Computing the coefficients of transformations between oscillator states

Victor D. Efros\textsuperscript{a,b}

\textsuperscript{a}National Research Centre "Kurchatov Institute", 123182 Moscow, Russia
\textsuperscript{b}National Research Nuclear University MEPhI, 115409 Moscow, Russia

Abstract. A program is created to compute recursively the Moshinsky brackets. It is very fast and provides highly accurate results. In the case of the double precision computations with a single-processor consumer notebook, the computing time per bracket at any not small oscillator excitations is on the scale of $10^{-8}$ s and the accuracy is very good for the total number of quanta up to 80. The program is easy to handle.

I. INTRODUCTION

The Talmi-Smirnov transformation of oscillator states is widely applied in calculations in various branches of physics. The transformation is especially useful in the microscopic studies of structure of matter on various levels. An important nuclear physics application is the calculation of matrix elements of nucleon-nucleon interaction in the oscillator shell-model basis, see, e.g., [1].

The coefficients of the Talmi-Smirnov transformation are called oscillator brackets. At present, large sets of oscillator states are frequently retained in calculations. Therefore, a fast program to compute oscillator brackets is needed. The program should provide accurate results up to high oscillator excitations. In the present work, such a program is presented.

II. PRELIMINARIES AND DEFINITIONS

Let us write the Hamiltonian of the three-dimensional isotropic oscillator as $\hbar \omega (q^2 + x^2)/2$ where $q$ and $x$ are canonically conjugated variables, $[q_j, x_k] = -i \delta_{jk}$. Denote the normalized oscillator eigenstates as $|nlm\rangle$ where $l$ and $m$ are the angular momentum and its projection, and $n$ is defined via the eigenenergy $\hbar \omega (2n + l + 3/2)$. The phase factors of the $|nlm\rangle$ states
are chosen such that the \(x\)-representation wave functions are

\[
\langle x|n_l n_m \rangle = \left[ \frac{2n!}{\Gamma(n + l + 3/2)} \right]^{1/2} x^n L_n^{l+1/2}(x^2) e^{-x^2/2} Y_{lm}(\mathbf{n}_x) \tag{1}
\]

where the Laguerre polynomials \(L_n^l\) are defined in the standard way \[2\], and the usual spherical harmonics \(Y_{lm}\) are employed which form the standard basis with respect to rotations.

Let \(|n_1 l_1 n_2 l_2 LM_L\rangle\) be the states that are obtained via coupling the above oscillator states, belonging to different spaces, to a given total angular momentum \(L\) and its projection \(M_L\),

\[
|n_1 l_1 n_2 l_2 LM_L\rangle = \sum_{m_1 + m_2 = M_L} C_{l_1 m_1 l_2 m_2}^{LM_L} |n_1 l_1 m_1\rangle |n_2 l_2 m_2\rangle. \tag{2}
\]

They are eigenstates of the Hamiltonian

\[
H = \hbar \omega (q_1^2 + q_2^2 + x_1^2 + x_2^2)/2 \tag{3}
\]

with the eigenvalues \(\hbar \omega (N_q + 3)\) where \(N_q\) denotes the total number of oscillator quanta,

\[
N_q = l_1 + l_2 + 2(n_1 + n_2). \tag{4}
\]

This notation is used below.

Let us perform a pseudo-orthogonal transformation

\[
x_1 = x'_1 \cos \varphi + x'_2 \sin \varphi, \quad x_2 = x'_1 \sin \varphi - x'_2 \cos \varphi. \tag{5}
\]

Denote the quantities canonically conjugated to \(x'_1\) and \(x'_2\) as, respectively, \(q'_1\) and \(q'_2\). The relations expressing \(q_1\) and \(q_2\) in terms of \(q'_1\) and \(q'_2\) are of the same form as Eqs. \[5\]. The Hamiltonian \[3\] preserves its form,

\[
H = \hbar \omega [(q'_1)^2 + (q'_2)^2 + (x'_1)^2 + (x'_2)^2]/2. \tag{6}
\]

Let \(|n'_1 l'_1 m'_1\rangle\) and \(|n'_2 l'_2 m'_2\rangle\) be, respectively, the eigenstates of the Hamiltonians \(\hbar \omega [(q'_1)^2 + (x'_1)^2]/2\) and \(\hbar \omega [(q'_2)^2 + (x'_2)^2]/2\). Let \(|n'_1 l'_1 n'_2 l'_2 LM_L\rangle\) be the eigenstates of the Hamiltonian \(H\) which are constructed from the \(|n'_1 l'_1 m'_1\rangle\) and \(|n'_2 l'_2 m'_2\rangle\) states in the same way as in Eq. \[2\]. The eigenstate \(|n_1 l_1 n_2 l_2 LM_L\rangle\) of Eq. \[2\] may be expanded over the \(|n'_1 l'_1 n'_2 l'_2 LM_L\rangle\) eigenstates. Only those expansion states that have the same energy as the original two-body harmonic oscillator state enter the expansion. Thus we have

\[
|n_1 l_1 n_2 l_2 LM_L\rangle = \sum_{n'_1 l'_1 n'_2 l'_2} \langle n'_1 l'_1 n'_2 l'_2|n_1 l_1 n_2 l_2\rangle_{LM_L}^\dagger |n'_1 l'_1 n'_2 l'_2 LM_L\rangle \tag{7}
\]
where the summation proceeds at the condition

$$l_1' + l_2' + 2(n_1' + n_2') = l_1 + l_2 + 2(n_1 + n_2) = N_q.$$  \hspace{1cm} (8)

The expansion coefficients

$$\langle n_1' l_1' n_2' l_2' | n_1 l_1 n_2 l_2 \rangle_{L}^r$$  \hspace{1cm} (9)

are called oscillator brackets or Talmi-Moshinsky-Smirnov coefficients (or brackets). Their computation is addressed here. The present work is based on the results of Ref. [3] but the notation of that paper is modified here for convenience of writing the computer program. The quantities $n_1'$ and $n_2'$ were denoted in Ref. [3] as $N$ and $n$, the quantities $l_1'$ and $l_2'$ as $L$ and $l$, and the quantities $L$ and $M$ as $\lambda$ and $\mu$.

The transformation (11) is used, in particular, to calculate matrix elements of two-body operators between the products of single-particle oscillator states. If $\mathbf{r}_{1,2}$ are particle positions and $\mathbf{p}_{1,2}$ are their momenta then the above $\mathbf{x}_{1,2}$, $\mathbf{q}_{1,2}$, $\mathbf{x}_1$, $\mathbf{q}_1$, $\mathbf{x}_2$, and $\mathbf{q}_2$ quantities are

$$\mathbf{x}_{1,2} = \mathbf{r}_{1,2} [\hbar/(m_{1,2}\omega)]^{-1/2}, \quad \mathbf{q}_{1,2} = \mathbf{p}_{1,2} (\hbar m_{1,2}\omega)^{-1/2}$$  \hspace{1cm} (10)

where $m_1$ and $m_2$ are masses of the particles.

