COMPUTATIONAL SCIENCE AND TECHNIQUES
Volume 7, 2020, 592-604

Publisher: Klaipėda University
http://journals.ku.lt/index.php/CST
Online ISSN: 2029-9966
DOI: 10.15181/csat.v7i0.1763

A ONE-PARTICLE GENERALIZED COEFFICIENTS OF FRACTIONAL PARENTAGE CALCULATION METHOD FOR ATOMIC NUCLEUS HARMONIC OSCILLATOR SHELL MODEL

Algirdas Deveikis
Department of Applied Informatics, Vytautas Magnus University,
Vileikos str. 8, LT-44404 Kaunas, Lithuania
algirdas.deveikis@vdu.lt

Abstract. A method for the calculation of the one-particle generalized coefficients of fractional parentage for an arbitrary number of *j*-orbits with isospin and an arbitrary number of oscillator quanta (generalized CFPs or GCFPs) is presented. The approach is based on a simple enumeration scheme for antisymmetric many-particle states, an efficient algorithm for the calculation of the CFPs for a single *j*-orbit with isospin, and a general procedure for the computation of the angular momentum (isospin) coupling coefficients describing the transformation between different momentum-coupling schemes. The method provides fast calculation of GCFPs for a given particle number and produces results possessing small numerical uncertainties. The introduced GCFPs make it feasible calculation of expectation values of one-particle nuclear shell-model operators within the isospin formalism.

Key words: atomic nuclear shell model, the harmonic oscillator basis, antisymmetric many-particle states, coefficients of fractional parentage, *jt*-coupling.

1. Introduction

The atomic nucleus harmonic oscillator (HO) shell model is widely used in present day calculations of nuclear properties. One ambitious project in large-scale nuclear calculations is the so-called *ab-initio* no-core shell model (NCSM) (Barrett et al., 2013). The *ab-initio* NCSM approach is known of its purity from a countless number of misleading modeling assumptions those severe aggravated its ancestors. The efficiency of NCSM calculations strongly depends on the scheme chosen to represent the many-particle basis states of nucleus. Until now, the most productive scheme for large-scale nuclear calculations is the simplest one, the so-called *m*-scheme, in which the many-particle basis states do not have a well-defined total angular momentum J (Navrátil et al., 2000). The main advantage of *m*-scheme approach is that it allows relatively easy to implement the antisymmetry of the many-particle basis states. However, the greatest disadvantage of the *m*-scheme basis is its exceptionally large dimension. Even for *ab-initio* NCSM calculations of light atomic nuclei, achieving convergence of results requires enormous computing resources far exceeding the possibilities of now day's supercomputers (Wang et al., 2016). An increasing number of particles and increasing of the maximum many-particle HO excitation energy (total oscillator quanta of excitations) $E_{\max}$ leads to an exponential increase in processing time and memory demands. For example, the calculations of the ^{6}Li nucleus were performed up to $E_{\max} = 18$ (Shin et al.,

2017) but more heavy nuclei with the atomic nucleus mass number values A = 18 and 19 were calculated only with E_{max} = 4 (Dikmen et al., 2015).

The well-known prescription of quantum physics to reduce the dimensionality of the problem is to impose on the basis states the characteristic symmetries of the many-particle system. However, the main deficiency of this way of solution is that the process of constructing the basis with additional symmetries is extremely complicated and difficult to perform. Nevertheless, numerous approaches beyond the *m*-scheme are now under development. The *ab-initio* symmetry-adapted no-core shell model takes advantage of symmetries inherent to the nuclear dynamics and classify the states according to the reduction of SU(3) group on SO(3) group (Dytrych et al., 2016). The method for constructing subspaces with well-defined total angular momentum by diagonalizing the J^2 operator in the *m*-scheme basis numerically has been demonstrated to work in (Aktulga et al., 2011). A large reduce of the model space has been achieved in Sp(3;R) symmetry-adapted basis (Draayer et al., 2008).

