

## CALCULATION OF FOUR-PARTICLE HARMONIC-OSCILLATOR TRANSFORMATION BRACKETS

D. Germanas<sup>a</sup>, R.K. Kalinauskas<sup>a</sup>, S. Mickevičius<sup>b</sup>, and R. Žemaičiūnienė<sup>c</sup>

<sup>a</sup> *Institute of Physics, Savanorių 231, LT-02300 Vilnius, Lithuania*

E-mail: dariusg@ar.fi.lt

<sup>b</sup> *Vytautas Magnus University, K. Donelaičio 58, LT-44248 Kaunas, Lithuania*

E-mail: s.mickevicius@gmf.vdu.lt

<sup>c</sup> *Šiauliai University, Vilniaus 88, LT-76285 Šiauliai, Lithuania*

Received 5 March 2008; revised 19 May 2008; accepted 9 June 2008

A procedure for precise calculation of the four-particle harmonic-oscillator (HO) transformation brackets is presented. The analytical expressions of the HO transformation brackets are given. The computer code for the calculations of HO transformation brackets proves to be fast, efficient and produces results with only small numerical uncertainties.

**Keywords:** mathematical methods in physics, algebraic methods, nuclear shell model

**PACS:** 03.65.Fd, 21.60.Cs

### 1. Introduction

The wave function of a self-bound system in the absence of external fields must be invariant in respect of spatial translations as well as antisymmetric in respect of all permutations of the fermions. Translational invariance of a wave function means that it is dependent only on intrinsic degrees of freedom of the system. The traditional applications, such as the nuclear shell model, however, are based on a model Hamiltonian with individual one-particle variables. These wave functions are very attractive because they allow employing a simple procedure of antisymmetrization. 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 a proper way because the centre of mass of a free nucleus (or a free hadron) should be described by the exponential function corresponding to a freely moving point mass. This should not be a problem in the case when the expression for the realistic wave function in a harmonic-oscillator (HO) basis is known. One of the possibilities to find a solution to the problem of translational invariance of any wave function is based on direct construction of the many-fermion wave function, which is independent of the centre of mass coordinate [1–3]. In this case, the HO basis set in terms of intrinsic (Jacobi) coordinates

is necessary. By a set of Jacobian coordinates for a system of  $N$  particles we have in mind the  $N - 1$  independent vectors each representing the displacement of the centre of mass of two different subsystems. For  $N > 2$ , there exist more than one set of Jacobi coordinates that can be assigned to the  $N$  particle system. In general, when the transformation from one set of Jacobi coordinates to another is performed, one obtains an expression for the wave function containing an infinite number of terms. Only the set of HO functions can be chosen so that the transformation from one set of Jacobi coordinates to another results in a corresponding expansion with a finite number of terms. In this approach, the essential feature is the Talmi–Moshinsky transformation [4–7] and corresponding HO brackets. Since HO brackets are constantly employed in various model calculations of nuclear and hadron structure, it is desirable to have a simple and efficient method to calculate them. Many papers have been devoted to the study of the Talmi–Moshinsky transformation brackets, and various methods for the calculation of these brackets and several explicit expressions for them are described in [8–10]. In the latter papers three-particle Talmi–Moshinsky transformations are presented. The goal of the current study is to work out a simple and efficient method of the calculation of four-particle HO transformation brackets.

## 2. Formalism

Let us define the four-particle wave function in intrinsic (Jacobi) coordinates [2] with bound momenta as

$$\begin{aligned} \{e_1 l_1(\mathbf{r}_1), e_2 l_2(\mathbf{r}_2)\}_{e_1 l_1, e_2 l_2}, e_3 l_3(\mathbf{r}_3) : lm \rangle &= \{ \{ \phi_{e_1 l_1}(\mathbf{r}_1) \otimes \phi_{e_2 l_2}(\mathbf{r}_2) \}_{e_1 l_1, e_2 l_2} \otimes \phi_{e_3 l_3}(\mathbf{r}_3) \}_{lm} \\ &\times \sum_{m_1 m_2 m_3} \begin{bmatrix} l_1 & l_2 & l_{12} \\ m_1 & m_2 & m_{12} \end{bmatrix} \begin{bmatrix} l_{12} & l_3 & l \\ m_{12} & m_3 & m \end{bmatrix} \phi_{e_1 l_1 m_1}(\mathbf{r}_1) \phi_{e_2 l_2 m_2}(\mathbf{r}_2) \phi_{e_3 l_3 m_3}(\mathbf{r}_3), \end{aligned} \quad (1)$$

and the properly orthonormalized HO function is given by [11]