The above $\mathbf{x}_1'$, $\mathbf{q}_1'$, $\mathbf{x}_2'$, and $\mathbf{q}_2'$ quantities may be taken as follows,

$$\mathbf{x}_1' = (\mathbf{r}_2 - \mathbf{r}_1) [\hbar/(\mu\omega)]^{-1/2}, \quad \mathbf{q}_1' = -\mathbf{p}_{rel}(\hbar\mu\omega)^{-1/2};$$  \hspace{1cm} \begin{align*} 
\mathbf{x}_2' &= \mathbf{R} [\hbar/(M_0\omega)]^{-1/2}, \quad \mathbf{q}_2' = \mathbf{P}(\hbar M_0\omega)^{-1/2}. \tag{11} 
\end{align*}

Another choice is

$$\mathbf{x}_1' = \mathbf{R} [\hbar/(M_0\omega)]^{-1/2}, \quad \mathbf{q}_1' = \mathbf{P}(\hbar M_0\omega)^{-1/2};$$  \hspace{1cm} \begin{align*} 
\mathbf{x}_2' &= (\mathbf{r}_1 - \mathbf{r}_2) [\hbar/(\mu\omega)]^{-1/2}, \quad \mathbf{q}_2' = \mathbf{p}_{rel}(\hbar\mu\omega)^{-1/2}. \tag{12} 
\end{align*}

In the above relations $M_0 = m_1 + m_2$, $\mu = m_1 m_2/M_0$ is the reduced mass, $\mathbf{p}_{rel} = (m_2 \mathbf{p}_1 - m_1 \mathbf{p}_2)/M_0$ is the relative momentum, $\mathbf{R} = (m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2)/M_0$, and $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$. These relations are the versions of the Smirnov [4] transformation.

The above quantities are defined in a way that the relations between ($\mathbf{x}_1$, $\mathbf{x}_2$) and ($\mathbf{x}_1'$, $\mathbf{x}_2'$) or ($\mathbf{q}_1$, $\mathbf{q}_2$) and ($\mathbf{q}_1'$, $\mathbf{q}_2'$) are, indeed, of the form of Eqs. (5). In the case of Eqs. (11) one gets

$$\cos \varphi = -\left( \frac{m_2}{m_1 + m_2} \right)^{1/2}, \quad \sin \varphi = \left( \frac{m_1}{m_1 + m_2} \right)^{1/2}.$$  \hspace{1cm} (13)
In the case of Eqs. (12), one gets
\[ \cos \varphi = \left( \frac{m_1}{m_1 + m_2} \right)^{1/2}, \quad \sin \varphi = \left( \frac{m_2}{m_1 + m_2} \right)^{1/2}. \] (14)

(This is seen at once if the inverse transformations are considered.)

The expansions (7) are also of use when solving three-particle problems in the oscillator basis. In the case of identical particles these expansions make possible to construct basis states that behave properly under particle permutations. If not all three particles are identical these expansions are helpful to calculate interaction matrix elements. This is discussed, e.g., in Ref. [5] as to the hyperspherical case.

If instead of the transformation (5) the orthogonal transformation
\[ x_1 = x'_1 \cos \varphi + x'_2 \sin \varphi, \quad x_2 = -x'_1 \sin \varphi + x'_2 \cos \varphi \] (15)
is considered then the coefficients of the corresponding expansion similar to (7) are obviously expressed in terms of the coefficients (9) as
\[ (-1)^l \langle n_1' n_2' | n_1 n_2 \rangle^\varphi_L. \] (16)

Use of the transformation (5) is preferable since in this case a simple symmetry relation
\[ \langle n_1' n_2' | n_1 n_2 \rangle^\varphi_L = \langle n_1 n_2 | n_1' n_2' \rangle^\varphi_L \] (17)
is valid. This has been pointed out in Ref. [6] for the case of equal masses \( m_1 = m_2 \) in Eqs. (10) and (12) and in Ref. [3] in the general form (17). As mentioned in [3] the relation (17) follows from general properties of the transformation (5) which is commented also in [5].

We shall deal with the transformation (5) and not with (15) in what follows.

Other symmetry relations for the brackets also exist [3] (as to the \( m_1 = m_2 \) case see also [6,7]). The symmetry relations for oscillator brackets presented as being original in [8] are in fact the same as those given previously in [3].

III. RELATIONS TO CALCULATE THE BRACKETS

Moshinsky [1] has suggested the following algorithm to calculate oscillator brackets. First the brackets with \( n_1 = n_2 = 0 \) are calculated. Next the rest brackets are obtained with the
help of \( n_1 - 1 \rightarrow n_1 \) and \( n_2 - 1 \rightarrow n_2 \) recurrence relations. He obtained such recurrence relations and an expression for the \( n_1 = n_2 = 0 \) brackets. He provided the formulae in the case of the transformation \([15]\) at \( \varphi = \pi/4 \) (which corresponds to the \( m_1 = m_2 \) case in Eq. \([11]\) type relations). Below we shall refer to such formulae pertaining to the transformations \([5]\) and \([15]\) at any \( \varphi \) as to Moshinsky-type relations.

In Ref. \([3]\) the recurrence relations realizing the Moshinsky algorithm have been obtained in a form different from the Moshinsky-type form. Also an expression for the initial \( n_1 = n_2 = 0 \) brackets different from the Moshinsky-type expression has been derived there. The present program is based on the corresponding relations of Ref. \([3]\), Eqs. \([20]\) and \([22]\) of the present paper.

The recurrence formulae in \([3]\) have been obtained for modified brackets, denoted as \([n'_1 l'_1 n'_2 l'_2 | n_1 l_1 n_2 l_2]_L^p\) and defined as follows,

\[
[n'_1 l'_1 n'_2 l'_2 | n_1 l_1 n_2 l_2]_L^p = \langle n'_1 l'_1 n'_2 l'_2 | n_1 l_1 n_2 l_2 \rangle_2^p \frac{A(n'_1, l'_1) A(n'_2, l'_2)}{A(n_1, l_1) A(n_2, l_2)},
\]

where

\[
A(n, l) = (-1)^n [(2n)!!(2n + 2l + 1)]^{-1/2}.
\]

Such a modification of brackets was done in \([6]\) in a different context and in \([9]\) in case of the hyperspherical brackets.