The traditional way of construction of shell model basis states for atoms and nuclei with any required symmetry uses the concept of coefficients of fractional parentage (CFPs). The foundation for this approach was developed in classical works (Bacher and Gousmit, 1934, Racah, 1943, Edmonds and Flowers, 1952, Redmond, 1954, de-Shalit and Talmi, 1963, Fano, 1965). The procedures for the evaluation of generalized CFPs for equivalent *p* shell, equivalent *d* shell and equivalent *f* shell electrons are presented in (Allison, 1969, Chivers, 1973, Allison and McNulty, 1974), the method for the calculation of CFPs for equivalent electrons in *jj*-coupling was developed by (Grant, 1972), and the procedure for the calculation of CFPs with well-defined seniority of identical fermion system was developed by (Wang et al. 1995). The symbolic techniques for analytical calculation of CFPs in *LS*-coupling and *jj*-coupling as well as in the isospin basis was implemented in (Gaigalas et al., 2001, Gaigalas et al., 2006, Fritzsche, 2009). To simplify the unique specification of the many-particle antisymmetrical states the additional integer quantum number (instead of precise labeling of the model wave-functions by quantum numbers of higher-order groups, such as seniority) was introduced for construction procedures of the CFPs by (Skouras and Kossionides, 1986), and (Kagawa 1992). One of the main disadvantages hindering the advantage of CFPs approach in the past is that their calculations are very time-consuming. However, for *ab initio* NCSM codes, the bottleneck is not floating point operations, but aggregate memory and memory access (Maris et al., 2012). This is the reason for the advent of the CFPs approach in the large-scale *ab-initio* NCSM calculations requiring the development of efficient algorithms of their run-time calculation instead of the traditional concept of their preliminary calculation and storage.

In this paper, we present a new method generating a list of one-particle generalized coefficients of fractional parentage (GCFPs) for an arbitrary number *j*-orbits with isospin and an arbitrary value of E_{max}. This is the coupled momentum approach that leads to the dimensions of the shell model basis that are at least an order of magnitude less than in the *m*-scheme (Dytrych et al., 2016). The method is based on the expression of the one-particle multishell coefficient of fractional parentage in terms of the single-shell coefficient of fractional parentage and the corresponding angular momentum coupling coefficient (Deveikis and Kamuntavičius, 1996). The efficiency of the method follows from the rejection of the higher-order group-theoretical classification of many-particle antisymmetrical

states simplifying the antisymmetrization procedure for *A*-particle states and to develop a simple enumeration scheme for antisymmetric many-particle states. Note that despite its simplicity, the adopted classification scheme of many-particle states have all quantum numbers that are used to specify the energy levels of nuclei: *J*, total isospin *T*, and parity $\Pi = (-1)^{E_{\max}}$. The introduced one-particle GCFPs are intended for the calculation of matrix elements of the physically relevant one-particle nuclear shell-model operators within the isospin formalism, such as nuclear magnetic and quadrupole moments.

The structure of this paper is as follows. The details of the method are presented in the next section. In section 3, we present the experiments for calculation of one-particle GCFPs and the investigation of the efficiency of the method. Finally, concluding remarks are given in section 4.

2. GCFPs Calculation Method

A simple and efficient approach for calculation of the CFPs for an arbitrary number of *j*-orbits with isospin, based on complete rejection of higher-order group-theoretical classification of many-particle antisymmetrical states, was introduced in (Deveikis and Kamuntavičius, 1995, Deveikis and Kamuntavičius, 1996). In this approach, *A*-particle antisymmetrical states are characterized by a set of quantum numbers containing the number of HO quanta *E*, the particle configuration *K* (a list of occupied *j*-orbits with a corresponding number of particles in each orbit and with a specified intermediate coupling), the total angular momentum *J*, the total isospin *T*, and only one additional integer quantum number $\Delta = 1 \dots r$, which is necessary for unambiguous enumeration of the states. Here *r* is the degeneracy of the many-particle antisymmetrical state characterized only by *EKJT* quantum numbers. By labeling of the model-space wave functions according to these quantum numbers, one obtains a great simplification of the one-particle GCFPs enumeration scheme. The one-particle GCFPs enable the antisymmetric *A*-particle oscillator wave-function Ψ to be expressed in terms of vector-coupled products of antisymmetric functions of (*A*-1) particles Φ and single particle wave functions ψ of *A*-th particle.

