d\xi_1 d\xi_2 = \rho^2 d\rho d\Omega$. The angles $\{\Omega\}$ are determined by the Jacobi vectors and it is convenient here to represent the dependence on $\{\Omega\}$ as that on the Jacobi vectors themselves, $Y_{KLM}^{l_1 l_2} = Y_{KLM}^{l_1 l_2}(\xi_1, \xi_2)$. The HH $Y_{KLM}^{l_1 l_2}$ with different quantum numbers are orthogonal at integrating with $d\Omega$ over the hypersphere. The HH are taken normalized,

$$\int d\Omega Y_{KLM}^{l_1 l_2}(\xi_1, \xi_2) Y_{K'LM'}^{l_1' l_2'}(\xi_1, \xi_2) = \delta(KLMl_1l_2, K'L'M'l_1'l_2).$$

Consider the expansion of the HH $Y_{KLM}^{l_1 l_2}(\xi_1, \xi_2)$ over the HH of the same form but depending on $\xi_1'$ and $\xi_2'$ vectors related with $\xi_1$ and $\xi_2$ via a pseudo orthogonal transformation

$$\xi_1 = \xi_1' \cos \varphi + \xi_2' \sin \varphi, \quad \xi_2 = \xi_1' \sin \varphi - \xi_2' \cos \varphi. \quad (3)$$

The HH $Y_{KLM}^{l_1 l_2}(\xi_1, \xi_2)$ when considered as functions of $\xi_1'$ and $\xi_2'$ are HH having the same $K$, $L$, and $M$ values. Therefore, the expansion is of the form

$$Y_{KLM}^{l_1 l_2}(\xi_1, \xi_2) = \sum_{l_1' l_2'} \langle l_1' l_2' | l_1 l_2 \rangle_{KLM}^\varphi Y_{KLM}^{l_1' l_2'}(\xi_1', \xi_2'). \quad (4)$$

The number of terms in the sum is given by Eq. (2). We address the coefficients

$$\langle l_1' l_2' | l_1 l_2 \rangle_{KLM}^\varphi \quad (5)$$

of this expansion. They are called hyperspherical brackets or Raynal–Revai coefficients, and they are real.

The matrix (5) is symmetric,

$$\langle l_1' l_2' | l_1 l_2 \rangle_{KLM}^\varphi = \langle l_1 l_2 | l_1' l_2' \rangle_{KLM}^\varphi. \quad (6)$$

This follows from the fact that the matrix of the transformation (3) coincides with its inverse. Indeed, then the matrix of the expansion of $Y_{KLM}^{l_1 l_2}(\xi_1', \xi_2')$ over $Y_{KLM}^{l_1 l_2}(\xi_1, \xi_2)$ is also given by Eq. (5) when written in the same form. But, at the same time, the latter matrix should be the transposed one to that of Eq. (5) since the transformation (3) conserves the norms of HH.

The coefficients of the expansion of $Y_{KLM}^{l_1 l_2}(\xi_1, \xi_2)$ over $Y_{KLM}^{l_1 l_2}(\xi_1', \xi_2')$ in case of an orthogonal transformation

$$\xi_1 = \xi_1' \cos \varphi + \xi_2' \sin \varphi, \quad \xi_2 = -\xi_1' \sin \varphi + \xi_2' \cos \varphi \quad (7)$$
may obviously be written in terms of the above coefficients as

\((-1)^l (l'_1 l'_2 | l_1 l_2)_{KL}^\varphi.\)

