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EFFECTIVE ALGORITHM FOR CALCULATION OF PROTONS AND NEUTRONS DISTRIBUTIONS IN ATOMIC NUCLEUS SHELLS

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Abstract. This paper presents the protons and neutrons distributions in atomic nucleus shells calculation algorithm which may be used for ab initio no-core nuclear shell model computations. The problem of enumeration of many-particle states is formulated on energetic basis instead of application of the traditional scheme for states classification. The algorithm provides calculations of protons and neutrons occupation restrictions for nuclear shells for an arbitrary number of oscillator quanta. The reported results show that the presented algorithm significantly outperforms the traditional approach and may fit the needs of state-of-the-art no-core shell model calculations of atomic nuclei.

Key words: atomic nuclear shell model, harmonic oscillator basis, antisymmetric many-particle states, combinatorial optimization

Introduction

The *ab initio* no-core shell model (NCSM) (Barrett et al., 2013) is one of the leading methods used to calculate the spectroscopic properties of light nuclei. This approach is aimed at the exact solution of the full many-particle problem for a system of nonrelativistic particles interacting with realistic inter-nucleon forces. One of the main advantages of *ab-initio* approaches is that they allow a physical insight of the results of large-scale calculations and elimination of the influence of a very large number of modelling assumptions. In the framework of *ab initio* NCSM, the *m*-scheme approach is widely used, in which the many-particle Schrödinger equation is solved using the large Slater determinant harmonic oscillator (HO) basis (Navrátil et al., 2000). The HO basis space dimension grows rapidly with achieving convergence of results and provide a major technical challenge (Wang et al., 2016). For example, until now the nuclei with the atomic nucleus mass number values A = 18 and 19 are calculated only with the maximum many-particle HO excitation energy E_{max} = 4 (Dikmen et al., 2015). Thus *ab initio* NCSM is actually limited only to light atomic nuclei, where calculations with higher values of E_{max} can be performed: for ^{7}Be and ^{7}Li nuclei E_{max} = 16 were achieved (Heng et al., 2017) and for the ^{6}Li nucleus the calculations were performed up to E_{max} = 18 (Shin et al., 2017). Therefore, further progress in the application of NCSM for the calculation of many-particle quantum systems should be supported by the development of new significantly more effective calculation techniques.

In particular, significant efforts in the *ab initio* NCSM *m*-scheme calculations are usually devoted to the initialization of a large number of characteristic parameters of *m*-scheme basis space that are used to set up the many-particle basis space and the management of computing resources. The aim of this work is to present an efficient algorithm that calculates the characteristic parameters of proton and neutron distributions in atomic nucleus shells for NCSM *m*-scheme calculations. The determination of the complete list of these distributions by considering the constraints imposed by the Pauli principle as well as the maximum many-particle HO excitation energy, is a well-known NP-complete problem. The traditional solution of which, based on the single-particle states treatment, is unacceptably slow for large values of A and E_{max} (Fedurtsya and Deveikis, 2011). The development of an efficient procedure for automatic calculation of input parameters for the NCSM *m*-scheme calculations may significantly facilitate the application of these calculations.

The structure of this paper is as follows. The details of the algorithm are presented in the next section. In section 3 we present the experiments for calculation of proton and neutron distributions in the shells of atomic nuclei. Finally, concluding remarks are given in section 4.

2. Protons and neutrons distributions algorithms

In the HO nuclear shell model a many-particle state consists of a number of single-particle states that can be occupied either by neutrons or protons. The most important from a computational point of view is that the number of possible single particle states has a significant effect on the scale size of the computational burden. The single particle state may be specified by three parameters (quantum numbers) (Basdevant, 2004): the principal quantum number e (number of HO quanta), angular momentum l and total angular momentum j. The e can take integer values from 0 to N-1 (here N is the number of nuclear shells), l is any integer satisfying the expression $e = 2n + l$ (here $n = 0, 1, 2 \ldots$) and j may take two values l-1/2 and l+1/2 if $l > 0$ or one value l+1/2 if $l = 0$. The neutron (proton) may be in any single-particle state characterized by the allowed values of these three quantum numbers. The nuclear shells are formed by single-particle states having the same number of HO quanta. When composing a many-particle state from the single-particle states, it is necessary to take into account the identity of the particles, i.e. any two neutrons (protons) cannot be in the same single-particle state. Since neutrons and protons are treated as different particles, the population of single-particle states by neutrons does not affect the population of single-particle states by protons and vice versa.