$$\Psi_{EK\Delta JT M_J M_T}(x_1 \dots x_A) = \sum_{\substack{\overline{(EK\Delta JT)} \\ (elj)_A}} \langle \overline{(EK\Delta JT)}; (elj)_A \| EK\Delta JT \rangle \times \left\{ \Phi_{\overline{(EK\Delta JT)}}(x_1 \dots x_{A-1}) \otimes \psi_{(elj)_A}(x_A) \right\}_{JT M_J M_T}. \quad (1)$$

A single bar over a list of quantum numbers marks the parent state with one particle removed. $(elj)_A$ denotes the *j*-orbit of the removed *A*-th particle. $\langle \dots ; \dots \| \dots \rangle$ is the one-particle GCFP. Semicolon means that the corresponding wave function is antisymmetric only with respect to permutations of the variables placed at the left-hand side of this sign. $\{\dots \otimes \dots\}_{JTM_J M_T}$ is a vector-coupled parent state function with the nonantisymmetrized last particle. The antisymmetric many-particle oscillator wave-functions are constructed from the eigenfunctions of the single-particle harmonic oscillator Hamiltonian, that in the *jj*-coupled representation are defined:

$$\psi_{eljtm_jm_t}(x) = R_{el}(r)\{Y_l(\hat{\vec{r}})\otimes\alpha_{1/2}(\vec{\sigma})\}_{jm_j}\alpha_{1/2m_t}(\vec{\tau}). \quad (2)$$

Here $R_{el}(r)$ is a radial function, $Y_{lm}(\hat{\vec{r}})$ is a spherical harmonics, $\alpha_{1/2m_s}(\vec{\sigma})$ is a spin-1/2 function in the spin space, and $\alpha_{1/2m_t}(\vec{\tau})$ is a spin-1/2 function in the isospin space. The single-particle variables are $x_i \equiv \vec{r}_i\vec{\sigma}_i\vec{\tau}_i$ (a set of the corresponding radius-vector, spin, and isospin variables).

The *e*, *l* and *j* are the principal, orbital, and total angular momentum quantum numbers, *m*, m_s, and m_j are the magnetic projection quantum numbers of orbital, spin, and total angular momentum, respectively. m_t is the projection of isospin *t* defined so that $m_t = +1/2$ corresponds to the neutron state and $m_t = +1/2$ to the proton state. Vector coupling of the angle and spin functions to form a state of a good total angular momentum is denoted by $\{\dots\otimes\dots\}_{jm_j}$. It should be stressed that practical calculations of GCFPs should imply the effective technique for management of all these quantum numbers in enumeration scheme for the shell model basis states of a nucleus.

The formula for the construction of multishell coefficients of fractional parentage was derived by (Levinson, 1957). Following his formula, there should be accomplished the separation of particle from the parent configuration in all possible ways consistent with the required triangular relations, thus producing the coupling coefficient describing the transformation between different momentum-coupling schemes. The coupling coefficients connect two vector-coupling schemes of subsystem angular momenta and can be written explicitly in terms of the Clebsch-Gordan expansion, as illustrated below for a case of three angular momenta:

$$\begin{aligned}\langle((j_1,j_2)j_{12},j_3)J|((j_3,j_2)j_{32},j_1)J\rangle \\ = \frac{1}{2j+1}\sum_{\substack{m_1m_2m_3\\ m_{12}m_{32}M}}\begin{bmatrix} j_1 & j_2 & j_{12}\\ m_1 & m_2 & m_{12}\end{bmatrix}\begin{bmatrix} j_{12} & j_3 & J\\ m_{12} & m_3 & M\end{bmatrix} \\ \times\begin{bmatrix} j_3 & j_2 & j_{32}\\ m_3 & m_2 & m_{32}\end{bmatrix}\begin{bmatrix} j_{32} & j_1 & J\\ m_{32} & m_1 & M\end{bmatrix}.\end{aligned} \quad (3)$$

Here j_1, j_2 and j_3 are the intermediate angular momenta. It is straightforward to generalize the expression (3) for the case of an arbitrary number of angular momenta and isospins. The great advantage of Levinson formula is that the definition of a one-particle GCFP contains only a single *j*-orbit CFP and the corresponding coupling coefficient, that is, no sum over any set of quantum numbers appear:

$$\langle\overline{(EK\Delta JT)};(eljt)_r\|EK\Delta JT\rangle$$
$$= (-1)^{\nu_r}\left(\frac{n_r}{A}\right)^{\frac{1}{2}}\langle(eljt)_r^{n_r-1}\overline{(\Delta JT)}_r;(eljt)_r\|(eljt)_r^{n_r}(\Delta JT)_r\rangle \quad (4)$$
$$\times\langle((J_1T_1\dots\overline{J_rT_r}\dots J_kT_k)\overline{JT},j_rt_r)JT|(J_1T_1\dots(\overline{J_rT_r},j_rt_r)J_rT_r\dots J_kT_k)JT\rangle.$$