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

where the corresponding dimensionless eigenvalue is equal to  $(e+3/2)$  and the principal quantum number  $n = (e-l)/2 = 0, 1, 2, \dots$ , with  $e = 2n + l$ , and  $l$  is the angular momentum. Momenta are coupled using Clebsch–Gordan coefficients (box brackets) [12]. Let us consider HO transformation brackets as a four-particle orbital coordinate transformation from one set, described by Eq. (1), to another:

$$\begin{aligned} \{e_1 l_1(\mathbf{r}_1), e_2 l_2(\mathbf{r}_2)\}_{e_1 l_1, e_2 l_2}, e_3 l_3(\mathbf{r}_3) : lm \rangle &= \\ \sum_{e'_1 l'_1, e'_2 l'_2, e'_3 l'_3} \langle \{e_1 l_1, e_2 l_2\}_{e_1 l_1, e_2 l_2}, e_3 l_3 : l \{e'_1 l'_1, e'_2 l'_2\}_{e'_1 l'_1, e'_2 l'_2}, e'_3 l'_3 : l \rangle & \{e'_1 l'_1(\mathbf{r}_1), e'_2 l'_2(\mathbf{r}_2)\}_{e'_1 l'_1, e'_2 l'_2}, e'_3 l'_3(\mathbf{r}_3) : lm \rangle, \end{aligned} \quad (3)$$

with the conservation of the total oscillator energy on both sides of the bracket:  $e_1 + e_2 + e_3 = e'_1 + e'_2 + e'_3$ .

In general, the transformation matrix should be the third-order matrix. It can be written as a product of three second order matrices in the following way:

$$\begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ \mathbf{r}_3 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} & 0 \\ \sqrt{\frac{d}{1+d}} & -\sqrt{\frac{1}{1+d}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} \\ 0 & \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} & 0 \\ \sqrt{\frac{d}{1+d}} & -\sqrt{\frac{1}{1+d}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{r}'_1 \\ \mathbf{r}'_2 \\ \mathbf{r}'_3 \end{pmatrix}. \quad (4)$$

Each of these three matrices describes the orthogonal two-particle coordinate transformation. We prefer the above order of the independent transformation variables  $d$ ,  $d_1$ , and the coupling of the angular momenta because this produces an orthogonal and, at the same time, symmetric transformation matrix [10]. Any orthogonal matrix of the second order can be represented in this form. Let us introduce new Jacobian variables

$$\boldsymbol{\eta}_1 = \sqrt{\frac{d}{1+d}} \mathbf{r}'_1 + \sqrt{\frac{1}{1+d_1}} \mathbf{r}'_2, \quad \boldsymbol{\eta}_2 = \sqrt{\frac{1}{1+d}} \mathbf{r}'_1 - \sqrt{\frac{d}{1+d_1}} \mathbf{r}'_2. \quad (5)$$

The new variables change the coupling scheme from  $\{ \phi_{e'_1 l'_1}(\mathbf{r}'_1) \otimes \phi_{e'_2 l'_2}(\mathbf{r}'_2) \}_{l'_{12}, m'_{12}}$  to  $\{ \phi_{\varepsilon_1 \lambda_1}(\boldsymbol{\eta}_1) \otimes \phi_{\varepsilon_2 \lambda_2}(\boldsymbol{\eta}_2) \}_{l'_{12}, m'_{12}}$ . The transformation is described by two-particle HO brackets [10]:

$$\{ \phi_{e'_1 l'_1}(\mathbf{r}'_1) \otimes \phi_{e'_2 l'_2}(\mathbf{r}'_2) \}_{l'_{12}, m'_{12}} = \sum_{\varepsilon_1 \lambda_1 \lambda_2} \langle \varepsilon_1 \lambda_1, \varepsilon_2 \lambda_2 : l'_{12} | e'_1 l'_1, e'_2 l'_2 : l'_{12} \rangle_d \{ \phi_{\varepsilon_1 \lambda_1}(\boldsymbol{\eta}_1) \otimes \phi_{\varepsilon_2 \lambda_2}(\boldsymbol{\eta}_2) \}_{l'_{12}, m'_{12}}. \quad (6)$$