The \( n_1 - 1 \rightarrow n_1 \) recurrence formula is

\[
[n'_1 l'_1 n'_2 l'_2 | n_1 l_1 n_2 l_2]_L^p = \cos^2 \varphi [n'_1 - 1l'_1 l'_2 l_2 | n_1 - 1l_1 n_2 l_2]_L^p + 
\sin^2 \varphi [n'_1 l'_1 n'_2 - 1l'_2 | n_1 - 1l_1 n_2 l_2]_L^p
\]

\[- \sin \varphi \cos \varphi \left\{ [n'_1 l'_1 - 1n'_2 l'_2 - 1n_1 - 1l_1 n_2 l_2]_L^p \psi_L^+(l'_1, l'_2) + [n'_1 - 1l'_1 + 1n'_2 - 1l'_2 + 1n_1 - 1l_1 n_2 l_2]_L^p \psi_L^-(l'_1 + 1, l'_2 + 1)
\]

\[ - [n'_1 - 1l'_1 + 1n'_2 l'_2 - 1n_1 - 1l_1 n_2 l_2]_L^p \psi_L^+(l'_1 + 1, l'_2) - [n'_1 l'_1 - 1n'_2 - 1l'_2 + 1n_1 - 1l_1 n_2 l_2]_L^p \psi_L^-(l'_1, l'_2 + 1) \right\} \]

where

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

(In Ref. \([3]\) the quantities \( \psi_L^+(p, q) \) were denoted as \( \alpha_L(p, q) \) and \( \psi_L^-(p + 1, q) \) as \( \beta_L(p, q) \). One then has \( \psi_L^-(p, q + 1) = \psi_L(q + 1, p) = \beta_L(q, p) \).
The $n_2 - 1 \rightarrow n_2$ recurrence formula is obtained from Eq. (20) via making the replacements $\cos^2 \varphi \leftrightarrow \sin^2 \varphi$ and changing the sign of $\sin \varphi \cos \varphi$.

The $[n'_1 n'_2 n''_2 | 0l_1 0l_2]_L^\varphi$ coefficients are calculated separately and they make possible to start the recursion. They are given by the following expression,

$$
[n'_1 n'_2 n''_2 | 0l_1 0l_2]_L^\varphi = (-1)^{n'} \prod_{i=1}^{2} 2^{-l'_i} [(2l_i + 1)(2l'_i + 1)]^{1/2} |A(n'_1, l'_i)|^2 \times [(l_1 + l_2 + L + 1)!(l_1 + l_2 - L)!]^{1/2} (\cos \varphi)^{l_1 + l_2} (\tan \varphi)^{n'_1 + n'_2} F_L^\varphi
$$

(22)

where $A(n'_1, l'_i)$ are from Eq. (19), and

$$
F_L^\varphi = \sum_{i=i_{\text{min}}}^{i_{\text{max}}} (-1)^{\alpha_{i4}} \frac{[\prod_{k=1}^{i}(2\alpha_{ik})!]}{\prod_{k=1}^{i} \alpha_{ik}!} \left( \begin{array}{ccc}
\tilde{l}_1 & \tilde{l}_2 & L \\
\tilde{l}'_1 - i & \tilde{l}'_2 - i & l'_2 - l'_1
\end{array} \right) \tan^i \varphi.
$$

(23)

Here $(.)$ is the $3j$-symbol,

$$
\alpha_{i1} = \frac{\tilde{l}_1 + \tilde{l}'_1 - i}{2}, \quad \alpha_{i2} = \frac{\tilde{l}_1 + \tilde{l}'_1 + i}{2}, \quad \alpha_{i3} = \frac{\tilde{l}_2 - \tilde{l}'_2 + i}{2}, \quad \alpha_{i4} = \frac{\tilde{l}_2 + \tilde{l}'_2 - i}{2}.
$$

(24)

The summation proceeds between the limits

$$
i_{\text{min}} = |\tilde{l}_1 - \tilde{l}'_1| \equiv |\tilde{l}_2 - \tilde{l}'_2|, \quad i_{\text{max}} = \min(\tilde{l}_1 + \tilde{l}'_1, \tilde{l}_2 + \tilde{l}'_2)
$$

within which the $3j$-symbol is different from zero. The summation variable takes only values of the same parity as these limits. This is related to the requirement that the quantities $|24|$ must be integers. (These quantities are non-negative.)

A remarkable feature of the recurrence formula (20) is that at a given $L$ value the coefficients $\psi_L^{\pm}$ depend on only two quantum numbers $l'_1$ and $l'_2$ and are independent of the quantum numbers $n'_1, n'_2, n_1, n_2, l_1,$ and $l_2$. In addition, these coefficients are expressed in terms of only two functions of Eq. (21). All this suggests precomputing these two functions which is very fast. Different from the above recurrence formulae, the Moshinsky-type recurrence formulae involve the initial brackets (9). The coefficients of such formulae are products

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1 Eq. (22) is Eq. (39) in [3] but it is written here for the modified coefficient $[\ldots |0l_1 0l_2]_L^\varphi$ instead of $(\ldots |0l_1 0l_2)\varphi$. Let us mention that the most simple derivation of the corresponding Eq. (23) in [3] is contained in Appendix there.
of six different functions depending on four quantum numbers and functions depending on two quantum numbers.

The quantity (23) depends on $l'_1$, $l'_2$, and on the difference $l_1 - l_2$. In our case, precomputing this quantity also proves to be helpful. The Moshinsky-type derivation leads to a different formula for the $n_1 = n_2 = 0$ brackets which includes full dependence on the four partial angular momenta and at given their values involves probably two-three times more computations than in case of Eq. (22).

IV. ANGULAR MOMENTUM VARIABLES

Permissible values of the quantum numbers $l_1$ and $l_2$, or $l'_1$ and $l'_2$, specifying a bracket are restricted by the requirement of a given parity and by the triangle inequalities involving the $L$ value. Aiming both to get compact arrays of brackets and avoid the restrictions in computations we shall use the following variables instead of $l_1$ and $l_2$, or $l'_1$ and $l'_2$,

$$M = \frac{l_1 + l_2 - L - \epsilon}{2}, \quad N = \frac{l_1 - l_2 + L - \epsilon}{2},$$

$$M' = \frac{l'_1 + l'_2 - L - \epsilon}{2}, \quad N' = \frac{l'_1 - l'_2 + L - \epsilon}{2} \quad (25)$$

where $\epsilon = 0$ or 1 when $N_q - L$ is even or odd, respectively. The inverse relations are $l_1 = M + N + \epsilon$, $l_2 = M - N + L$ and $l'_1 = M' + N' + \epsilon$, $l'_2 = M' - N' + L$. These variables have been introduced in [10] in the case of hyperspherical brackets. One has

$$(N_q - L - \epsilon)/2 = M + n_1 + n_2 = M' + n'_1 + n'_2. \quad (26)$$

When $l_1$, $l_2$, $l'_1$, and $l'_2$ take all the values allowed at a given $L$ and a given parity, the $M$ or $M'$ and $N$ or $N'$ variables take all the integer values from zero up to, respectively,

$$M_{\text{max}} = (N_q - L - \epsilon)/2, \quad N_{\text{max}} = L - \epsilon. \quad (27)$$

(The case $L = 0, \epsilon = 1$ is, obviously, not possible.) Thus the discussed variables densely fill intervals independent of each other.

V. THE PROGRAMS

We suggest that often the most convenient form of the output would be an array, or 'table', of all the brackets pertaining to states with $N_q$ values up to some $(N_q)_{\text{max}}$, with
total angular momenta in a range from $L_{\text{min}}$ to $L_{\text{max}}$, and with a given parity. In particular, if such an array is available then one can avoid repeated computations of the same brackets at the calculation of matrix elements. In the framework of the present algorithm, such an array is composed of groups of brackets having the same $l_1, l_2, \text{and } L$ values. The brackets of each group are related by the recursion.