The standard procedure for determining all distributions of protons and neutrons in the shells of atomic nuclei is based on enumeration of all single-particle states constituting the many-particle state, that is, it is assumed that each neutron iterates over all single-particle states allowed for neutrons and for each of these cases, the protons iterates over all single-particle states permissible for protons. The number of single-particle states that may be involved in this procedure is determined by the number of shells N, which in turn is determined by the selected maximum many-particle HO excitation energy E_{max}. The E_{max} is defined as the maximum number of total HO quanta over the minimal HO energy for the selected nucleus. The many-particle state is formed by all populated by neutrons and protons single-particle states with total excitation quanta less than or equal to E_{max}. Particularly, E_{max}

= 0 is the lowest population of such single-particle states by energy for each nucleus consistent with the Pauli principle. This widely used definition of E_{max} makes it possible to completely solve the problem of spurious center-of-mass excitations in the HO nuclear shell model calculations (Caprio et al., 2012). It should be noted, that for large values of E_{max} the number of single-particle states increases rapidly and the HO nuclear shell model calculations may soon become intractable (Wang et al., 2016). Another factor that seriously affects the computational burden is the number of particles. An increasing number of particles leads to an exponential increase in the number of allowed populations of single-particle states. The main deficiency of the standard enumeration procedure is a large number of its iteration parameters, that is, a large number of single-particle states and a large number of quantum numbers that specify these states.

In this paper, we reformulate the procedure for determining all distributions of protons and neutrons in the shells of atomic nuclei and propose to iterate not over the large number of parameters as in the case of the standard enumeration procedure, but only one parameter, the nuclear shell energy. The calculation of neutrons distributions in atomic nucleus shells should begin with calculating the maximum excitation energy of one neutron E_{max_n} and finding the contribution of neutrons to the minimal many-particle HO energy E_{min} (when all particles are in states with a minimal total energy, that is, E_{max} = 0). Algorithm 1 shows a pseudocode for calculating of these quantities for neutrons based on the known formula for the maximum number of neutrons in the shell $(E_{sh}+1)(E_{sh}+2)$, here E_{sh} is the energy corresponding to the shell.

Algorithm 1. A maximum excitation energy of one neutron computation algorithm.

Input: N_n, E_{max}
Output: E_{min}, E_{max_n}
Initial values: $E_{min} \leftarrow 0$, $x \leftarrow N_n$, $E_{sh} \leftarrow 0$
1: **while** $(E_{sh}+1)(E_{sh}+2) \leq x$ **do**
2: $E_{min} \leftarrow E_{min} + E_{sh}(E_{sh}+1)(E_{sh}+2)$
3: $x \leftarrow x - (E_{sh}+1)(E_{sh}+2)$
4: $E_{sh} \leftarrow E_{sh} + 1$
5: **end while**
6: $E_{min} \leftarrow E_{min} + xE_{sh}$
7: **if** $E_{sh} > 0$ **then**
8: **if** $x > 0$ **then**
9: $E_{max\_n} \leftarrow E_{max} + E_{sh}$
10: **else**
11: $E_{max\_n} \leftarrow E_{max} + E_{sh} - 1$
12: **end if**
13: **end if**

Algorithm 1 takes as input parameters the number of neutrons in the nucleus N_n and E_{max}. At the core of this algorithm is a loop (steps 1 to 5) that is responsible for the population by N_n neutrons of nuclear shells in the increasing order of their energy and the determination of the highest occupied shell energy E_{sh}. Finally, E_{max_n} is computed based on the definitions of e and E_{sh}. The algorithm for the subsystem of N_n protons is essentially the same, but to

take into account the contribution of both neutrons and protons, it must begin with the E_{min} value obtained for the neutron subsystem.

