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КОМПЬЮТЕРНЫЕ ТЕХНОЛОГИИ В ФИЗИКЕ

ELIMINATION OF THE CENTRE-OF-MASS MOTION IN THE NUCLEAR SHELL MODEL WITH ISOSPIN

A. Deveikis [1], *A. Fedurtsya* [2]

Department of Applied Informatics, Vytautas Magnus University, Kaunas, Lithuania

An efficient procedure for large-scale calculations of the two-particle translational invariant coefficients of fractional parentage (CESOs) for several j-shells with isospin is presented. The approach is based on a simple enumeration scheme for antisymmetric many-particle states and efficient algorithms for calculation of the coefficients of fractional parentage for a single j-shell and several j-shells with isospin. The CESOs may be obtained by diagonalizing the centre-of-mass Hamiltonian in the basis set of antisymmetric A-particle oscillator functions with singled out dependence on intrinsic coordinates of two last particles and choosing the subspace of its eigenvectors corresponding to the minimal eigenvalue equal to $3/2$. An arbitrary number of oscillator quanta can be involved. The characteristics of the introduced CESO's basis are investigated.

Представлена эффективная процедура расчета двухчастичных трансляционно-инвариантных генеалогических коэффициентов (CESOs) для нескольких j-орбит с изоспином. Подход основан на простом методе классификации многочастичных состояний и эффективных процедурах расчета генеалогических коэффициентов как для одной, так и для нескольких j-орбит с изоспином. Расчет CESOs производится путем диагонализации матрицы гамильтониана центра масс ядра, рассчитанной на A-частичных осцилляторных функциях с выделенной зависимостью от внутренних координат двух последних частиц, и выделения подпространства собственных векторов, соответствующих минимальному собственному значению $3/2$. Представленная процедура применима для любого числа осцилляторных квантов. Исследуются характеристики введенного базиса CESOs.

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INTRODUCTION

The calculations of light atomic nuclei properties should obey the principle of translational invariancy. One of the most known problems in which resolution assists the principle of translational invariancy is the problem of spurious states elimination in the nuclear spectra. In the last decade, significant progress in the nuclear calculations of light atomic nuclei presents the m-scheme method of *ab initio* No Core Nuclear Structure calculations [1]. It is a method to solve the full A-body problem for a system of nonrelativistic particles that interact by realistic two- plus three-body forces. However, this method is not explicitly translationally invariant and even does not follow the coulped momentum approach. The main

[1] E-mail: a.deveikis@if.vdu.lt
[2] E-mail: anton@fedurtsya.com

goal of this paper is to present the efficient procedure for large-scale calculations of the two-particle translational invariant coefficients of fractional parentage (CESOs) for several j-shells with isospin. Introducing translational invariant coefficients of fractional parentage instead of m-scheme basis (Slater determinants) may significantly reduce the dimensions of the diagonalized Hamiltonian matrices. In order to simplify shell-model states classification and formation algorithms, the many-particle antisymmetrical states are characterized only by well-defined set of quantum numbers: the configuration K (with a specified intermediate coupling), the total angular momentum J, the total isospin T, and one additional integer quantum number which is necessary for unambiguous enumeration of the states. Rejection of the higher-order group-theoretical classification of many-particle antisymmetrical states allows one to significantly simplify the antisymmetrization procedure for A-particle states. The efficiency of the proposed procedure for calculation of coefficients of fractional parentage uprises from the possibility to perform the calculation of translationally invariant CFPs in the ordinary one-particle basis. The introduced CESOs may be used most effectively for *ab initio* No Core Nuclear Structure calculations with oscillator intrinsic density matrices within the framework of Reduced Hamiltonian Method (RHM) [2].

1. DEFINITION OF CESOs

Since the antisymmetrization procedure is rather cumbersome in Jacobi coordinates, it is convenient to introduce the expansion of the product of centre-of-mass ground-state function and intrinsic harmonic oscillator wave function in terms of antisymmetric but not translationally invariant shell model wave functions [3]

$$\Psi_{00}(\boldsymbol{\xi}_0)\Psi_{E\Gamma JTM_JM_T}(\xi_1 \cdots \xi_{A-1}) = \sum_{K\Delta} \Psi_{EK\Delta JTM_JM_T}(x_1 \cdots x_A) a^{EJT}_{K\Delta;00,\Gamma}. \qquad (1)$$

Here $\Psi_{00}(\boldsymbol{\xi}_0)$ is the nucleus centre-of-mass ground-state wave function with principal and orbital angular momentum quantum numbers equal to zero. The summation in this formula runs over all configurations K and additional quantum number Δ (Γ is the additional quantum number for differentiation of translationally invariant states). The functions from the subspace of the nonspurious motion are the eigenfunctions of the centre-of-mass Hamiltonian. Thus, the coefficients of this expansion $a^{EJT}_{K\Delta;00,\Gamma}$ can be obtained by diagonalizing the centre-of-mass Hamiltonian in the basis of osillator shell-model wave functions $\Psi_{EK\Delta JTM_JM_T}\ (x_1 \cdots x_A)$.