The sum runs over only one energy quantum number  $\varepsilon_1$ , because according to the conservation of the total oscillator energy of the system  $\varepsilon_2 = e'_1 + e'_2 - \varepsilon_1$ . Now we introduce another set of Jacobian variables

$$\boldsymbol{\chi}_1 = \sqrt{\frac{d_1}{1+d_1}} \boldsymbol{\eta}_2 + \sqrt{\frac{1}{1+d_1}} \mathbf{r}'_3, \quad \boldsymbol{\chi}_2 = \sqrt{\frac{1}{1+d_1}} \boldsymbol{\eta}_2 - \sqrt{\frac{d_1}{1+d_2}} \mathbf{r}'_3 \quad (7)$$

and change the coupling scheme from  $\{ \{ \phi_{\varepsilon_1 \lambda_1}(\boldsymbol{\eta}_1) \otimes \phi_{\varepsilon_2 \lambda_2}(\boldsymbol{\eta}_2) \}_{l'_{12}, m'_{12}} \otimes \phi_{e'_3 l'_3}(\mathbf{r}'_3) \}_{l', m'}$  to  $\{ \phi_{\varepsilon_1 \lambda_1}(\boldsymbol{\eta}_1) \otimes \phi_{E_1 \mu_1}(\boldsymbol{\chi}_1) \otimes \phi_{E_2 \mu_2}(\boldsymbol{\chi}_2) \}_{l', m'}$ .

In this case the transformation matrix element is as follows:

$$\begin{aligned} & \{ \{ \phi_{\varepsilon_1 \lambda_1}(\boldsymbol{\eta}_1) \otimes \phi_{\varepsilon_2 \lambda_2}(\boldsymbol{\eta}_2) \}_{l'_{12} m'_{12}} \otimes \phi_{\varepsilon'_3 l'_3}(\mathbf{r}'_3) \}_{l' m'} = \sum_{E_1 \mu_1 \mu_2 l'_b} (-1)^{\lambda_1 + \lambda_2 + l'_3 + l'} \sqrt{(2l'_{12} + 1)(2l'_b + 1)} \\ & \times \left\{ \begin{matrix} \lambda_1 & \lambda_2 & l'_{12} \\ l'_3 & l' & l'_b \end{matrix} \right\} \langle E_1 \mu_1, E_2 \mu_2 : l'_b | \varepsilon_2 \lambda_2, \varepsilon'_3 l'_3 : l'_b \rangle_{d_1} \{ \phi_{\varepsilon_1 \lambda_1}(\boldsymbol{\eta}_1) \otimes \{ \phi_{E_1 \mu_1}(\boldsymbol{\chi}_1) \otimes \phi_{E_2 \mu_2}(\boldsymbol{\chi}_2) \}_{l'_b m'_b} \}_{l' m'}. \end{aligned} \quad (8)$$

After these changes the transformation Eq. (4) becomes

$$\begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ \mathbf{r}_3 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} & 0 \\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{\eta}_1 \\ \boldsymbol{\chi}_1 \\ \boldsymbol{\chi}_2 \end{pmatrix}. \quad (9)$$

As can be seen from Eq. (9), coordinates  $\mathbf{r}_3$  and  $\boldsymbol{\chi}_2$  are equal. It means that energies and angular momenta representing these coordinates are also equal:  $e_3 l_3 = E_2 \mu_2$ . The final transformation is transformation from the coordinates  $\boldsymbol{\eta}_1, \boldsymbol{\chi}_1$  to  $\mathbf{r}_1, \mathbf{r}_2$ , and its matrix element, with the help of the  $6j$  coefficients, is

$$\begin{aligned} & \{ \phi_{\varepsilon_1 \lambda_1}(\boldsymbol{\eta}_1) \otimes \{ \phi_{E_1 \mu_1}(\boldsymbol{\chi}_1) \otimes \phi_{\varepsilon_3 l_3}(\mathbf{r}_3) \}_{l'_b} \}_{lm} = \delta_{el, e'l'} (-1)^{\lambda_1 + \mu_1 + l'_3 + l} \sqrt{(2l'_b + 1)(2l_{12} + 1)} \\ & \times \left\{ \begin{matrix} \lambda_1 & \mu_1 & l_{12} \\ l_3 & l & l'_b \end{matrix} \right\} \langle e_1 l_1, e_2 l_2 : l_{12} | \varepsilon_1 \lambda_1, E_1 \mu_1 : l_{12} \rangle_d \{ \{ \phi_{e_1 l_1}(\mathbf{r}_1) \otimes \phi_{e_2 l_2}(\mathbf{r}_2) \}_{e_{12} l_{12}} \otimes \phi_{e_3 l_3}(\mathbf{r}_3) \}_{lm}. \end{aligned} \quad (10)$$