In the present work, brackets sought for are produced by a subroutine written in two versions. One of them is named ALLOSBRAC and its output is just the mentioned array.

The parameters of the ALLOSBRAC subroutine are NQMAX, LMIN, LMAX, CO, SI, and BRAC. Here NQMAX, LMIN, and LMAX are the input parameters defined above. (NQMAX $\equiv (N_q)_{\text{max}}$, LMIN $\equiv L_{\text{min}}$, etc. We use capital letters for quantities entering the programs.) CO and SI are the input parameters $\cos \varphi$ and $\sin \varphi$ from Eq. (5). BRAC is the output array of brackets. Values of $N_q$ pertaining to all these brackets are such that $(N_q)_{\text{max}} - N_q$ is even.

In the present programs, the quantities like $N', n_1', \text{etc.}$, are denoted like NP, N1P, etc., where P symbolizes 'primed'. The mentioned output array BRAC is of the form $\text{BRAC}(NP,N1P,MP,N1,N2,N,M,L)$. The value of N2P is determined by Eq. (26). Thus the arguments of BRAC represent all quantum numbers specifying a bracket. The order of arguments of BRAC corresponds to the nesting of loops in the subroutine at the computation of brackets since such an order is preferable. In accordance with the bounds of the BRAC array in the dimension list, the size of this array is

$$\left(L_{\text{max}} - L_{\text{min}} + 1\right)\left(L_{\text{max}} + 1\right)^2\left\{\text{Int}\left[\left[(N_q)_{\text{max}} - L_{\text{min}}\right]/2\right] + 1\right\}^5.$$  

In many cases such a size is acceptable. (At the double precision calculations when $(N_q)_{\text{max}} = 40$ and $L_{\text{min}} = L_{\text{max}} = L$ this size is about or less 1 GB at any $L$. When $(N_q)_{\text{max}} = L_{\text{max}} = 20$ and $L_{\text{min}} = 0$ it is about 12 GB.)

The other version of the subroutine, named OSBRAC, produces the above mentioned subsets of brackets with given $l_1, l_2, \text{and } L$ values or, which is the same, with given $M, N, \text{and } L$ values. As mentioned above, these brackets pertain to states with $N_q$ values up to some $(N_q)_{\text{max}}$ and with given parity determined by the $(N_q)_{\text{max}}$ value. This version is required, in particular, in the cases of memory restrictions. (Of course, one can also compute an array at given $l_1'$ and $l_2'$ values instead of given $l_1$ and $l_2$ values, see [17].)

The parameters of the OSBRAC subroutine are N, M, L, NQMAX, CO, SI, FIRSTCALL,
and BRAC. All the listed parameters but BRAC are input ones. All of them except FIRSTCALL represent the quantities defined above. The FIRSTCALL parameter is discussed below. The BRAC parameter represents the output array of brackets. In this case, it is of the form BRAC(NP,N1P,MP,N1,N2). It thus represents the subset of brackets pertaining to given input N, M, and L values. Again, N2P is determined by Eq. (26) and the arguments of BRAC along with N, M, and L represent all quantum numbers specifying a bracket.

Describing the programs, let us first discuss the issue of possible overflows at large quantum numbers. When the double precision is set in the present programs, the allowed values of NQMAX are as follows, \( (N_q)_{\text{max}} \leq 84 \). At this restriction, the computation as real numbers of all the factorials and double factorials entering Eqs. (19), (22), and (23), apart from the \( 3j \) symbols in Eq. (22), does not lead to overflows/underflows. (To conclude this, one needs to take into account that in Eq. (24) \( \alpha_{ik} \leq N_q \).) This restriction may be considerably weakened if square roots of factorials are calculated with the quadrupole precision and all the rest with the double precision. This is not done here because, at \( (N_q)_{\text{max}} \) values already not much higher than 84, accuracy of the present double precision computation becomes insufficient in general, see Table V in the next section. Let us mention in this connection that e.g., passing from the double precision to the quadrupole precision everywhere in the calculation of Ref. [11] increased the running time more than 15 times.

Still, products of several factorials entering the usual expressions for \( 3j \) symbols may lead to overflows. To avoid this, we employed the expression [12] (see also [13]) for \( 3j \) symbols in terms of binomial coefficients,

\[
\binom{j_1 - j_2 - m_3}{m_1 - m_2 - m_3} = (-1)^{j_1 - j_2 - m_3} \left( \frac{Bi(\gamma_2, 2j_1)Bi(\gamma_3, 2j_2)}{(2j_3 + 1)Bi(\gamma_3, j_1 + j_2 + j_3 + 1)\Pi} \right)^{1/2} S,
\]

\[
\Pi = Bi(j_1 + m_1, 2j_1)Bi(j_2 + m_2, 2j_2)Bi(j_3 + m_3, 2j_3),
\]

\[
S = \sum_{k=k_{\text{min}}}^{k_{\text{max}}} (-1)^k Bi(k, \gamma_3)Bi(j_1 - m_1 - k, \gamma_2)Bi(j_2 + m_2 - k, \gamma_1)
\]

where \( Bi(m, n) = n!/\lfloor m!(n-m)! \rfloor \) are the binomial coefficients, \( \gamma_i = j_1 + j_2 + j_3 - 2j_i \), and

\[
k_{\text{min}} = \max(0, j_1 - j_3 + m_2, j_2 - j_3 - m_1), \quad k_{\text{max}} = \min(\gamma_3, j_1 - m_1, j_2 + m_2).
\]

We note that if one writes the binomial coefficients entering here in terms of factorials then Eq. (28) turns to the standard Van der Waerden formula [13] for \( 3j \) symbols. In Ref. [14]
it has been realized that Eq. (28) type expressions are advantageous for computations. In Ref. [15], their utility to cope with the overflow issue has been noted. Due to the fact that $Bi(m,n)$ grow with the increase of $n$ slower than factorials, $Bi(m,n) \leq 2^n$, no overflows can arise in double precision computations at use of the expression (28) with the above restriction on $(N_q)_{max}$.

The structures and details of the present programs should be clear from generous comments they include. Below an outline is presented. Both subroutines ALLOSBRAC and OSBRAC first call for the simple subroutines ARR and COE that precompute the required factorials, double factorials, quantities $[(2I)!]^{1/2}/I!$ from Eq. (23), and the binomial coefficients. Then the quantities (19) are precomputed. Next both ALLOSBRAC and OSBRAC call for the subroutine named FLPHI to precompute the array of the quantities (23) multiplied by $(2I_1+1)(2I_2+1)$. The FLPHI subroutine calls for the function WIGMOD that provides the quantity $S$ from Eq. (28) times the factors from there depending on $m_1$ and $m_2$. Furthermore, to precompute the arrays representing the coefficients (21) of the recurrence formulae, the subroutine named COEFREC is called. In the ALLOSBRAC case, FLPHI and COEFREC are called inside the loop over $L$.