The expectation value of the two-particle operator (centre-of-mass Hamiltonian) can be obtained by expressing them in the single-particle form. This may be accomplished by means of Jacobi coordinates

$$\begin{cases} \boldsymbol{\xi}_{-1} = \dfrac{1}{\sqrt{2}}(\mathbf{x}_{(A-1)} + \mathbf{x}_A), \\ \boldsymbol{\xi}_2 = \dfrac{1}{\sqrt{2}}(\mathbf{x}_{(A-1)} - \mathbf{x}_A). \end{cases} \qquad (2)$$

The antisymmetric two-particle oscillator shell model functions may be expanded in terms of vector coupled products of the functions depending on the intrinsic Jacobi variable $\boldsymbol{\xi}_2$ with

the functions depending on the Jacobi coordinate with the nonpositive index $\boldsymbol{\xi}_{-1}$

$$|((elj)_{A-1},(elj)_A)J''T''\rangle = \sum_{(el)_{-1},elsj} |((el)_{-1},elsj)J''T''\rangle\times$$
$$\times\,\langle((elj)_{A-1},(elj)_A)J''T''||((el)_{-1},elsj)J''T''\rangle. \quad (3)$$

Here the coefficients for the transition from the antisymmetrical two-particle shell model functions to the function of $\boldsymbol{\xi}_2$ are introduced [4] and further will be called Jacobi coefficients. It is convenient to introduce the coefficients of expansion of the oscillator shell model functions in terms of the ones with singled out dependence on the intrinsic coordinates of two last particles (SCFPs)

$$\langle\overline{\overline{(EK\Delta JT)}};((el)_{-1},elsj)J''T''||EK\Delta JT\rangle =$$
$$= \sum_{(elj)_{A-1},(elj)_A} \langle\overline{\overline{(EK\Delta JT)}};\ ((elj)_{A-1},(elj)_A)J''T''||EK\Delta JT\rangle\times$$
$$\times\,\langle((elj)_{A-1},(elj)_A)J''T''|((el)_{-1},elsj)J''T''\rangle. \quad (4)$$

Here is expansion in terms of two-particle multishell CFPs [5]. The procedure for spurious state elimination is based on projecting out the unexcited centre-of-mass subspace by diagonalizing centre-of-mass Hamiltonian matrix in the basis of the antisymmetric A-particle oscillator functions with singled out dependence on intrinsic coordinates of two last particles — SCFPs [3]

$$\langle EK\Delta JT|\frac{H_{\rm cm}}{\hbar\omega}|EK'\Delta'JT\rangle = (E+3/2)\,\delta_{K\Delta,K'\Delta'} -$$
$$-\,(A-1)\sum_e e \sum_{\overline{\overline{(EK\Delta JT)}}} \sum_{(el)_{-1},lsj,J''T''} \times$$
$$\times\,\langle\overline{\overline{(EK\Delta JT)}};\ ((el)_{-1},elsj)J''T''||EK\Delta JT\rangle\times$$
$$\times\,\langle\overline{\overline{(EK\Delta JT)}};\ ((el)_{-1},elsj)J''T''||EK'\Delta'JT\rangle. \quad (5)$$

The real symmetric centre-of-mass Hamiltonian matrix is expressible as the spectral decomposition of idempotent matrices that may be expressed in terms of the original matrix and its eigenvalues

$$\mathbf{P}_\alpha = \prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{s}\left(\lambda_\beta - \frac{\mathbf{H}_{\rm cm.}}{\hbar\omega}\right)\Bigg/\prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{s}(\lambda_\beta-\lambda_\alpha)\,. \quad (6)$$

The diagonalization of P matrices was performed with `rs()` procedure from EISPAC and obtained eigenvectors are coefficients $a^{EJT}_{K\Delta;00,\Gamma}$.

CESOs are the coefficients of expansion of the oscillator shell model functions in terms of A-particle oscillator functions with singled-out dependence on intrinsic coordinates of two

last particles and with eliminated spurious states

$$\overline{\overline{\langle (EK\Delta JT)};\ ((el)_{-1}, elsj)J''T''||E\Gamma JT\rangle} = \\ = \sum_{K\Delta} \overline{\overline{\langle (EK\Delta JT)};\ ((el)_{-1}, elsj)J''T''||EK\Delta JT\rangle} a^{EJT}_{K\Delta;00,\Gamma}. \quad (7)$$