III. APPLICATIONS OF HYPERSPHERICAL BRACKETS

Five angles parametrizing the 6–dimensional sphere may be chosen to be ones determining a unit vector \(\mathbf{n}_1\) in the direction of \(\xi_1\), a unit vector \(\mathbf{n}_2\) in the direction of \(\xi_2\), and an extra angle \(\theta\) such that \(\xi_1 = \rho \sin \theta\) and \(\xi_2 = \rho \cos \theta\). The HH \(Y_{KLM}^{l_1 l_2}(\xi_1, \xi_2)\) are of the structure

\[ [Y_{l_1}(\mathbf{n}_1) Y_{l_2}(\mathbf{n}_2)]_{LM} f_{Kl_1 l_2}(\theta) \]

where \(Y_{lm}(\mathbf{n})\) are spherical harmonics and the brackets \([\ldots]\) represent the coupling to a total momentum. The function \(f_{Kl_1 l_2}\) is as follows,

\[ f_{Kl_1 l_2}(\theta) = N_{Kl_1 l_2} \sin^{l_1} \theta \cos^{l_2} \theta P_{(K-l_1-l_2)/2}^{(l_1+1/2; l_2+1/2)}(\cos 2\theta) \]

where \(P_{n}^{(\alpha,\beta)}\) is the Jacobi polynomial and \(N_{Kl_1 l_2}\) is the normalization factor assumed to be positive. The integration element \(d\Omega\) is \(d\mathbf{n}_1 d\mathbf{n}_2 \sin^{2} \theta \cos^{2} \theta d\theta\).

The relative–motion kinetic energy operator of a three–particle system written in terms of the above Jacobi vectors is

\[ T = -\left(\hbar^2/2m\right)(\Delta\xi_1 + \Delta\xi_2). \]

The Hamiltonian \(H\) is \(T + V\) and we suppose that the interaction operator \(V\) is of the form \(V = V(12) + V(13) + V(23)\) where \(V(ij)\) are interactions between pairs of particles.

Suppose here that the particles are not all identical. In the approach we discuss, basis functions contain the HH \(Y_{KLM}^{l_1 l_2}(\xi_1, \xi_2)\) coupled with the spin functions to a total momentum. The expansion coefficients depend on \(\rho\). In turn, they may be expanded over a suitable basis. Kinetic energy matrix elements between the resulting basis functions are simple. In accordance with Eq. \(N\) such basis functions are also suitable to calculate the matrix elements of the \(V(12)\) interaction. And in order to calculate the matrix elements of the \(V(13)\) interaction, the HH \(Y_{KLM}^{l_1 l_2}(\xi'_1, \xi'_2)\) which are of the same form but depend on the other Jacobi vectors,

\[ \xi'_1 = \sqrt{\mu_{13}}(r_3 - r_1), \quad \xi'_2 = \sqrt{\mu_{13,2}}(r_2 - (m_1 r_1 + m_3 r_3)/M), \]

(9)
would be suitable. The definition (9) corresponds to the substitution \( r_2 \leftrightarrow r_3, m_2 \leftrightarrow m_3 \) in the definition (1). The vectors (1) are expressed in terms of the vectors (9) via a transformation of the form (3). The transformation matrix is the following,

\[
\cos \varphi = \left[ \frac{m_2 m_3}{(m_1 + m_2)(m_1 + m_3)} \right]^{1/2}, \quad \sin \varphi = \left[ \frac{m_1(m_1 + m_2 + m_3)}{(m_1 + m_2)(m_1 + m_3)} \right]^{1/2}.
\] (10)

The calculation is then performed with the help of the corresponding expansion of Eq. (4) form.

If any two of the three particles are not identical then the calculation of matrix elements of the \( V(23) \) interaction is required in addition. The Jacobi vectors \( \xi'_1 \) and \( \xi'_2 \) suitable for this purpose are obtained from the vectors (1) via the substitution \( r_1 \leftrightarrow r_3, m_1 \leftrightarrow m_3 \). The vectors (1) are expressed in terms of such vectors via a transformation of the form (3) with the following transformation matrix,

\[
\cos \varphi = \left[ \frac{m_1 m_3}{(m_1 + m_2)(m_2 + m_3)} \right]^{1/2}, \quad \sin \varphi = -\left[ \frac{m_2(m_1 + m_2 + m_3)}{(m_1 + m_2)(m_2 + m_3)} \right]^{1/2}.
\] (11)

The calculation is then performed in the same way.