All the mentioned routines are contained in the file allosbrac.f90 in the case of the first mentioned version of the program and in the file osbrac.f90 in the case of the second one.

The recurrence procedures are realized as follows. First the recursion $n_2 - 1 \rightarrow n_2$ discussed in Sec. III is performed at $n_1 = 0$. Then the recursion $n_1 - 1 \rightarrow n_1$ is performed at each $n_2$ value starting from the obtained brackets with $n_1 = 0$.

One should require that the arguments of the array BRAC in the right-hand sides of the recurrence relations like (20) do not go beyond their bounds prescribed at the preceding step of the recursion. When this condition is not fulfilled, the corresponding contributions to the recurrence relations are to be omitted. The arising restrictions are summarized in comment lines in the subroutines. One case of the restrictions is as follows.

Consider a step of the recursion. According to Eq. (26), the N1P and MP values pertaining to this step are such that $N1P+MP \leq M_{max}$. The $N_q$ value increases by two at each step of the recursion. Correspondingly, the $M_{max}$ value given by Eq. (27) increases by one. Let us write the array BRAC as BRAC(K1,K2,K3...) where K2 and K3 represent, respectively, the N1P and MP variables. Then, according to the said above, for the array BRAC in the right-hand sides of the recurrence relations the condition $K2+K3 \leq M_{max} - 1$ should
be fulfilled since the array BRAC there corresponds to the preceding step of the recursion. At given N1P and MP values mentioned above, possible K2 and K3 values pertaining to the preceding step of the recursion are the following, K2=N1P or N1P-1 and K3=MP or MP-1, or MP+1. This is seen from Eq. [20] rewritten in terms of the $M'$ and $N'$ variables.

All the combinations of these K2 and K3 values except for (K2,K3)=(N1P,MP+1) are present in the recurrence relations. When (K2,K3)=(N1P,MP-1), or (K2,K3)=(N1P-1,MP-1), or (K2,K3)=(N1P-1,MP) the above condition $K2+K3 \leq M_{\text{max}} - 1$ fulfills automatically. But when (K2,K3)=(N1P,MP) or (K2,K3)=(N1P-1,MP+1) the requirement $N1P+MP \neq M_{\text{max}}$ is to be imposed in order this condition fulfills. (The restriction we described matters if the BRAC array includes non-zero elements at the time of the call of the OSBRAC or ALLOSBRAC routine.)

The FIRSTCALL parameter of the OSBRAC subroutine is a logical variable. This variable makes possible not to call for the subroutine FLPHI by OSBRAC at all, except for the first, sequential calls for OSBRAC with a given $L$ value and with each of $N$ (i.e., $l_1 - l_2$) values. To achieve this, it is to be said FIRSTCALL=.FALSE. in the proper place of the program that calls for OSBRAC. Then, a change of $L$ in that program is to be accompanied by the statement FIRSTCALL=.TRUE. Examples of use of the variable FIRSTCALL are given in the appended program TESTOSBRAC, tests 3 and 4. (The statement FIRSTCALL=.FALSE. also removes most of unnecessary calls of other subroutines by OSBRAC but this is not important.)

Of course, there exists also a possibility not to use the described option and to call for OSBRAC always at FIRSTCALL=.TRUE. The effect of the variation of FIRSTCALL is not very large, see the last section.

VI. TESTS

Tests can be readily performed with the help of the appended programs TESTALLOSBRAC and TESTOSBRAC. In addition to checks of brackets, these programs provide commented examples of implementation of ALLOSBRAC and OSBRAC. Outcomes of the tests are contained, respectively, in the files named allosoutput and osoutput. The tests as well as the calculations in the next section were performed at $m_1 = m_2$ in Eq. [13]. The tests were the following.
1. For the brackets with \( n'_2 = l'_2 = 0 \) and thus with \( l'_1 = L \) and \( n'_1 = (N_q - L)/2 \) there exists a simple explicit expression \(^2\)

\[
\langle n'_1 L00|n_1 l_1 n_2 l_2 \rangle^\varphi_L = \cos^{2n_1 + l_1} \varphi \sin^{2n_2 + l_2} \varphi \\
\times (-1)^L [(2l_1 + 1)(2l_2 + 1)]^{1/2} \left( \begin{array}{ccc} l_1 & l_2 & L \\ 0 & 0 & 0 \end{array} \right) \frac{A(n_1, l_1)A(n_2, l_2)}{A(n'_1, L)} \tag{29}
\]

where the notation \(^19\) is used. The bracket computed with the programs has been compared with this expression.

2. Symmetry \(^17\) of brackets computed with the programs has been verified.

3. Consider the relation

\[
\sum_{i,i',j,L;N_q=\text{const}} \langle j|i \rangle^\varphi_L \langle j|i' \rangle^\varphi_L = \nu(N_q). \tag{30}
\]

Here \( i, i' \), and \( j \) symbolize various \( n_1 l_1 n_2 l_2 \) sets. The summations proceed over all such sets existing at a given \( N_q \) value. The quantities \( \langle...|.. \rangle^\varphi_L \) thus represent the brackets we deal with. The quantity \( \nu(N_q) \) is the number of all the \( |n_1 l_1 n_2 l_2 LM_L \rangle \) states, with the same \( M_L \), existing at a given \( N_q \) value.

This number is \( \sum_{allL} \nu(N_q, L) \) where \( \nu(N_q, L) \) is the number of all such states at given \( N_q \) and given \( L \) values. The latter number equals \( (N_{max} + 1)(M_{max} + 1)(M_{max} + 2)/2 \) where \( N_{max} \) and \( M_{max} \) are given by Eq. \(^27\). Indeed, according to Eq. \(^25\) the number of such states at a given \( M \) value with all possible \( N \) values equals \( (N_{max} + 1)[(M_{max} - M) + 1] \).

Thus the left-hand side of Eq. \(^30\) computed with the programs has been verified.

4. The quantity equal to zero

\[
\delta = \sum_{i,i',L;N_q \leq (N_q)_{max}} \left| \left[ \sum_j \langle j|i \rangle^\varphi_L \langle j|i' \rangle^\varphi_L \right] - \delta_{ii'} \right| \tag{31}
\]

has been computed with the programs. Here the notation is as in Eq. \(^30\) and the summations proceed over all the brackets with \( N_q \) values that do not exceed some \( (N_q)_{max} \).

\(^2\) This expression has been derived in \(^16\) for the case of pseudo-orthogonal transformations \(^15\). For orthogonal transformations \(^5\) considered here the result is the same and the derivation is a bit simpler due to the symmetry relation \(^17\).
VII. ACCURACIES AND RUNNING TIMES

All the calculations below have been performed with a consumer notebook Intel core of the first generation i5-750 2.67 GHz (2009). Since the computer had a small active memory (3.6 GB) the ALLOSBRAC routine was employed at $L_{\text{min}} = L_{\text{max}} = L$ to make the calculation executable in all the cases. To determine small running times, the computations were done repeatedly. Times to print out the outputs were disregarded. In the present computations and those of other authors discussed below the double precision has been set.