Here $(eljt)_r^{n_r}$ denotes a single *j*-orbit with n_r particles in it. The subscript *r* refers to the *r*-th orbit in the configuration. It is also an orbit from which a particle is removed. *k* is the total number of *j* orbits. *r*-th $(eljt)_r$ specifies the quantum numbers of the *r*-th orbit from which the particle is removed. The phase factor $\nu_r = \sum_{i=r+1}^{k} n_i$, where the sum runs over all orbits standing to the right from the *r*-th orbit. A term having a form $\langle(eljt)_r^{n_r-1}\overline{(\Delta JT)}_r;(eljt)_r\|(eljt)_r^{n_r}(\Delta JT)_r\rangle$ denotes single *j*-orbit CFP. Their calculation is described in (Deveikis, 2002) and was implemented in the computer program CFPjOrbit in (Deveikis, 2005). The last bracketed term on the right side of (4) is the coupling coefficient. It describes a transformation from (a) the vector-coupling scheme where separated particle is coupled to the remaining particles in the same *j*-orbit forming a subsystem to (b) the coupling scheme where this separated particle is coupled to the vector-coupled subsystem of (*A* - 1) particles. In the definition of single *j*-orbit CFP and the coupling coefficient, the angular momenta (and isospins) are coupled from left to right and parentheses increase the priority.

Finally, the accuracy of GCFPs calculation is evaluated using their normalization condition:

$$\sum_{\substack{\overline{(EK\Delta JT)}\\(elj)_r}}\langle\overline{(EK\Delta JT)};(elj)_r\|EK\Delta JT\rangle^2 = 1. \quad (5)$$

This normalization condition serves as a sensitive test of correctness and completeness of the constructed GCFPs representing the shell model basis states of a nucleus.

3. Computational Experiments

The efficiency of the proposed method for the calculation of one-particle GCFPs (GCFP1s) for higher excitations was tested on i7 2.4 GHz PC with 8 GB RAM. The FORTRAN90 program for this method was run on Fortran PowerStation 4.0. We limit ourselves to examples for which the complete set of one-particle GCFPs can be calculated within our current limits of computing resources. The benchmark calculations for four representative nuclei subject to the current state-of-the-art *ab-initio* no-core nuclear shell model calculations were performed. Let us present the illustration of the performance of the method for the chosen nucleus atomic mass number values *A* in (Fig. 1).

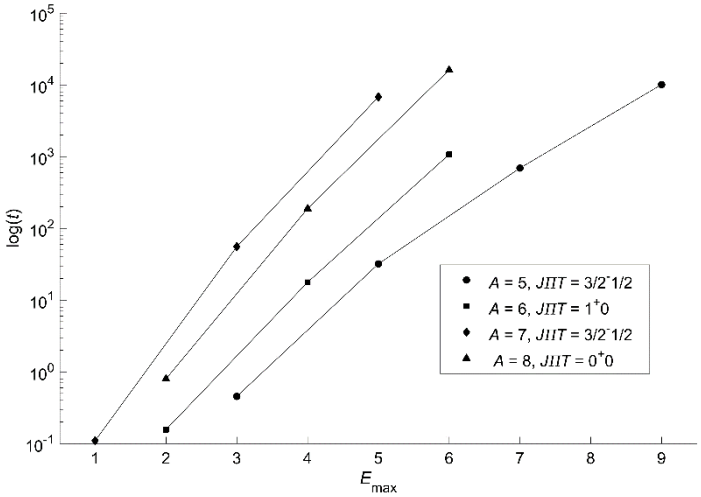

Figure 1. **The dependence of the processing time (in seconds) of GCFP1s on the maximum total oscillator quanta of excitations specified by E_{max}.**

In figure, the quantum numbers $J\Pi T$ specify the lowest energy level of the nucleus from isobaric spin multiplet with a given value of A: ^{5}He, ^{6}Li, ^{7}Li, and ^{8}Be. The points represent chosen sample cases and correspond to those listed in the legend. In this and in the following figures the presented results are connected by straight-line segments to guide the eye. It should be stressed that the observed processing time shows an exponential dependence on the maximum many-particle HO excitation energy $E_{\max}$. Nevertheless, this strong dependency does not point to the deficiency of the presented method, but is rather quite common feature of the *ab-initio* NCSM calculations.