Hyperspherical brackets can also be applied to construct an HH basis for identical particles. Let us speak of the three–nucleon case. Basis functions include spin and isospin variables. These functions should be antisymmetric with respect to particle permutations. They may be constructed from HH and spin–isospin functions both of which also transform in a simple way under permutations. In dynamics calculations, such basis functions provide maximum separation of space and spin–isospin degrees of freedom.

In the three–particle case, there exist three types of irreducible representations of the corresponding permutation group. The representations of the first type are realized by states denoted as \( \phi^s \) that are symmetric with respect to any permutations of particles. The representations of the second type are realized by states denoted as \( \phi^a \) that are antisymmetric, i.e. change their signs under particle transpositions. Those of the third type are realized by the so called states of mixed symmetry denoted as \( (\phi'^s, \phi'^a) \) that form a two–dimensional space invariant with respect to permutations. The states of mixed symmetry may be specified by the transformation formulae (see, e.g., [3], Chapt. 7)

\[
(12) \begin{pmatrix} \phi' \\ \phi'' \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \phi' \\ \phi'' \end{pmatrix}, \quad (13) \begin{pmatrix} \phi' \\ \phi'' \end{pmatrix} = \begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} \begin{pmatrix} \phi' \\ \phi'' \end{pmatrix}.
\] (12)
where \((i\hat{j})\) are transpositions of particles \(i\) and \(j\). The transformation matrices for other permutations may be obtained from here.

Correspondingly, basis HH having given symmetries and given \(K\), \(L\), and \(M\) values are denoted as \(Y_{KLM}^{s}\), \(Y_{KLM}^{r}\), and \(Y_{KLM}^{\alpha}\). Basis spin–isospin functions of given symmetries are denoted as \(\theta^{s}\), \(\theta^{r}\), and \(\theta^{\alpha}\). The resulting basis antisymmetric states belong to one of the following three types,

\[
Y_{KLM}^{s} \theta^{\alpha}, \quad 2^{-1/2}(Y_{KLM}^{r} \theta^{\alpha} - Y_{KLM}^{\alpha} \theta^{r}), \quad Y_{KLM}^{\alpha} \theta^{r}\quad (13)
\]

(The hyperradial variable \(\rho\) is invariant with respect to particle permutations so that in each case the \(\rho\) dependence leads merely to a factor.)

Basis HH entering Eq. (13) may be constructed via the application of the three–particle symmetrization (or Young) operators to the HH \(Y_{KLM}^{l_{1}l_{2}}(\xi_{1}, \xi_{2})\). These operators may be represented in the following form,

\[
P_{[s]} = 3^{-1} \left[ 1 + (\hat{1}3) + (\hat{2}3) \right] P_{+}, \quad P_{[s]} = 3^{-1} \left[ 1 - (\hat{1}3) - (\hat{2}3) \right] P_{-}, \quad (14)
\]

\[
P_{[n]_{(l)}} = 3^{-1} \left[ 2 - (\hat{1}3) - (\hat{2}3) \right] P_{+}, \quad P_{[m]_{(l)}} = 3^{-1/2} \left[ (\hat{2}3) - (\hat{1}3) \right] P_{+}, \quad (15)
\]

\[
P_{[m]_{(l)}} = 3^{-1/2} \left[ (\hat{2}3) - (\hat{1}3) \right] P_{-}, \quad P_{[m]_{(l)}} = 3^{-1} \left[ 2 + (\hat{1}3) + (\hat{2}3) \right] P_{-} \quad (16)
\]

where

\[
P_{\pm} = 2^{-1} \left[ 1 \pm (\hat{1}2) \right]. \quad (17)
\]

The transpositions \((i\hat{j})\) act as follows, \((i\hat{j})F(\xi_{1}, \xi_{2}) = F((i\hat{j})\xi_{1}, (i\hat{j})\xi_{2})\). When the operators \((14)\)–\((16)\) are applied to the HH \(Y_{KLM}^{l_{1}l_{2}}(\xi_{1}, \xi_{2})\) the result equals one or zero depending on the parity of the angular momentum \(l_{1}\). Either pair of the operators \(P_{[n]_{(l)}} \), \(P_{[m]_{(l)}} \) or \(P_{[m]_{(l)}} \), \(P_{[m]_{(l)}} \) may be used to construct mixed symmetry states \(\phi^{\alpha}, \phi^{\prime}\).

