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CALCULATION OF FOUR-PARTICLE HARMONIC-OSCILLATOR TRANSFORMATION BRACKETS

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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

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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 instrinsic 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.

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2. Formalism

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

$$|\{e_1l_1(\mathbf{r}_1),e_2l_2(\mathbf{r}_2)\}e_{12}l_{12},e_3l_3(\mathbf{r}_3):lm\rangle=\{\{\phi_{e_1l_1}(\mathbf{r}_1)\otimes\phi_{e_2l_2}(\mathbf{r}_2)\}_{e_{12}l_{12}}\otimes\phi_{e_3l_3}(\mathbf{r}_3)\}_{lm}$$

$$\times\sum_{m_1m_2m_{12}m_3}\begin{bmatrix}l_1 & l_2 & l_{12}\\ m_1 & m_2 & m_{12}\end{bmatrix}\begin{bmatrix}l_{12} & l_3 & l\\ m_{12} & m_3 & m\end{bmatrix}\phi_{e_1l_1m_1}(\mathbf{r}_1)\phi_{e_2l_2m_2}(\mathbf{r}_2)\phi_{e_3l_3m_3}(\mathbf{r}_3)\,, \tag{1}$$

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

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

where the corresponding dimensionless eigenvalue is equal to $(e+3/2)$ and the principal quantum number $n=(e-l)/2=0,1,2,\ldots$, 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:

$$|\{e_1l_1(\mathbf{r}_1),e_2l_2(\mathbf{r}_2)\}e_{12}l_{12},e_3l_3(\mathbf{r}_3):lm\rangle= \tag{3}$$

$$\sum_{e_1'l_1'e_2'l_2'e_{12}'l_{12}'e_3'l_3'}\big\langle\{e_1l_1,e_2l_2\}e_{12}l_{12},e_3l_3:l|\{e_1'l_1',e_2'l_2'\}e_{12}'l_{12}',e_3'l_3')\,:\,l\big\rangle|\{e_1'l_1'(\mathbf{r}_1),e_2'l_2'(\mathbf{r}_2)\}e_{12}'l_{12}',e_3'l_3'(\mathbf{r}_3):lm\big\rangle\,,$$

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:

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

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

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

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]:

$$\{\phi_{e_1'l_1'}(\mathbf{r}_1')\otimes\phi_{e_2'l_2'}(\mathbf{r}_2')\}_{l_{12}'m_{12}'}=\sum_{\varepsilon_1\lambda_1\lambda_2}\big\langle\varepsilon_1\lambda_1,\varepsilon_2\lambda_2:l_{12}'\big|e_1'l_1',e_2'l_2':l_{12}'\big\rangle_d\{\phi_{\varepsilon_1}\lambda_1(\boldsymbol{\eta}_1)\otimes\phi_{\varepsilon_2}\lambda_2(\boldsymbol{\eta}_2)\}_{l_{12}'m_{12}'}\,. \tag{6}$$

The sum runs over only one energy quantum number ε_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

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

and change the coupling scheme from $\{\{\phi_{\varepsilon_1\lambda_1}(\boldsymbol{\eta}_1)\otimes\phi_{\varepsilon_2\lambda_2}(\boldsymbol{\eta}_2)\}_{l_{12}'m_{12}'}\otimes\phi_{\varepsilon_3'l_3'}(\mathbf{r}_3')\}_{l'm'}$ to $\{\phi_{\varepsilon_1\lambda_1}(\boldsymbol{\eta}_1)\otimes\{\phi_{E_1\mu_1}(\boldsymbol{\chi}_1)\otimes\phi_{E_2\mu_2}(\boldsymbol{\chi}_2)\}_{l_b'm_b'}\}_{l'm'}$.

In this case the transformation matrix element is as follows:

$$\{\{\phi_{\varepsilon_1\lambda_1}(\boldsymbol{\eta}_1)\otimes\phi_{\varepsilon_2\lambda_2}(\boldsymbol{\eta}_2)\}_{l'_{12}m'_{12}}\otimes\phi_{\varepsilon'_3l'_3}(\mathbf{r}'_3)\}_{l'm'}=\sum_{E_1\mu_1\mu_2l'_b}(-1)^{\lambda_1+\lambda_2+l'_3+l'}\sqrt{(2l'_{12}+1)(2l'_b+1)}$$

$$\times\begin{Bmatrix}\lambda_1 & \lambda_2 & l'_{12}\\ l'_3 & l' & l'_b\end{Bmatrix}\langle E_1\mu_1,E_2\mu_2:l'_b|\varepsilon_2\lambda_2,\varepsilon'_3l'_3:l'_b\rangle_{d_1}\{\phi_{\varepsilon_1\lambda_1}(\boldsymbol{\eta}_1)\otimes\{\phi_{E_1\mu_1}(\boldsymbol{\chi}_1)\otimes\phi_{E_2\mu_2}(\boldsymbol{\chi}_2)\}_{l'_bm'_b}\}_{l'm'}\,. \quad (8)$$