The accuracy of CESOs calculation may be evaluated using their normalization condition

$$\sum_{\substack{\overline{\overline{(EK\Delta JT)}} \\ (el)_{-1}, elsj, J''T''}} \overline{\overline{\langle (EK\Delta JT)};\ ((el)_{-1}, elsj)J''T''||E\Gamma JT\rangle} \times \\ \times \overline{\overline{\langle (EK\Delta JT)};\ ((el)_{-1}, elsj)J''T''||E\Gamma' JT\rangle} = \delta_{\Gamma,\Gamma'}. \quad (8)$$

2. CALCULATIONS AND RESULTS

The efficiency of the proposed procedure for calculation of CESOs for higher excitations was tested on Pentium 3 GHz PC with 1 GB RAM. The FORTRAN90 program for CESOs calculation were run on Fortran PowerStation 4.0. The computational results for $A = 6$, $JT = 10$ and $A = 11$, $JT = 1/2\ 3/2$ are presented in Tables 1 and 2, correspondingly. The columns of the tables are: E is the number of excitation quanta; #GCFP is the number of two-particle multishell CFPs; #J is the number of the Jacobi coefficients; #SCFP is the number of SCFPs; $H_{\rm cm}$ is the dimension of centre-of-mass Hamiltonian matrix; P is the rank of P matrix; $\#a$ is the number of $a^{EJT}_{K\Delta;00,\Gamma}$ coefficients; #CESO is the number of CESOs; accuracy is the accuracy of CESOs computation; time is the computing time of CESOs computation procedure.

Table 1. **The $A = 6$, $JT = 10$ calculation data of CESOs for up to 5 excitation quanta**

E	#GCFP	#J	#SCFP	$H_{\rm cm}$	P	$\#a$	#CESO	Accuracy	Time
0	44	32	72				138	3.33E–15	
1	538	80	1098	15	11	165	3223	3.99E–15	
2	5540	172	13655	77	45	3465	61200	9.10E–15	3 s
3	33697	332	99842	283	136	38488	681632	1.33E–14	66 s
4	180911	592	664893	955	387	369585	6228765	2.50E–14	32.3 min
5	799357	992	3610794	2774	950	2635300	43792150	4.24E–14	14 h

Table 2. **The $A = 11$, calculation data of CESOs for up to 2 excitation quanta**

E	#GCFP	#J	#SCFP	$H_{\rm cm}$	P	$\#a$	#CESO	Accuracy	Time
0	829	32	1740				4875	3.99E–15	
1	53960	80	124679	89	77	6853	1246014	1.44E–14	2 min
2	1391178	172	3642641	836	623	520828	82169962	3.66E–14	15 h

CONCLUSION

The considered calculation procedure for evaluation of two-particle translationally invariant coefficients of fractional parentage for higher excitations (CESOs) has good perspectives for calculation of intrinsic density matrices and matrix elements of two-particle nuclear shell-model operators within the isospin formalism. The proposed procedure consistently outlines the principles of antisymmetrization and translational invariancy. A distinct feature of this procedure is the complete rejection of group-theoretical classification of antisymmetric many-particle states. This is remarkable, because a benefit could be gained due to simplicity and comprehensibility of such a kind of calculations. The efficiency of the proposed procedure was illustrated by calculation of CESOs in a complete $0-5\hbar\omega$ basis for ^{6}Li and in a complete $0-2\hbar\omega$ basis for ^{11}Be nuclei. The accuracy of calculated CESOs is extremely high ($\approx 10^{-13}$). At the same time, the dimensions of matrices involved (centre-of-mass Hamiltonian) are very low. It should be noted that, as is common in the *ab initio* shell-model calculations, the CESO's calculation time grows exponentially with the number of nucleons and the excitation energy. However, due to the simplified method for enumeration of A-particle states, the effective classification procedures of A-particle states may be applied and computation of CESOs may be efficiently managed.

REFERENCES

1. *Navratil P. et al.* The Reduced Hamiltonian Method in the Theory of the Identical Particles Systems Bound States // J. Phys. G: Nucl. Part. Phys. 2009. V. 36. P. 083101.

2. *Kamuntavicius G. P.* The Reduced Hamiltonian Method in the Theory of the Identical Particles Systems Bound States // Sov. J. Part. Nucl. 1989. V. 20, No. 2. P. 261–292.

3. *Deveikis A., Kamuntavicius G. P.* Elimination of Spurious States of Oscillator Shell Model // Lithuan. Phys. J. 1997. V. 37, No. 5. P. 371–383.

4. *Deveikis A., Kamuntavicius G. P.* Intrinsic Density Matrices of the Nuclear Shell Model // Lithuan. Phys. J. 1996. V. 36, No. 2. P. 83–95.

5. *Deveikis A., Juodagalvis A.* A Computer Program for Two-Particle Generalized Coefficients of Fractional Parentage // Comp. Phys. Commun. 2008. V. 179. P. 607–613.