Let us denote the operators \((14)\)–\((16)\) as \(P_{[f]_{\mu(\nu)}}\). When these operators are applied to a complete set of HH like \(Y_{KLM}^{l_{1}l_{2}}(\xi_{1}, \xi_{2})\) the sets of HH of given permutational symmetries arise which are over-complete. It is possible to get bases in the spaces of the latter sets via orthogonalization of the HH thus obtained. Besides, matrix elements of kinetic energy between orthonormalized HH are simple. Therefore, one aims to construct orthonormalized complete sets in the spaces of the \(P_{[f]_{\mu(\nu)}} \cdot Y_{KLM}^{l_{1}l_{2}}(\xi_{1}, \xi_{2})\) states.

Basis states forming these sets are to be obtained in the form of expansions over the initial HH \(Y_{KLM}^{l_{1}l_{2}}(\xi_{1}, \xi_{2})\). This is needed to calculate the interaction matrix elements and
related to the fact that the matrix elements of an interaction $V(12)+V(13)+V(23)$ between the states of Eq. (13) type are the same as matrix elements of $3 \cdot V(12)$. A three–particle interaction may also consist of three terms that differ in numbering of particles and are such that for calculating matrix elements of one of them, which is sufficient, the mentioned expansion is suitable.

Thus, first one has to obtain expansions of the form

$$ P^{l_1 l_2}_{-\mu(-\nu)} Y_{KLM}^{l_1 l_2} (\xi_1, \xi_2) = \sum_{l_1', l_2'} c_{KL}(l_1', l_2') Y_{KLM}^{l_1' l_2'} (\xi_1, \xi_2). $$

According to Eqs. (14)–(16) the expansion coefficients $c_{KL}(l_1', l_2')$ are sums of the delta–symbol contribution and the contributions

$$ \int d\Omega Y_{KLM}^{l_1 l_2*} (\xi_1, \xi_2) Y_{KLM}^{l_1 l_2} ((\hat{1}3)\xi_1, (\hat{1}3)\xi_2) $$

where $(\hat{1}3)$ are transpositions $(\hat{1}3)$ and $(\hat{2}3)$. The $(\hat{2}3)$ contribution is readily expressed in terms of the $(\hat{1}3)$ contribution.

Calculating the latter, one may write

$$ (\hat{1}3)\xi_1 = \xi_1 \cos \varphi + \xi_2 \sin \varphi, \quad (\hat{1}3)\xi_2 = \xi_1 \sin \varphi - \xi_2 \cos \varphi. $$

Therefore, in accordance with the definition of Eq. (4) the matrix element (19) is equal to the hyperspherical bracket $\langle l_1' l_2' | l_1 l_2 \rangle_{KL}$.

The transformation (20) is reverse to the transformation of Eqs. (3) and (11) with $m_1 = m_2 = m_3$. The matrices of the transformation (3) and its reverse are the same. Hence the matrix of the transformation (20) is the matrix in Eq. (12).

In conclusion of this section let us comment on the orthogonalization procedure. It should be sufficiently stable if, as usual, the number (2) of HH with given $K$, $L$, and $M$ is not very high. Anyway, it may be performed with the quadrupole precision. In the $(Y''_{KLM}, Y'_{KLM})$ case it is not required to orthogonalize independently $Y''_{KLM}$ and $Y'_{KLM}$ states. Selecting linear independent states one needs to check whether their net number obtained coincides with that given by Eq. (2). It is simpler to deal with the multiplicities of the spaces of given permutational symmetries themselves when they known in advance. In the general case these multiplicities can be obtained as the traces of projection operators [4]. And in the three–particle case we have obtained them analytically. We shall list the formulae without derivation.
To this aim, define three subsidiary functions \( n_s(i), n_m(i), \) and \( n_a(i), \)