Programs to calculate oscillator brackets have been published in Refs. [8, 11, 17–22]. Of them, the programs [8, 11, 22] are written in a contemporary programming language. They are based on an explicit expression [23] for the brackets. Comparison of the results of the present calculations with those of Refs. [8, 11, 22] is done below.

The programs of Refs. [17–21] are written in Fortran - IV (1965). The too complicated program [17] is based on the formulae of Ref. [1] (taken from [24]). It is applicable only in a limited range of quantum numbers. It was stated [20], see also [6], that the recurrence relations of Ref. [1] are very time consuming and somewhat inefficient to compute the brackets. In the programs of Refs. [18–21] explicit expressions [4, 6, 25, 26] have been employed. In [20, 21] ingredients of such expressions which are independent of $n$’s were precomputed. This speeds up the computations in the cases when sets of brackets with many $n$’s and limited $l$’s are required. In the case of the programs of Refs. [17–21] no information on stability of the computation algorithms is available. Contrary to our results below, only brackets at rather low oscillator excitations were considered in the mentioned papers.

In Table I the computed values of the sum $\delta$ of Eq. (31) and the corresponding running times are presented for a number of $(N_q)_{\text{max}}$ values. The computations were performed with both ALLOSBRAC and OSBRAC. The calling programs here are the same as in the appended files mentioned in the preceding section. The contributions of even and odd $N_q$ values were added up. (In the OSBRAC case arrays of brackets were not stored. Otherwise, the calculation would had been equivalent to use of ALLOSBRAC.) The $\delta$ values produced

---

3 Methods to calculate the brackets were also worked out in Refs. [27–33]. Refs. [28, 30] deal with explicit formulae, Ref. [31] deals with the matrix diagonalization, and Refs. [27, 32, 33] deal with the recurrence relations different from the present ones.
TABLE I: Accuracy and running times at calculating the quantity $\delta$ of Eq. (31) in comparison with Ref. [8]. First column: $(N_q)_{\text{max}}$ value in Eq. (31). Second column: the values of $\delta$ obtained. Third column: running times $t_1$ in seconds calculated with ALLOSBRAC. Fourth column: running times $t_2$ in seconds calculated with OSBRAC. Fifth column: the values of Ref. [8] for $\delta$ denoted as $\delta'$. Last column: the ratios of the running time $t'$ of Ref. [8] to that in the third column. These ratios are commented in the text.

| $(N_q)_{\text{max}}$ | $\delta$       | $t_1$, [s]   | $t_2$, [s]   | $\delta'$ [8] | $t'/t_1$ |
|----------------------|----------------|--------------|--------------|----------------|----------|
| 8                    | $7.9 \cdot 10^{-13}$ | $1.9 \cdot 10^{-4}$ | $1.3 \cdot 10^{-3}$ | $7.0 \cdot 10^{-10}$ | $9.2 \cdot 10^6$ |
| 12                   | $6.8 \cdot 10^{-12}$ | $1.3 \cdot 10^{-3}$ | $2.0 \cdot 10^{-2}$ | $3.5 \cdot 10^{-5}$ | $1.9 \cdot 10^8$ |
| 16                   | $3.5 \cdot 10^{-11}$ | $6.8 \cdot 10^{-3}$ | 0.19         | -              | -        |
| 20                   | $1.4 \cdot 10^{-10}$ | $2.7 \cdot 10^{-2}$ | 1.2          | -              | -        |
| 24                   | $4.75 \cdot 10^{-10}$ | $9.1 \cdot 10^{-2}$ | 5.65         | -              | -        |
| 28                   | $1.5 \cdot 10^{-9}$  | 0.28         | 22           | -              | -        |

by the two programs coincide with each other. This should be the case since eventually the same operations are performed in the same order in the two computations. (Although in the OSBRAC case some repetitions occur.) The $\delta$ values obtained are shown in the second column. The running times in seconds pertaining to ALLOSBRAC and OSBRAC are presented in the third and fourth column, respectively. They are denoted as $t_1$ and $t_2$. It is seen that at higher $(N_q)_{\text{max}}$ values OSBRAC is much slower. This is because of the repeated calculations of the same brackets required in the OSBRAC case. If the varying of FIRSTCALL is not applied then the running time $t_2$ becomes more than twice larger than in the table at $(N_q)_{\text{max}} = 12$ and by 30% larger at $(N_q)_{\text{max}} = 28$.

The values of $\delta$ obtained in Ref. [8] are listed in the fifth column and denoted as $\delta'$. It is seen that the algorithm based on an explicit expression for the brackets employed in Ref. [8] leads to much faster deterioration of accuracy with the increase of $(N_q)_{\text{max}}$ than in the case of the present approach.

In the last column the ratios of the running times of Ref. [8], denoted as $t'$, to the present running times $t_1$ are listed. Discussing them, we shall take into account that, as it can be seen, the contribution to the considered running times of summations in Eq. (31) can be disregarded. The drastic difference in the running times is caused by several reasons and
one of them is the following. The numbers of computed brackets listed in Ref. [8] show that the same brackets were computed there repeatedly for many times. And in case of use of our ALLOSBRAC routine all the brackets are computed only once. But this is not the only point, and also average running times per one computed bracket are much larger in the case of Ref. [8] than in the present case. The ratio of these running times equals \(8.2 \times 10^3\) at \((N_q)_{\text{max}} = 8\) and \(4.5 \times 10^4\) at \((N_q)_{\text{max}} = 12\). Probably, in accordance with the Moore’s law, about two digits in these ratios may be attributed to the difference between the performances of the computer used in the present calculation and of the older PC of Ref. [8]. If one accepts this, then it may be concluded that the average number of operations to calculate a bracket in Ref. [8] is larger more than 80 times at \((N_q)_{\text{max}} = 8\) and about 450 times at \((N_q)_{\text{max}} = 12\) than in the case of the present program.

In Table II the running times \(t_{\Sigma}\) are listed which pertain to the calculation of all existing brackets with a given \(L\) value and with \(N_q\) values such that \(N_q \leq (N_q)_{\text{max}}\) and \((N_q)_{\text{max}} - N_q\) is even. These running times refer to use of ALLOSBRAC. When OSBRAC is used the running times are almost the same. This is because the number of arithmetic operations performed is the same in this case except for some repetitions of fast precomputations. See also the next table in this connection.

Comparison with the running times \(t'\) of Ref. [11] is presented as well in the table. These times refer to the calculation at \(N_q = (N_q)_{\text{max}}\) only. Considering the listed ratios \(t'/t_{\Sigma}\) one should take into account that in the present calculation a single processor having the nominal performance less than 11 Gflops has been used. Whereas the calculation in Ref. [11] has been performed with a supercomputer and used in parallel 32 processors having the nominal performance about 16 Gflops each. Also the numbers of corresponding brackets in our \(N_q \leq (N_q)_{\text{max}}\) computations exceed more than twice the numbers of brackets in the \(N_q = (N_q)_{\text{max}}\) computations of Ref. [11].