Having determined these quantities, we can calculate the total many-particle HO energy $E_{tot} = E_{min} + E_{max}$, and the maximum number of shells in the model space $N_{sh} = \max(E_{max\_n}, E_{max\_p}) + 1$, here E_{max_p} is the maximum excitation energy of a single proton. Once E_{tot} and N_{sh} are calculated, the calculation of the distributions of protons and neutrons in the shells of atomic nuclei can begin. The main steps of the proposed method are described in Algorithm 2.

Algorithm 2. The main steps of calculating the distributions of protons and neutrons in the shells of atomic nuclei.

Input: N_n, N_p, E_{tot}, N_{sh}
Output: e_{max}, N^p_{min}, N^p_{max}, N^n_{min}, N^n_{max}, N^{pn}_{min}, N^{pn}_{max}
Initial values: 1. obtain neutrons and protons distribution with $E_{max} = 0$
2. compute E^p_{min}

1: **repeat until** all neutrons have been selected
2: find E_n
3: **if** $E^p_{min} + E_n > E_{tot}$ **then**
5: populate the neutrons for the next distribution
6: **end if**
7: reset the proton subsystem to distribution with minimal energy
8: **repeat until** all protons have been selected
9: find E_p
10: **if** $E_p + E_n = E_{tot}$ **then**
11: find the number of neutrons and protons in the shells
12: obtain: e_{max}, N^p_{min}, N^p_{max}, N^n_{min}, N^n_{max}, N^{pn}_{min}, N^{pn}_{max}
13: **end if**
14: populate the protons for the next distribution
15: **end repeat**
16: **end repeat**

The algorithm begins with the population of nuclear shells by neutrons and protons, when $E_{max} = 0$ and finding the minimal energy of the proton subsystem N^p_{min}. Algorithm 2 is implemented in two nested loops (steps 1 to 16). The outer loop is responsible for the iteration over the energies of the shells occupied by neutrons. The sum of the neutron energies for their current population of shells E_n is calculated in step 2. If the resulting E_n gives an energy greater than the E_{tot}, then in step 5 the next distribution of neutrons over nuclear shells will be established. The population of protons over the nuclear shells with the minimal energy for each neutron distribution is performed in step 7. The inner loop (steps 8 to 15) iterates over the energies of shells occupied by protons according to the same rules as in the case of neutrons. Now, the sum of the proton energies for their current population of shells E_p is calculated in step 9. If the sum of the energies of protons and neutrons is equal to the total many-particle HO energy, this distribution of neutrons and protons over nuclear shells is accepted as valid in step 10. The accepted distribution of protons and neutrons is used to find the number of neutrons and protons in each shell of the nucleus in step 11. These numbers of neutrons and protons in nuclear shells

are used for accumulation of the extreme values of the characteristic parameters of the distributions of protons and neutrons over nuclear shells in step 12: the maximum excitation energy of two nucleons (neutron and/or proton) e_{max}, the minimum number of protons for all shells N^{p}_{min}, the maximum number of protons for all shells N^{p}_{max}, the minimum number of neutrons for all shells N^{n}_{min}, the maximum number of neutrons for all shells N^{n}_{max}, the minimum number of neutrons and protons for all shells N^{pn}_{min}, and the maximum number of neutrons and protons for all shells N^{pn}_{max}. The next distribution of protons over nuclear shells is established in step 14. When Algorithm 2 ends, the accumulated parameters will contain the true values of the characteristic parameters of the *m*-scheme basis space: e_{max}, N^{p}_{min}, N^{p}_{max}, N^{n}_{min}, N^{n}_{max}, N^{pn}_{min}, and N^{pn}_{max}.