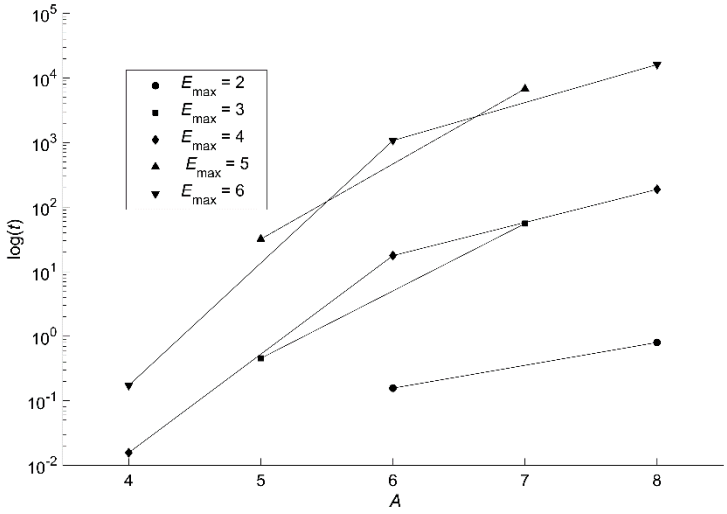

Figure 2. **The dependence of the processing time (in seconds) of GCFP1s on the atomic mass number specified by A.**

The dependence of the processing time on A for selected $E_{\max}$ values is presented in (Fig. 2). The calculations are performed for the same nuclei as those presented in (Fig. 1), except that the results corresponding to the ground state $J\Pi T = 0^{+}0$ of ^{4}He are included.

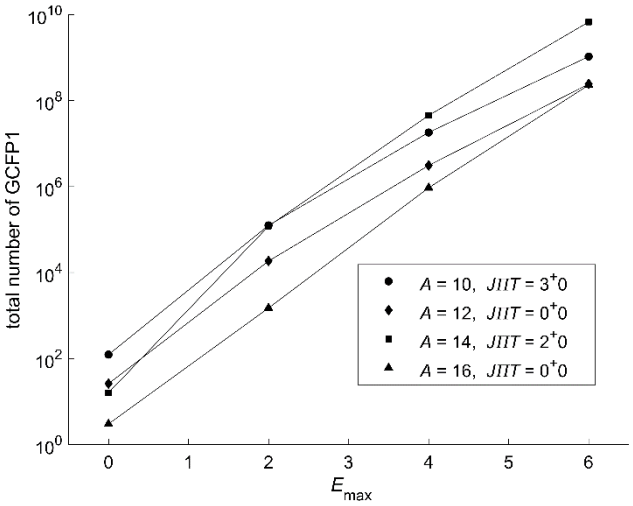

Figure 3. **The total number of GCFP1s as a function of the maximum total oscillator quanta of excitations specified by E_{max}.**

In these calculations, the approximately exponential character of the dependence of the processing time on A is established as in the previous case. Therefore, the processing time of one-particle GCFPs calculations depends exponentially on two parameters: the number of nucleons A and the maximum many-particle HO excitation energy $E_{\max}$. It should be highlighted that this quick grow of processing time shows the scale of the problem and is one of the main reasons why the *ab-initio* NCSM applications are restricted in most cases for *p*-shell nuclei calculations.