In Table III the running times for calculating all the existing brackets with even \(N_q\) values that do not exceed \((N_q)_{\text{max}}\) are listed. (These are brackets with all possible \(L\) values.) The net numbers of such brackets at given \((N_q)_{\text{max}}\) are denoted as \(\mathcal{N}\). The running times, \(t_1\) and \(t_2\), refer, respectively, to use of ALLOSBRAC and OSBRAC. At \((N_q)_{\text{max}} = 80\) only the calculation with OSBRAC is done because of insufficient memory. The running times \(t_2\) are a bit larger at low \((N_q)_{\text{max}}\). At higher \((N_q)_{\text{max}}\) they are somewhat smaller. This is probably because of memory restrictions in the ALLOSBRAC case. The running times per bracket
TABLE II: Third column: the running times $t_x$ in seconds for the calculation of the sets of all brackets with a given $L$ value and with $N_q$ values such that $N_q \leq (N_q)_{\text{max}}$ and $(N_q)_{\text{max}} - N_q$ is even. Last column: the ratios $t'/t_x$, where $t'$ are the running times of Ref. [11], for the calculation of the brackets with $N_q = (N_q)_{\text{max}}$ only. These ratios are commented in the text as well as those in the tables below.

| $(N_q)_{\text{max}}$ | $L$ | $t_x$, [s] | $t'/t_x$ |
|----------------------|-----|------------|----------|
| 21                   | 11  | 1.7 · 10^{-3} | 68 |
| 22                   | 8   | 3.3 · 10^{-3} | 110 |
| 23                   | 9   | 4.0 · 10^{-3} | 120 |
| 24                   | 8   | 5.9 · 10^{-3} | 130 |
| 25                   | 9   | 7.3 · 10^{-3} | 150 |
| 26                   | 10  | 8.5 · 10^{-3} | 170 |
| 27                   | 9   | 1.2 · 10^{-2} | 210 |
| 28                   | 10  | 1.4 · 10^{-2} | 240 |

prove to vary slowly and they stabilize when $(N_q)_{\text{max}}$ increases. In the OSBRAC case they equal $1.4 \cdot 10^{-8}$ s at $(N_q)_{\text{max}} \geq 30$.

In the last column the corresponding running times of Ref. [22], deduced from the table there, are compared with the present running times. In contrast to our case, in the case of Ref. [22] the running times per bracket sharply increase with $(N_q)_{\text{max}}$. Comparing the running times one should take into account that, contrary to the present single-processor calculation with the computer described above, the calculation in Ref. [22] was performed in parallel using 12 processors. The same refers to the results in Table IV below.

In Table IV the quantities equal to zero

\[
\delta_1(N_q) = \sum_{i,i',L; N_q=\text{const}} \left| \sum_j \langle j|i \rangle \langle j|i' \rangle \delta_{ii'} \right| 
\]

\[
\delta_2(N_q) = \left| \sum_{i,i',L; N_q=\text{const}} \sum_j \langle j|i \rangle \langle j|i' \rangle \delta_{ii'} \right| 
\]

are calculated. Here the summations proceed at given $N_q$ values and the other notation is as in Eq. [31]. The computation was done with ALLOSBRAC. In the fourth column the values of the sum obtained in Ref. [22] are listed. They are denoted as $\delta'$. It is not
TABLE III: The running times for the calculation of the sets of all existing brackets with even $N_q$ values such that $N_q \leq (N_q)_{\text{max}}$. The net numbers of such brackets are denoted as $\mathcal{N}$. The running times in seconds for the computation with ALLOSBRAC and OSBRAC are denoted as $t_1$ and $t_2$, respectively. The running time of Ref. [22] is denoted as $t'$.

| $(N_q)_{\text{max}}$ | $\mathcal{N}$ | $t_1$, [s] | $t_2$, [s] | $t_1/\mathcal{N}$, [s] | $t'/t_1$ |
|----------------------|--------------|------------|------------|----------------|----------|
| 12                   | 41424        | 8.2 $\cdot$ 10^{-4} | 9.8 $\cdot$ 10^{-4} | 2.0 $\cdot$ 10^{-8} | 33       |
| 16                   | 243705       | 4.1 $\cdot$ 10^{-4} | 4.5 $\cdot$ 10^{-4} | 1.7 $\cdot$ 10^{-8} | 94       |
| 20                   | 1040468      | 1.6 $\cdot$ 10^{-2} | 1.7 $\cdot$ 10^{-2} | 1.5 $\cdot$ 10^{-8} | 90       |
| 24                   | 3555825      | 5.3 $\cdot$ 10^{-2} | 5.3 $\cdot$ 10^{-2} | 1.5 $\cdot$ 10^{-8} | 390      |
| 26                   | 6165680      | 9.4 $\cdot$ 10^{-2} | 9.0 $\cdot$ 10^{-2} | 1.5 $\cdot$ 10^{-8} | 540      |
| 30                   | 16743504     | 0.25        | 0.24       | 1.5 $\cdot$ 10^{-8} | -        |
| 40                   | 131288025    | 1.9         | 1.8        | 1.5 $\cdot$ 10^{-8} | -        |
| 50                   | 674606556    | 9.9         | 9.3        | 1.5 $\cdot$ 10^{-8} | -        |
| 80                   | 23084445209  | -           | 330        | -                | -        |

known whether this was the sum (32) or (33). The calculation completely loses stability at $N_q > 20$. In the fifth column the running times are given for the calculation of the sums $\sum_{N_q} \delta_{1,2}(N_q')$. The summations proceed over $N_q'$ values of the same parity as $N_q$ and such that $N_q' \leq N_q$. These running times are denoted as $t_{\Sigma}$. In the last column the ratios of such running times $t'_{\Sigma}$ of Ref. [22], deduced from the table there, to the above running times are presented. As in the tables above, these ratios strongly increase as $N_q$ increases.

The quantity equal to zero

$$\delta_{\text{rel}} = \frac{1}{2} \max_{i, \mathcal{L}} \left| \sum_{j; N_q = \text{const}} \left( \langle j | i \rangle_{\mathcal{L}}^2 \right)^2 - 1 \right|$$

is also calculated. The notation is as above. This quantity represents an estimate of the relative error of computed brackets at a given $N_q$ value. Indeed, in the presence of errors $\Delta(j, i, \mathcal{L})$ in values of the brackets one has

$$\frac{1}{2} \left\{ \left[ \sum_{j; N_q = \text{const}} \left( \langle j | i \rangle_{\mathcal{L}}^2 \right)^2 \right] - 1 \right\} \simeq \sum_{j; N_q = \text{const}} \left( \langle j | i \rangle_{\mathcal{L}}^2 \right)^2 \frac{\Delta(j, i, \mathcal{L})}{\langle j | i \rangle_{\mathcal{L}}^2}.$$ 