\[
\begin{align*}
n_s(i) &= \left(\frac{i + 6}{6}\right), & n_m(i) &= \frac{i}{3}, & n_a(i) &= \left(\frac{i + 3}{6}\right) \quad \text{at } i \mod 3 = 0, \\
n_s(i) &= \left(\frac{i + 2}{6}\right), & n_m(i) &= \frac{i + 2}{3}, & n_a(i) &= \left(\frac{i - 1}{6}\right) \quad \text{at } i \mod 3 = 1, \\
n_s(i) &= \left(\frac{i + 4}{6}\right), & n_m(i) &= \frac{i + 1}{3}, & n_a(i) &= \left(\frac{i + 1}{6}\right) \quad \text{at } i \mod 3 = 2.
\end{align*}
\]

(21)

Here \([\ldots]\) is the integer part of a number. (In all the cases \( n_s + 2n_m + n_a = i + 1. \))

Let \( N_m(K, L, M), N_s(K, L, M), \) and \( N_a(K, L, M) \) be, respectively, the number of independent subspaces \( Y''_{KLM}, Y'_{KLM} \) of mixed symmetry HH contained in the space of HH with given \( K, L, M \), the number of linearly independent HH with given \( K, L, M \) that are symmetric with respect to particle permutations, and the number of such HH that are antisymmetric with respect to them. One has \( N_s + 2N_m + N_a = N \) where \( N(K, L, M) \) is given by Eq. (2). The quantities \( N_s, N_m, \) and \( N_a \) sought for are the following,

\[
\begin{align*}
N_s(K, L, M) &= n_s(i_1)n_s(i_2) + n_m(i_1)n_m(i_2) + n_a(i_1)n_a(i_2), \\
N_m(K, L, M) &= n_s(i_1)n_m(i_2) + n_m(i_1)n_s(i_2) + n_a(i_1)n_m(i_2) + n_m(i_1)n_a(i_2), \\
N_a(K, L, M) &= n_s(i_1)n_a(i_2) + n_m(i_1)n_m(i_2) + n_a(i_1)n_s(i_2) \quad \text{(22)}
\end{align*}
\]

where \( i_1 \) and \( i_2 \) are defined according to Eq. (2).

The schemes of three–body HH expansions may somewhat differ from those outlined above but the applications of the HH brackets are anyway the same.

IV. RELATIONS TO CALCULATE THE BRACKETS

These relations, Eqs. (25) and (27) below, which were obtained in Ref. [5] are the following. It is convenient to deal with the modified brackets

\[
[l'_1l'_2|l_1l_2]_{KL}^e = \langle l'_1l'_2|l_1l_2\rangle_{KL}^e A_{Kl_1l_2}/A_{Kl'_1l'_2} \quad \text{(23)}
\]

where

\[
A_{Kl_1l_2} = \left[\left(\frac{K - l_1 - l_2}{2}\right)! \left(\frac{K + l_1 + l_2}{2} + 1\right)! (K - l_1 + l_2 + 1)! (K + l_1 - l_2 + 1)!!\right]^{1/2}.
\]

(24)
First, the brackets with \( K = l_1 + l_2 \) are calculated using the formula\(^1\)

\[
\frac{l_1 l_2}{n_!} \left. \prod_{l_1 + l_2 + L + 1}^{l_1 + l_2 - L} \sin \varphi \cos \varphi \right|_{l_1 + l_2 - l_2 - m} \sum_{m=m_{\text{min}}}^{m_{\text{max}}} (-1)^n \left( \frac{\prod_{i=1}^4 (\nu_i)!}{(2\nu_i)!} \right) \left( \frac{l_1 - n_+ l_2 - n_+ L}{l_1 - m - n_+ l_2' + l_1'} \right) \tan \nu \varphi
\]

where the notation like \([l] = \sqrt{2l + 1}\) is used, \(n_+ = (l_1 + l_2 - l_2')/2\), \(n_+ = (l_1 + l_2 + l_1' + l_2')/2\), the expression in the round brackets is the \(3j\)-symbol, and

\[
\nu_1 = (l_1 - n_+ + l_1' - m)/2, \quad \nu_2 = (l_1 - n_+ - l_1' + m)/2, \\
\nu_3 = (l_2 - n_+ - l_2' + m)/2, \quad \nu_4 = (l_2 - n_+ + l_2' - m)/2.
\]