After these changes the transformation Eq. (4) becomes

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

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: $e_3l_3=E_2\mu_2$. 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

$$\{\phi_{\varepsilon_1\lambda_1}(\boldsymbol{\eta}_1)\otimes\{\phi_{E_1\mu_1}(\boldsymbol{\chi}_1)\otimes\phi_{\varepsilon_3l_3}(\mathbf{r}_3)\}_{l'_b}\}_{lm}=\delta_{el,e'l'}(-1)^{\lambda_1+\mu_1+l'_3+l}\sqrt{(2l'_b+1)(2l_{12}+1)}$$

$$\times\begin{Bmatrix}\lambda_1 & \mu_1 & l_{12}\\ l_3 & l & l'_b\end{Bmatrix}\langle e_1l_1,e_2l_2:l_{12}|\varepsilon_1\lambda_1,E_1\mu_1:l_{12}\rangle_d\{\{\phi_{e_1l_1}(\mathbf{r}_1)\otimes\phi_{e_2l_2}(\mathbf{r}_2)\}_{e_{12}l_{12}}\otimes\phi_{e_3l_3}(\mathbf{r}_3)\}_{lm}\,. \quad (10)$$

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):

$$\langle\{e_1l_1,e_2l_2\}e_{12}l_{12},e_3l_3:l|\{e'_1l'_1,e'_2l'_2\}e'_{12}l'_{12},e'_3l'_3:l\rangle=(-1)^{l_3+l'_3}\sqrt{(2l_{12}+1)(2l'_{12}+1)}$$

$$\times\sum_{\varepsilon_1\lambda_1\lambda_2l'_b\mu_1}(-1)^{(\lambda_2+\mu_1)}(2l'_b+1)\langle\varepsilon_1\lambda_1,\varepsilon_2\lambda_2:l'_{12}|e'_1l'_1,e'_2l'_2:l'_{12}\rangle_d\begin{Bmatrix}\lambda_1 & \lambda_2 & l'_{12}\\ l'_3 & l & l'_b\end{Bmatrix}$$

$$\times\langle E_1\mu_1,e_3l_3:l'_b|\varepsilon_2\lambda_2,e'_3l'_3:l'_b\rangle_{d_1}\begin{Bmatrix}\lambda_1 & \mu_1 & l_{12}\\ l_3 & l & l'_b\end{Bmatrix}\langle e_1l_1,e_2l_2:l_{12}|\varepsilon_1\lambda_1,E_1\mu_1:l_{12}\rangle_d\,. \quad (11)$$

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)):

$$\delta(E_0)=\sum_0^{E_0}\Bigg[\sum_{\overline{e}_1\overline{l}_1\overline{e}_2\overline{l}_2\overline{e}_{12}\overline{l}_{12}\overline{e}_3\overline{l}_3}\langle\{e_1l_1,e_2l_2\}e_{12}l_{12},e_3l_3:l|\{\overline{e}_1\overline{l}_1,\overline{e}_2\overline{l}_2\}\overline{e}_{12}\overline{l}_{12},\overline{e}_3\overline{l}_3:l\rangle$$

$$\times\langle\{\overline{e}_1\overline{l}_1,\overline{e}_2\overline{l}_2\}\overline{e}_{12}\overline{l}_{12},\overline{e}_3\overline{l}_3:l|\{e'_1l'_1,e'_2l'_2)\}e'_{12}l'_{12},e'_3l'_3:l\rangle-\delta_{e_1l_1e_2l_2e_3l_3,e'_1l'_1e'_2l'_2e'_3l'_3}\Bigg], \quad (12)$$

where the sum runs over free parameters $\overline{e}_1\overline{l}_1\overline{e}_2\overline{l}_2$ $\overline{e}_{12}\overline{l}_{12}\overline{e}_3\overline{l}_3$ 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.

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KETURIŲ DALELIŲ SISTEMOS HARMONINIO OSCILIATORIAUS TRANSFORMACIJOS KOEFICIENTŲ SKAIČIAVIMAS

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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 koordinačių. Kiekvienai sistemai, kurios dalelių skaičius $N > 2$, egzistuoja daugiau kaip viena Jakobio koordinačių sistema. Bendru atveju pereinant nuo vienos Jakobio koordinačių sistemos prie kitos reikia begalinio funkcijos skleidinio narių skaičiaus. Tik harmoninio osciliatoriaus (HO) funkcijų atveju pakanka baigtinio funkcijos skleidinio narių skaičiaus. Pereinant nuo vienos Jakobio koordinačių sistemos prie kitos naudojami HO transformacijos koeficientai. Pateikta keturių dalelių sistemos HO transformacijos koeficientų išraiška (11), koeficientų skaičius esant tam tikrai sužadinimo energijai, skaičiavimo tikslumas bei koeficientų skaičiavimo laikas naudojant 2,2 GHz Athlon 32 bitų asmeninį kompiuterį su GNU / Linux sistema.