The latter quantity is the relative error averaged over the $(\langle j | i \rangle_{\mathcal{L}}^2)$ distribution. The obtained values of the quantity (34) are presented in Table V. The results at the highest $N_q$ values
TABLE IV: Accuracies at calculating the sums \(33\) and \(32\) and related running times in comparison with Ref. [22]. Second column: the computed values of the quantity \(\delta_1(N_q)\) of Eq. \(32\). Third column: the computed values of the quantity \(\delta_2(N_q)\) of Eq. \(33\). Fourth column: the quantity of Eq. \(32\) or \(33\) computed in Ref. [22] which is denoted as \(\delta'(N_q)\). Fifth column: the running times \(t_\Sigma\) for the calculation of the sums \(\sum_{N_q'}\delta_{1,2}(N_q')\). The summations proceed over \(N_q'\) values of the same parity as \(N_q\) and such that \(N_q' \leq N_q\). Last column: the ratios of such running times \(t'_\Sigma\) of Ref. [22] to the above running times.

| \(N_q\) | \(\delta_1(N_q)\) | \(\delta_2(N_q)\) | \(\delta'(N_q)\) \([22]\) | \(t_\Sigma\), [s] | \(t'_\Sigma/t_\Sigma\) |
|---|---|---|---|---|---|
| 12 | \(2.55 \cdot 10^{-12}\) | \(1.3 \cdot 10^{-11}\) | \(3.2 \cdot 10^{-9}\) | \(8.1 \cdot 10^{-4}\) | \(4.35 \cdot 10^{3}\) |
| 16 | \(1.1 \cdot 10^{-11}\) | \(4.6 \cdot 10^{-12}\) | \(1.5 \cdot 10^{-6}\) | \(4.0 \cdot 10^{-3}\) | \(2.2 \cdot 10^{4}\) |
| 20 | \(3.8 \cdot 10^{-11}\) | \(1.2 \cdot 10^{-11}\) | \(6.1 \cdot 10^{-4}\) | \(1.6 \cdot 10^{-2}\) | \(8.8 \cdot 10^{4}\) |
| 25 | \(1.65 \cdot 10^{-10}\) | \(3.2 \cdot 10^{-11}\) | \(0.72\) | \(7.0 \cdot 10^{-2}\) | \(3.6 \cdot 10^{5}\) |
| 30 | \(7.1 \cdot 10^{-10}\) | \(6.7 \cdot 10^{-11}\) | - | 0.25 | - |
| 35 | \(3.5 \cdot 10^{-9}\) | \(1.2 \cdot 10^{-10}\) | - | 0.75 | - |

TABLE V: Dependence of the calculated quantity \(34\) on \(N_q\).

| \(N_q\) | \(\delta_{rel}\) |
|---|---|
| 10 | \(1.6 \cdot 10^{-15}\) |
| 20 | \(5.4 \cdot 10^{-15}\) |
| 30 | \(1.6 \cdot 10^{-13}\) |
| 40 | \(4.0 \cdot 10^{-12}\) |
| 50 | \(1.1 \cdot 10^{-10}\) |
| 60 | \(3.3 \cdot 10^{-9}\) |
| 70 | \(1.1 \cdot 10^{-7}\) |
| 80 | \(2.7 \cdot 10^{-6}\) |

indicate the limitations of the double precision computation.

In conclusion, the programs to calculate oscillator brackets have been created. The listed runs show that the programs are fast and results they produce are accurate up to very high oscillator excitations. Contrary to the programs based on the explicit expression for the brackets, the amount of computations per bracket practically does not change as
quantum numbers increase. Output arrays of the brackets are quite convenient for majority of applications. These arrays are made compact due to use of the suitable combinations of partial orbital momenta as array arguments. The programs are easy to implement and follow.

[1] M. Moshinsky, Nucl. Phys. 13 (1959) 104.
[2] I.S. Gradshteyn and I.M Ryzhik, *Table of Integrals, Series and Products* (Elsevier, 2015).
[3] V.D. Efros, Nucl. Phys. A202 (1973) 180.
[4] Yu.F. Smirnov, Nucl. Phys. 27 (1961) 177.
[5] V.D. Efros, Comput. Phys. Comm. 255 (2020) 107281.
[6] M. Baranger and K.T.R. Davies, Nucl. Phys. 79 (1966) 403.
[7] M. Moshinsky, *The harmonic oscillator in modern physics; from atoms to quarks* (Gordon and Breach, N.Y., 1969).
[8] G.P. Kamuntavičius, R.K. Kalinauskas, B.R. Barrett, S. Mickevičius, and D. Germanas, Nucl. Phys. A695 (2001) 191.
[9] Ja.A. Smorodinsky and V.D. Éfros, Yad. Fiz. 17, 210 (1973) [Sov. J. Nucl. Phys. 17, 107 (1973)].
[10] V.D. Efros, Comput. Phys. Comm. 261 (2021) 107817.
[11] A. Stepšys, S. Mickevičius, D. Germanas, and R.K. Kalinauskas, Comput. Phys. Comm. 185 (2014) 3062.
[12] T. Shimpuku, J. Math. Analysis and Applications 7 (1963) 397; Progr. Theor. Phys. Suppl. 13 (1960) 1.
[13] D.A. Varshalovich, A.N. Moskalev, and V.K. Khersonskij, *Quantum Theory of Angular Momentum* (World Scientific, Singapore, 1988).
[14] S.T. Lai and Y.N. Chiu, Comput. Phys. Comm. 61 (1990) 350.
[15] L. Wei, Comput. Phys. Comm. 120 (1999) 222.
[16] V.D. Efros, Phys. Rev. C 99 (2019) 034620.
[17] A. Lejeune and J.P. Jeukenne, Comput. Phys. Comm. 2 (1971) 231.
[18] M. Sotona and M. Gmitro, Comput. Phys. Comm. 3 (1972) 53.
[19] O. Zohni, Comput. Phys. Comm. 3 (1972) 61.
[20] D.H. Feng and T. Tamura, Comput. Phys. Comm. 10 (1975) 87.
[21] J. Dobeš, Comput. Phys. Comm. 16 (1979) 373.
[22] D. Germanas, A. Stepšys, S. Mickevičius, and R.K. Kalinauskas, Comput. Phys. Comm. 215 (2017) 259.
[23] B. Buck and A.C. Merchant, Nucl. Phys. A600 (1996) 387.
[24] T.A. Brody and M. Moshinsky, *Tables of transformation brackets* (Gordon and Breach, London, 1967).
[25] L. Trlifaj, Phys. Rev. C 5 (1972) 1534.
[26] J. Dobeš, J. Phys. A: Math. Gen. 10 (1977) 2053; 11 (1978) 2131.
[27] A. Arima and T. Terasawa, Progr. Theor. Phys. 23 (1960) 115.
[28] Yu.F. Smirnov, Nucl. Phys. 39 (1962) 346.
[29] K. Kumar, J. Math. Phys. 7 (1966) 671.
[30] M.M. Bakri, Nucl. Phys. A 96 (1967) 115.
[31] J.D. Talman and A. Lande, Nucl. Phys. A163 (1971) 249.
[32] J. Raynal, Nucl. Phys. A 259 (1976) 272.
[33] J. Dobeš, Czech. J. Phys. 41 (1991) 31.