The summation goes between the limits

\[
m_{\text{min}} = \left| (l_1 - l_1') - (l_2 - l_2') \right|/2, \quad m_{\text{max}} = \min\{l_1 + l_1' - n_+, l_2 + l_2' - n_+\}
\]

within which the \(3j\) symbol is different from zero. The summation variable takes only the values of the same parity as these limits. This is related to the requirement that the quantities \([25]\) should be integer.

Proceeding from the brackets of Eq. \(25\) the general type brackets are calculated with the help of the \(K \rightarrow K + 2\) recursion relation

\[
[l_1 l_2 l_3 l_4]_{K+2,L} = \cos 2\varphi [l_1 l_2 l_3 l_4]_{K,L} + \sin \varphi \cos \varphi
\]

\[
\times \{l_1' - 1l_2' - 1l_1 l_2\} \left. \alpha_L(l_1', l_2') - [l_1' + 1l_2' + 1l_1 l_2] \right. + \left. \beta_L(l_1', l_2') - [l_1' - 1l_2' + 1l_1 l_2] \right. \}
\]

where

\[
\alpha_L(p, q) = \left[ \frac{(p + q - L - 1)(p + q - L)(p + q + L)(p + q + L + 1)}{(4p^2 - 1)(4q^2 - 1)} \right]^{1/2}, \\
\beta_L(p, q) = \left[ \frac{(q - p + L - 1)(q - p + L)(q - p + L + 1)(q - p + L + 2)}{(2p + 1)(2p + 3)(4q^2 - 1)} \right]^{1/2}.
\]

Let us also mention that the oscillator (or Moshinsky) brackets can be calculated in a similar way \([6]\).

\(^1\) Denote the product \([l_1][l_2][l_1'][l_2']\) in Eq. \(25\) times the numerator of the ratio of factorials and double factorials from the second line in this equation as \(A\) and the denominator of the mentioned ratio as \(B\). In the formula in Ref. \([3]\) the quantity \(A/B\) was listed as \(A^{1/2}/B\) which is an obvious misprint.
V. THE PROGRAM

The double precision is set in the program. Factorials and double factorials entering the above listed formulae are to be calculated as real numbers. The factors entering the product $[...]$ in the third line in Eq. (25) are extracted from the array $\sqrt{(2\nu)!/\nu!}$ calculated in advance.

At calculating the second line factor in Eq. (25) the values of the products of factorials and double factorials entering it and even those quantities themselves may become larger than the maximum real number allowed in a double precision calculation. To avoid this, the mentioned factor is calculated as $\exp(\ln A)$, $A$ being this factor up to a sign. When a calculation is performed in this way, the large numbers cancel each other to a sufficient degree and the outcome is never too large or too small. The quantity $\ln A$ includes the logarithms of factorials and double factorials. The arrays of these logarithms are calculated in advance. The ratio of the quantities $[24]$ is calculated similarly.

The point as to such large numbers arises also at calculating the $3j$ symbols entering Eq. (25). We wrote a routine to calculate $3j$ symbols utilizing the expression for them of the structure $F^{1/2} \sum_n (-1)^n u_n^{-1}$ where $F$ is the ratio of products of factorials and $u_n$ are also products of them, see, e.g., [7]. The calculation is performed in the form $\sum_n (-1)^n \exp[(1/2) \ln F - \ln u_n]$ which also in this case leads to cancellation to a sufficient degree of large numbers entering $F$ and $u_n$.

We tried also to proceed in another way constructing $F^{1/2} u_n^{-1}$ from the quantities like $(i!)^{1/j}$ where $j$ is a sufficiently large integer. This makes possible to avoid the calculation of many exponentials. However, this made the net program faster by less than only 30%. Therefore, in order not to complicate the program we decided not to release this version. We got rid of the difficulty also via calculating the $3j$ symbols in their primary form with the quadrupole precision. However, in the case of brackets with large quantum numbers this increased the net computation time by 5 - 10 times and we abandoned also this version.