From Eq. (10) it can be seen that  $E_1 = e_1 + e_2 - \varepsilon_1$  and the sum over  $E_1$  vanishes. Now we can describe four-particle HO transformation brackets as products of matrix elements from Eqs. (6), (8), and (10):

$$\begin{aligned} & \langle \{ e_1 l_1, e_2 l_2 \}_{e_{12} l_{12}}, e_3 l_3 : l | \{ e'_1 l'_1, e'_2 l'_2 \}_{e'_{12} l'_{12}}, e'_3 l'_3 : l \rangle = (-1)^{l_3 + l'_3} \sqrt{(2l_{12} + 1)(2l'_{12} + 1)} \\ & \times \sum_{\varepsilon_1 \lambda_1 \lambda_2 l'_b \mu_1} (-1)^{(\lambda_2 + \mu_1)} (2l'_b + 1) \langle \varepsilon_1 \lambda_1, \varepsilon_2 \lambda_2 : l'_{12} | e'_1 l'_1, e'_2 l'_2 : l'_{12} \rangle_d \left\{ \begin{matrix} \lambda_1 & \lambda_2 & l'_{12} \\ l'_3 & l & l'_b \end{matrix} \right\} \\ & \times \langle E_1 \mu_1, e_3 l_3 : l'_b | \varepsilon_2 \lambda_2, e'_3 l'_3 : l'_b \rangle_{d_1} \left\{ \begin{matrix} \lambda_1 & \mu_1 & l_{12} \\ l_3 & l & l'_b \end{matrix} \right\} \langle e_1 l_1, e_2 l_2 : l_{12} | \varepsilon_1 \lambda_1, E_1 \mu_1 : l_{12} \rangle_d. \end{aligned} \quad (11)$$

### 3. Calculations

Using the above results we have developed a Fortran code for the HO transformation brackets. Such a computer code is needed because certain types of nuclear calculation require large matrices. Detailed information regarding calculation techniques for Clebsch–Gordan, binomial,  $6j$ , and  $9j$  coefficients can be obtained in our previous article [10]. For demonstration purposes of our code we have calculated the error  $\delta(E_0)$  for the HO energy  $E_0$  of the normalization condition of the HO transformation bracket matrix (Eq. (11)):

$$\begin{aligned} \delta(E_0) = & \sum_0^{E_0} \left[ \sum_{\bar{e}_1 \bar{l}_1 \bar{e}_2 \bar{l}_2 \bar{e}_{12} \bar{l}_{12} \bar{e}_3 \bar{l}_3} \langle \{ e_1 l_1, e_2 l_2 \}_{e_{12} l_{12}}, e_3 l_3 : l | \{ \bar{e}_1 \bar{l}_1, \bar{e}_2 \bar{l}_2 \}_{\bar{e}_{12} \bar{l}_{12}}, \bar{e}_3 \bar{l}_3 : l \rangle \right. \\ & \left. \times \langle \{ \bar{e}_1 \bar{l}_1, \bar{e}_2 \bar{l}_2 \}_{\bar{e}_{12} \bar{l}_{12}}, \bar{e}_3 \bar{l}_3 : l | \{ e'_1 l'_1, e'_2 l'_2 \}_{e'_{12} l'_{12}}, e'_3 l'_3 : l \rangle - \delta_{e_1 l_1 e_2 l_2 e_3 l_3, e'_1 l'_1 e'_2 l'_2 e'_3 l'_3} \right], \end{aligned} \quad (12)$$

where the sum runs over free parameters  $\bar{e}_1 \bar{l}_1 \bar{e}_2 \bar{l}_2 \bar{e}_{12} \bar{l}_{12} \bar{e}_3 \bar{l}_3$  of the normalization condition, taking all allowed values between 0 and  $E_0$ . The total number of HO brackets for a given value of  $E_0$  equals  $N(E_0)$ . Calculations have been performed on 2.2 GHz Athlon 32-bit personal computer, compiled with the GNU gfortran compiler with default settings, operating system is GNU/Linux. The processor time (in seconds) to perform these calculations is  $T(E_0)$ . The results of calculations are presented in Table 1.

Table 1. The total number of HO brackets  $N(E_0)$  for a given value of HO energy  $E_0$ , error  $\delta(E_0)$ , and computation time  $T(E_0)$  in seconds.

$E_0$	$N(E_0)$	$\delta(E_0)$	$T(E_0)$
3	7 345	$0.8878 \cdot 10^{-13}$	0.36
4	68 499	$0.3298 \cdot 10^{-12}$	6.05
5	580 473	$0.1061 \cdot 10^{-11}$	89
6	3 723 983	$0.5509 \cdot 10^{-10}$	1 009
7	21 299 949	$0.2164 \cdot 10^{-10}$	9 692
8	102 734 460	$0.1079 \cdot 10^{-9}$	81 942
9	448 443 764	$0.5667 \cdot 10^{-9}$	597 874

#### 4. Conclusions

Using Eq. (11) we have updated our earlier research [10] that was applicable only to the system of three particles. The current approach is suitable for fast and precise calculations of four-particle harmonic-oscillator transformation brackets. The numerical procedure is based on independent calculations of Clebsch–Gordan coefficients with zero-valued angular momentum projections, the  $6j$ ,  $9j$  symbols, and binomial coefficients [10], which are precalculated and stored in appropriate arrays.