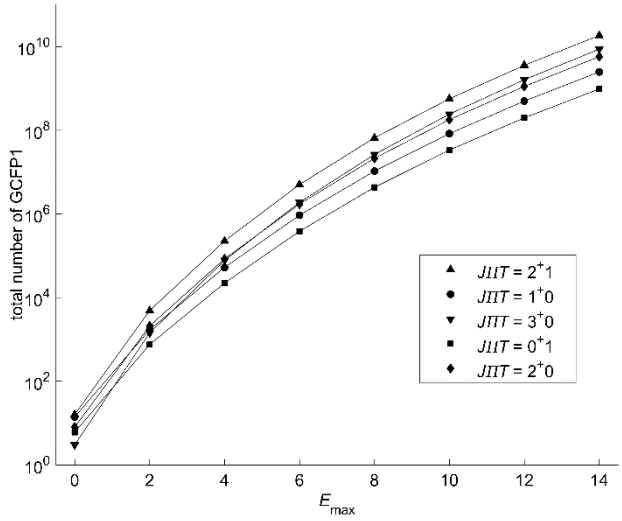

Figure 4. **Calculated total number of GCFP1s as a function of the maximum total oscillator quanta of excitations $E_{\max}$, for selected sample cases displayed in the legend.**

The important characteristic of the GCFPs calculation method is the number of coefficients it produces for the given nuclear states. The total number of one-particle GCFPs in the complete set of them for the chosen nucleus mass number values A is displayed in (Fig. 3).

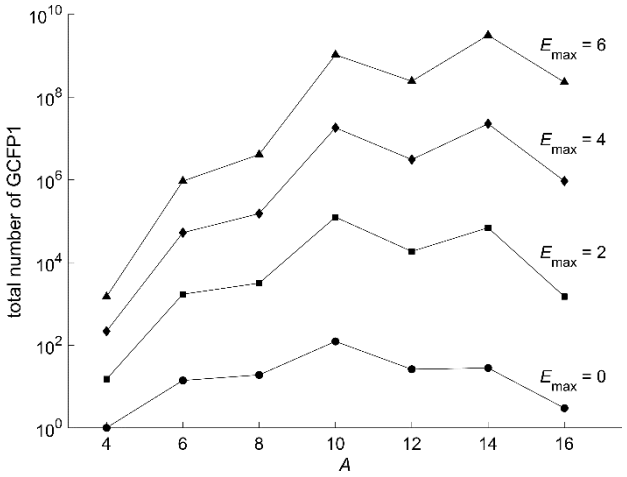

Figure 5. **Calculated total number of GCFP1s as a function of atomic mass number *A* at various values of the maximum total oscillator quanta of excitations E_{max}.**

Here are shown the quantum numbers $J\Pi T$ specify the lowest energy level of the nucleus from isobaric spin multiplet with a given value of *A*: ^{10}B, ^{12}C, ^{14}N, and ^{16}O. The obtained dependencies imply that the total number of GCFPs does not necessary grows monotonically with the value of *A*. The observed complicated interplay of the total number of GCFP1s with *A* is determined by the closing of the *p*-shell for a given nucleus.

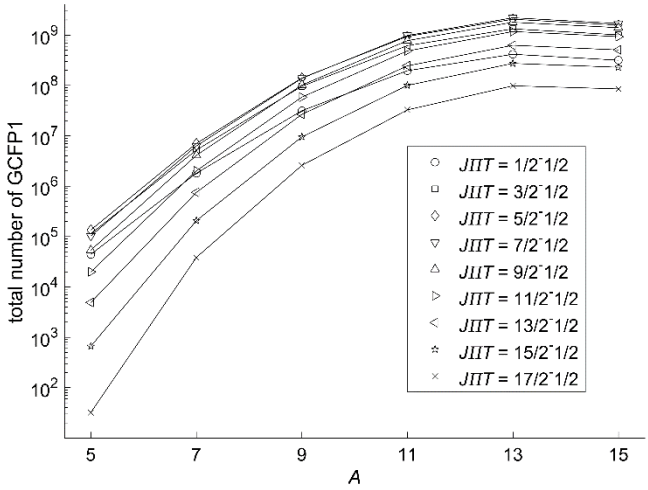

Figure 6. **Calculated total number of GCFP1s as a function of atomic mass number *A* at various values of the total angular momentum and fixed total isospin of the nucleus.**

One of the main advantages of the coefficients of fractional parentage approach is the possibility to perform the shell model calculations separately for every particular nuclear state. Here, the shell model basis is factored in separate subspaces and the dimensionality of the problem is effectively reduced. For illustrative purposes and data comparability, the total number of one-particle GCFPs for lower part of ^{6}Li spectra are presented in (Fig. 4). In these graphics, it can be seen that the obtained total number of one-particle GCFPs show complicated dependency on the E_{max} and do not follow the actual sequence of levels: $J\Pi T = 1^{+}0, 3^{+}0, 0^{+}1, 2^{+}0, 2^{+}1$.