The brackets are calculated with the help of the subroutine named

\texttt{HHBRACKETS(K,L,L1,L2,CO,SI,DLFAC,DL2FAC,RFAC,N0,BRAC)}

that is called from a main program. \texttt{HHBRACKETS} returns the array \texttt{BRAC} of the brackets of Eq. (5) with all $l_1'$ and $l_2'$ values allowed at given $K$, $L$, $l_1$, and $l_2$. All the parameters of the
subroutine but BRAC are input ones. CO and SI are $\cos \varphi$ and $\sin \varphi$. DLFAC, DL2FAC, and RFAC are arrays ranging from zero to $N_0$ where $N_0$ is an arbitrary integer larger than $2K$. The first two arrays contain, respectively, the above mentioned quantities $\ln(m!)$ and $\ln[(2m+1)!!]$, and the last one is the array of the above mentioned quantities $\sqrt{(2\nu)!/\nu!}$. To get these three arrays, a main program may call for the appended small subroutine FACT(DLFAC,DL2FAC,RFAC,N0).

The subroutine HHBRACKETS we discuss calls for the function WIGN(JJ1,JJ2,JJ3,MM1,MM2,DLFAC,N0) that calculates the $3j$ symbols entering Eq. (25). It calls also for the small routines AL and BE providing the quantities (28). Thus the set of our routines consists of HHBRACKETS, WIGN, AL, BE, and FACT.

The output array of brackets reads as BRAC(M,N) where $M$ and $N$ variables are related to the $l_1'$ and $l_2'$ orbital momenta entering the brackets (5) as follows,

$$l_1' = \frac{K - (L - \epsilon)}{2} + N - M, \quad l_2' = \frac{K + L - \epsilon}{2} - M - N + 2 \quad (29)$$

where $\epsilon$ is as in Eq. (2). The ranges of $M$ and $N$ are the following,

$$1 \leq M \leq i_2 + 1, \quad 1 \leq N \leq i_1 + 1 \quad (30)$$

where $i_1(K, L)$, and $i_2(K, L)$ are as in Eq. (2). It can be seen that the expressions (29) set up a one-to-one correspondence between the $M$, $N$ values of Eq. (30) and all the allowed $l_1'$, $l_2'$ values. The allowed $M$ and $N$ values are independent of each other in the difference to the allowed $l_1'$ and $l_2'$ values. When performing the summations at the calculations of matrix elements one may consider the brackets as depending on $M$ and $N$ and employ the relations (29). One may also use the expressions $M(l_1', l_2')$ and $N(l_1', l_2')$ reverse to those of Eqs. (29) to extract brackets from the BRAC(M,N) array.

VI. TESTS

Tests were conducted at $\cos \varphi = 1/2$, $\sin \varphi = -\sqrt{3}/2$, see Eq. (20). The orthogonality relations

$$\sum_{all l_1',l_2'} (l_1' l_2'|l_1l_2)_K^\varphi (l_1' l_2'|l_3l_4)_K^\varphi = \delta_{l_1l_3}\delta_{l_2l_4} \quad (31)$$
were tested for various $K$ and $L$ values of both parities at $K$ up to 201 and $L$ up to 31. This presumably covers all the possible applications. The relations with $l_3 = l_1$ and $l_2 = l_4$ were tested for all allowed $l_1$ and $l_2$ values. In each $K \simeq 200$, $L \simeq 30$ case, for example, the number of these relations is about 2700 and they involve about $7 \cdot 10^6$ brackets thus controlled. In both $K = 200$, $L = 30$ and $K = 200$, $L = 0$ cases the largest among such relations deviation from unity was $3 \cdot 10^{-9}$. At $K = 30$, $L = 5$, for example, the largest such deviation was $9 \cdot 10^{-14}$. The accuracy is mostly determined by the accuracy at calculating the $3j$ symbols.