#### Acknowledgement

This work was supported by the Lithuanian State Science and Studies Foundation under the project No. T-12/06.

#### References

- [1] V. Vanagas, *Algebraic Methods in Nuclear Theory* (Mintis, Vilnius, 1971) [in Russian].
- [2] G.P. Kamuntavičius, The reduced Hamiltonian method in the theory of the identical particle systems of bound states, *Sov. J. Part. Nucl.* **20**, 261–292 (1989).
- [3] P. Navratil, G.P. Kamuntavičius, and B.R. Barrett, Few-nucleon systems in a translationally invariant harmonic oscillator basis, *Phys. Rev. C* **61**, 044001 (2000).
- [4] I. Talmi, Nuclear spectroscopy with harmonic-oscillator wave-functions, *Helv. Phys. Acta* **25**, 185–234 (1952).
- [5] M. Moshinsky, Transformation brackets for harmonic-oscillator functions, *Nucl. Phys.* **13**, 104–116 (1959).
- [6] Yu.F. Smirnov, Talmi transformations for particles with different masses, *Nucl. Phys.* **27**, 177–187 (1961).
- [7] Yu.F. Smirnov, Talmi transformation for particles with different masses (II), *Nucl. Phys.* **39**, 346–352 (1962).
- [8] L. Trlifaj, Simple formula for the general oscillator brackets, *Phys. Rev. C* **5**, 1534–1539 (1972).
- [9] B. Buck and A.C. Merchant, A simple expression for the general oscillator bracket, *Nucl. Phys. A* **600**, 387–402 (1996).
- [10] G.P. Kamuntavičius, R.K. Kalinauskas, B.R. Barrett, S. Mickevičius, and D. Germanas, The general harmonic-oscillator brackets: Compact expression, symmetries, sums and Fortran code, *Nucl. Phys. A* **695**, 191–201 (2001).
- [11] A. Bandzaitis and D. Grabauskas, *Quantum Mechanics* (Mokslas, Vilnius, 1975) [in Lithuanian].
- [12] A.P. Jucys and A.A. Bandzaitis, *Theory of Angular Momentum in Quantum Mechanics* (Mokslas, Vilnius, 1977) [in Russian].

## KETURIŲ DALELIŲ SISTEMOS HARMONINIO OSCILIATORIAUS TRANSFORMACIJOS KOEFICIENTŲ SKAIČIAVIMAS

D. Germanas<sup>a</sup>, R.K. Kalinauskas<sup>a</sup>, S. Mickevičius<sup>b</sup>, R. Žemaičiūnienė<sup>c</sup>

<sup>a</sup> Fizikos institutas, Vilnius, Lietuva

<sup>b</sup> Vytauto Didžiojo universitetas, Kaunas, Lietuva

<sup>c</sup> Šiaulių universitetas, Šiauliai, Lietuva

#### Santrauka

Susirišusioms fizikinėms sistemoms, tarp jų ir atomo branduoliui, matematiškai aprašyti naudojamos transliaciškai invariantinės banginės funkcijos, priklausančios tik nuo sistemos vidinių laisvės laipsnių. Invariantiškumas pasiekiamas, pasirenkant erdvines bangines funkcijas, kurios priklauso nuo Jakobio koordinatų. Kiekvienai sistemai, kurios dalelių skaičius  $N > 2$ , egzistuoja daugiau kaip viena Jakobio koordinatų sistema. Bendru atveju pereinant nuo vienos Jakobio koordinatų sistemos prie kitos reikia begali-

nio funkcijos skleidinio narių skaičiaus. Tik harmoninio osciliatoriaus (HO) funkcijų atveju pakanka baigtinio funkcijos skleidinio narių skaičiaus. Pereinant nuo vienos Jakobio koordinatų sistemos prie kitos naudojami HO transformacijos koeficientai. Pateikta keturių dalelių sistemos HO transformacijos koeficientų išraiška (11), koeficientų skaičius esant tam tikrai sužadinto energijai, skaičiavimo tikslumas bei koeficientų skaičiavimo laikas naudojant 2,2 GHz Athlon 32 bitų asmeninį kompiuterį su GNU/Linux sistema.