The influence of the nonmonotonic character of *p*-shell closing on the total number of one-particle GCFPs is illustrated in (Fig. 5). The obtained significant relative reduce of the total number of one-particle GCFPs for values of A = 4, 8, 12, 16 should be associated with the well-known effect of α-clasterization in atomic nuclei. So this type of calculation is valuable for recognition and investigation of nuclear clasterization phenomena.

The dependence of the total number of one-particle GCFPs on the total angular momentum when the total isospin of the nucleus is fixed is displayed in (Fig. 6). The decrease in the slope of the dependencies with an increasing number of nucleons is related to the closing of the *p*-shell. This effect decreases the number of combinatorial combinations of single-particle states that should form the given many-particle nuclear state. At the same time the combinatorics produces more combinations of single-particle states for middle values of the total angular momentum and gives a larger number of corresponding one-particle GCFPs.

The opposite type of dependency when the total isospin vary but total angular momentum is fixed is illustrated in (Fig. 7). In figure, the *p*-shell closing effect on the obtained dependencies is observed as in the previous case. The decreasing value of one-particle GCFPs with isospin should be related to the larger difference in the number of protons and neutrons for a given nucleus. The obtained results imply that nuclei with a more equal number of protons and neutrons have a larger number of one-particle GCFPs. It is well-known that more stable light nuclei are characterized by the close numbers of protons and neutrons. So the number of GCFPs is related to the stability of the nucleus.

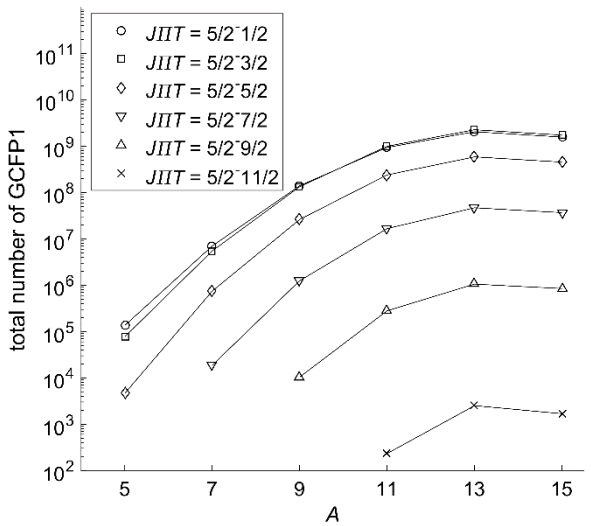

Figure 7. **Calculated total number of GCFP1s as a function of atomic mass number A at various values of the total isospin and fixed total angular momentum of the nucleus.**

In Table 1, we give the accuracies of our one-particle GCFPs for $J\Pi T = 0^+1$ state of the ^{6}Li nucleus for up to the E_{max} = 8. The columns of the table are: E_{max} is the number of excitation quanta; #shells is the total number of *j*-shells; #terms is the total number of terms; #CFPs is the total number of single *j*-orbit CFPs involved in the calculation of the corresponding GCFPs; #confs is the total number of calculated configurations; #GCFPs is the total number of one-particle GCFPs for all configurations; *accuracy* is the accuracy of one-particle GCFPs computation; *time* is the program running time.

Table 1. The A = 6, $J\Pi T = 0^+1$ calculation data of one-particle GCFPs for up to $8\hbar\omega$ excitation quanta.

E_{max}	#shells	#terms	#CFPs	#confs	#GCFPs	*accuracy*	*time*
0	3	11	11	2	6	1.33E-15	–
1	3	17	25	6	75	2.89E-15	–
2	4	32	57	18	752	4.88E-15	–
3	4	38	83	40	3998	4.88E-15	–
4	5	63	149	96	22190	6.44E-15	6.0 s
5	5	60	137	197	96706	7.33E-15	50.0 s
6	6	100	348	401	383830	8.66E-15	6.7 min
7	6	123	453	760	1407064	9.77E-15	38.5 min
8	6	172	1008	1412	4310601	1.39E-14	2.8 h

The accuracy of the one-particle GCFPs calculation was evaluated by testing the orthonormality condition (5) for a set of GCFPs in the listed nuclear state. Considering that calculations were performed on a personal computer, the obtained accuracy and computation time of the calculated one-particle GCFPs is very high.