At $K = 200$ and $L = 4$ the zero values of the sum of Eq. (31) were reproduced as $10^{-14} - 10^{-15}$ for some sets of randomly chosen allowed $l_1$, $l_2$, $l_3$, and $l_4$ values such that $l_3 \neq l_1$ or $l_4 \neq l_2$. The symmetry of the calculated brackets was also verified at the same conditions. The two brackets coincided in 13 digits.

One more test was the following. In the $L = 0$ case a complete set of HH that transform in a simple way under the coordinate transformation [9] or [17] was found in a closed form [8]. In Ref. [9] it was (unexpectedly) found that the transformation coefficients between that set and the $Y_{K,L=0}^{ll'}$ set have the form of the usual Clebsch–Gordan coefficients of the $SO(3)$ group. In Ref. [5] this was employed to calculate the $L = 0$ brackets also in another way using the HH of Ref. [8] as intermediate ones. The corresponding expression includes a summation. At zero Jacobi orbital momenta, performing it directly one comes to the relation

$$\langle 00|00 \rangle_{K,L=0}^\varphi = \frac{2}{K + 2} \frac{\sin(K + 2)\varphi}{\sin 2\varphi}$$

obtained in an implicit form in Ref. [10]. The brackets entering this relation were tested at $K \simeq 200$ and they coincided with its right-hand side in 14 digits.

Some results of the tests are presented in the appended file named "output". Tests at any quantum numbers can be readily performed with the appended program TESTHHBRACKETS.

VII. RUNNING TIMES

The calculations below have been performed with a notebook Intel core i5, 2.67 GHz (2010). Brackets [13] with all $l_1$, $l_2$, $l'_1$, and $l'_2$ values allowed at given $K$ and $L$ were computed. The numbers of these brackets are the squares of the
numbers of states given by Eq. (2). In the Table the times are listed to compute all these brackets (fourth column) along with the average times per computing one of them (last column). The latter ones are the former ones divided by the number of states listed in the the third column (In all the cases except for the first one the same calculation was done repeatedly in a loop to have a detectable net CPU time value.) In Refs. [11] and [12]

**TABLE I: Computing times in seconds**

| $K$ | $L$ | net number of brackets | net running time | average time per one bracket |
|-----|-----|------------------------|------------------|------------------------------|
| 200 | 30  | 7107556                | 48.7             | $6.9 \cdot 10^{-6}$        |
| 200 | 0   | 10201                  | $2.62 \cdot 10^{-2}$ | $2.6 \cdot 10^{-6}$          |
| 20  | 10  | 4356                   | $1.71 \cdot 10^{-3}$ | $3.9 \cdot 10^{-7}$          |
| 20  | 0   | 121                    | $4.14 \cdot 10^{-5}$ | $3.4 \cdot 10^{-7}$          |
| 6   | 2   | 81                     | $1.47 \cdot 10^{-5}$ | $1.8 \cdot 10^{-7}$          |
| 6   | 1   | 9                      | $2.26 \cdot 10^{-6}$ | $2.5 \cdot 10^{-7}$          |
| 6   | 0   | 16                     | $3.27 \cdot 10^{-6}$ | $2.0 \cdot 10^{-7}$          |

programs to calculate the HH brackets based on different algorithms were created. The program of Ref. [12] was tested there in the $K = 6$ case. 60 brackets pertaining to $L = 0$, 1, and 2 were calculated. The average computation time per one bracket equaled 2.4 s. In Ref. [11] where the brackets with $K = 6, L = 2$ were calculated the computation time was about the same. Our computation times for these cases are presented in the last three lines in the Table. Basing on the flops, the increase in the speed of computation of the present notebook with respect to the VAX machine employed in Ref. [12] is about $3 \cdot 10^4$. Very probably that it is about the same also with respect to the computer of Ref. [11]. With this factor taken into account, one concludes that at $K = 6$ the present program is more than 400 times faster as compared with the program of Ref. [12] and, very probably, with that of Ref. [11]. It is also not known whether the codes [11, 12] can produce sufficiently accurate results at higher $K$ values.
VIII. ACKNOWLEDGMENT

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