3. Experiments

The efficiency of the algorithm was tested on i7 2.4 GHz PC with 8 GB RAM. The FORTRAN90 program for this algorithm was run on Fortran PowerStation 4.0. We limit ourselves to examples for which the characteristic parameters of the *m*-scheme basis space can be calculated within our current limits of computing resources. The benchmark calculations for several representative nuclei that are subject to current state-of-the-art *ab initio* no-core nuclear shell model calculations were performed. It should be noted, that the traditional algorithm is so slow compared to the new one, that in fact it is impossible to present the performance of both algorithms on the same plot. The processing time of the traditional algorithm may take hours when the new algorithm for the same problem ends in such a short time that its measurement is really unreliable. For example, the nucleus with 8 neutrons and 8 protons for E_{max} = 20, takes 7437 seconds with the ordinary algorithm and only 0.047 seconds with the new algorithm. So the speed up of the new algorithm in comparison with the traditional one is about 150000 times. Let us present the illustration of the performance of the traditional algorithm for a number of nucleus mass number values *A* in Figure 1.

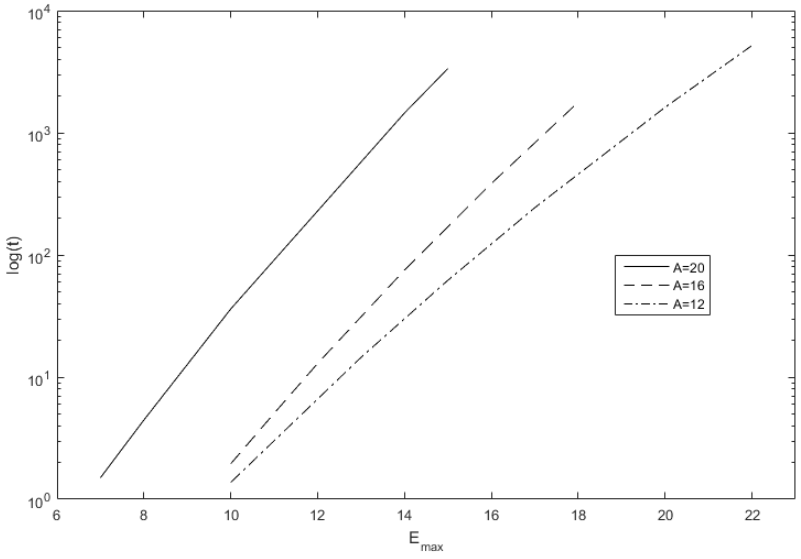

Figure 1. **The dependence of processing time (in seconds) of the traditional algorithm on the E_{max}**

The observed exponential dependence of the processing time on the maximum many-particle HO excitation energy E_{max} is quite common in the problems of calculating the distributions of protons and neutrons in the shells of atomic nuclei. It should be stressed that the processing time of the traditional algorithm grows very quickly with A and is computationally infeasible for large scale calculations. For comparison, we present the performance of the new algorithm in Figure 2.

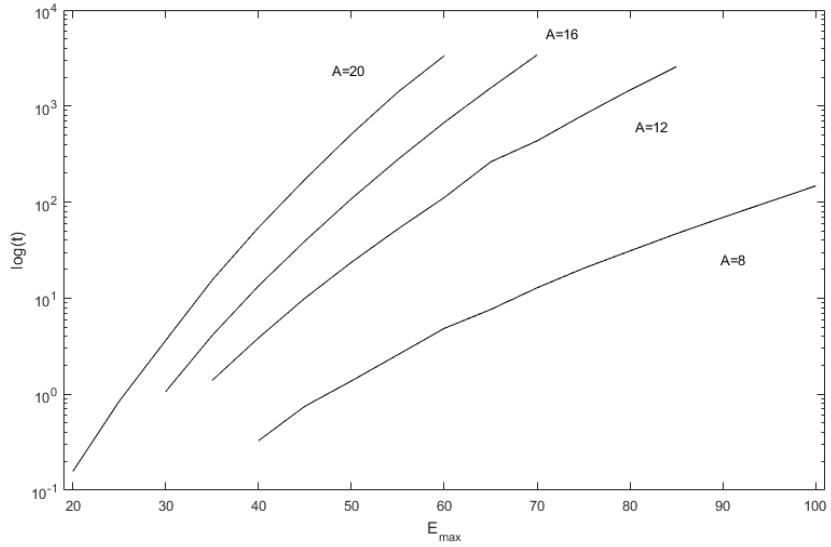

Figure 2. **The dependence of the processing time (in seconds) of the new algorithm on the E_{max}**

The obtained results confirm that the new algorithm shows performance that covers the current needs of nuclear computations. The dependence of the processing time on the difference in the number of protons and neutrons for a number of values of A is illustrated in Figure 3.