The proposed method for one-particle GCFPs calculation is applicable not only for light nuclei, but also for heavier nuclei. However, since the running time depends strongly on the number of nucleons A and the excitation energy of the system E_{max}, we present here the illustration only for zero number of excitation quanta. For example, the A = 24 nucleon nucleus with JT = 01 took approximately 27 s at E_{max} = 0. For comparison, the computation of the A = 46 nucleon nucleus with JT = 01 on the same machine requires approximately 3.1 h at E_{max} = 0. These results are quite impressive, considering the used computing resources.

Note that the restriction to A and E_{max} for calculations of higher j-orbits is related to the efficiency and accuracy of the available 6j, Clebsch-Gordan and single j-orbit CFPs subroutines for large momenta. At this time, the subroutine for calculation of single j-orbit CFPs allows computation of full sets of GCFPs up to the j = 9/2 orbit. The higher orbits cannot get full, however this is not the critical restriction to the present day *ab-initio* NCSM calculations. It is worth noting that the real efficiency of the presented method for one-particle GCFPs calculation should be revealed in calculations on super-computers.

4. Conclusions

A new method for the calculation of one-particle generalized coefficients of fractional parentage for an arbitrary number of *j*-orbits with isospin has been developed and experimentally investigated by solving different instances of the problem of the construction of many-particle basis for nuclear shell model. A distinct feature of this method is in the complete rejection of group-theoretical classification of antisymmetric many-particle states. By rejecting the precise labeling of the model-space wave functions according to quantum numbers of higher-order groups, such as seniority, we obtain a great simplification of the GCFPs construction procedure and considerably extend the scale of the calculations. The results of the experimental investigation of the proposed method showed that the accuracy of the calculated one-particle GCFPs is very high and is more than sufficient for large-scale shell-model calculations. The important advantage of our method is its universality. The application of the method does not require special preparations of the calculation procedure for every different instance of the problem. The couplings of the nucleons moments and enumeration of the antisymmetric many-particle states are realized for an arbitrary number of orbits, nucleons, and harmonic oscillator quanta. Therefore, the new generalized coefficients of fractional parentage calculation method is valuable for the development of effective and universal large-scale nuclear computation schemes of light as well as heavy nuclei.

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A. Deveikis is an associate professor at the Department of Applied Informatics, Faculty of Informatics, Vytautas Magnus University. He received a PhD degree (Physics) in 1996 from Vytautas Magnus University, Kaunas, Lithuania. His research interests include iteration schemes of continuous analog of the Newton method, antisymmetrization of many-particle basis and calculation of matrix eigenvalues algorithms, numerical modeling of light atomic nuclei and few body systems.

VIENDALELIŲ APIBENDRINTŲ KILMINIŲ KOEFICIENTŲ SKAIČIAVIMO METODAS ATOMO BRANDUOLIO HARMONINIO OSCILIATORIAUS SLUOKSNIŲ MODELIUI

Algirdas Deveikis

Santrauka

Straipsnyje siūlomas naujas metodas skaičiuoti viendaleliams apibendrintiems kilminiams koeficientams esant bet kokioms nuklonų konfigūracijoms ir bet kokiai osciliatorinio sužadinimo energijai. Metodo, grįsto paprasta antisimetrinių daugiadalelių būsenų klasifikavimo schema ir universalia vektorinių momentų perrišimo procedūra, efektyvumas vertinamas sprendžiant įvairius daugiadalelių antisimetrinių banginių funkcijų bazės sudarymo uždavinius, aktualius *ab-initio* atomo branduolio sluoksnių modelio skaičiavimams. Eksperimentinio tyrimo rezultatai parodė, kad siūlomas kilminių koeficientų sudarymo metodas efektyviai sprendžia minėtus uždavinius, vertinant pagal pilnos bazės normavimo tikslumą.

Pagrindiniai žodžiai: atomo branduolio sluoksnių modelis, harmoninio osciliatoriaus būsenų bazė, antisimetrinės daugiadalelės būsenos, kilminiai koeficientai, *jt*-ryšys