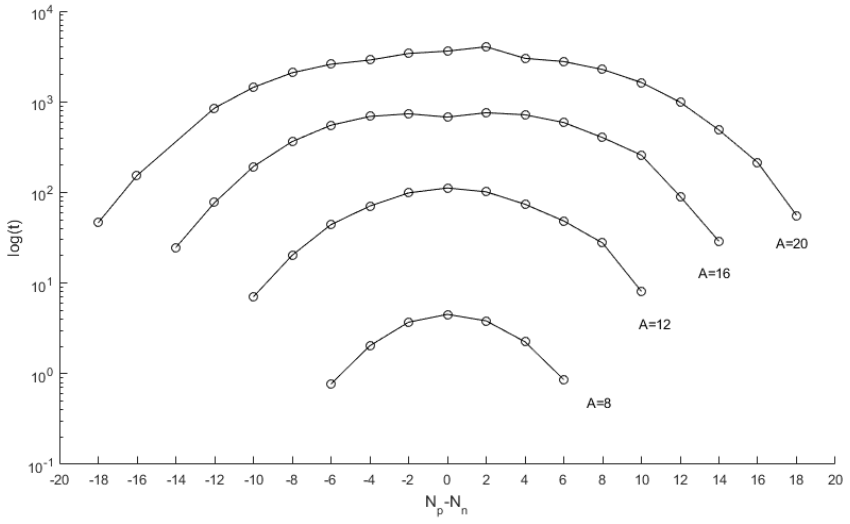

Figure 3. **The dependence of the processing time (in seconds) of the new algorithm on the difference in the number of protons and neutrons**

The obtained results imply that nuclei with a more equal number of protons and neutrons are more computationally involved. It is interesting to note, that more stable light nuclei usually satisfy this condition.

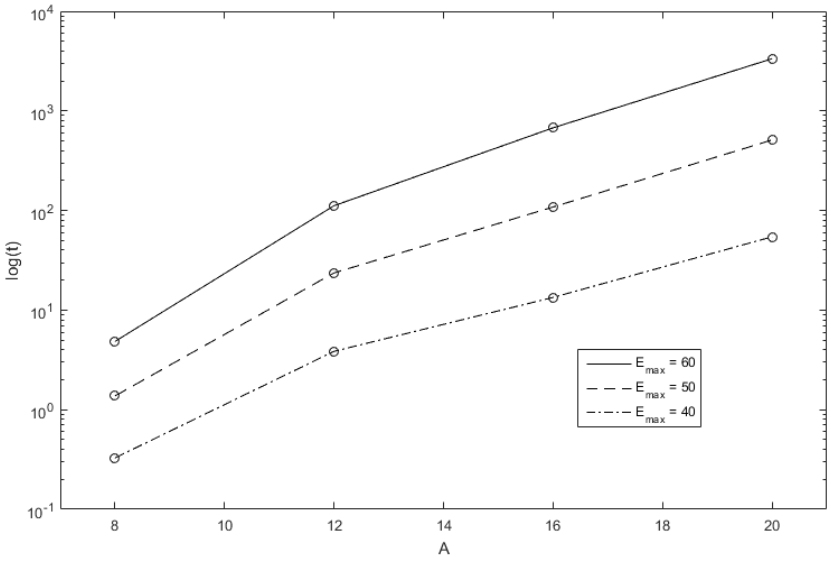

Figure 4. **The dependence of the processing time (in seconds) of the new algorithm on the** *A*

The dependence of processing time on A for a number of E_{max} values is presented in Figure 4. In this calculations the almost exponential character of the dependence is established. Finally, we present an investigation of the dependence of the processing time of the new algorithm on the asymmetry of neutron and proton subsystems in Figure 5.

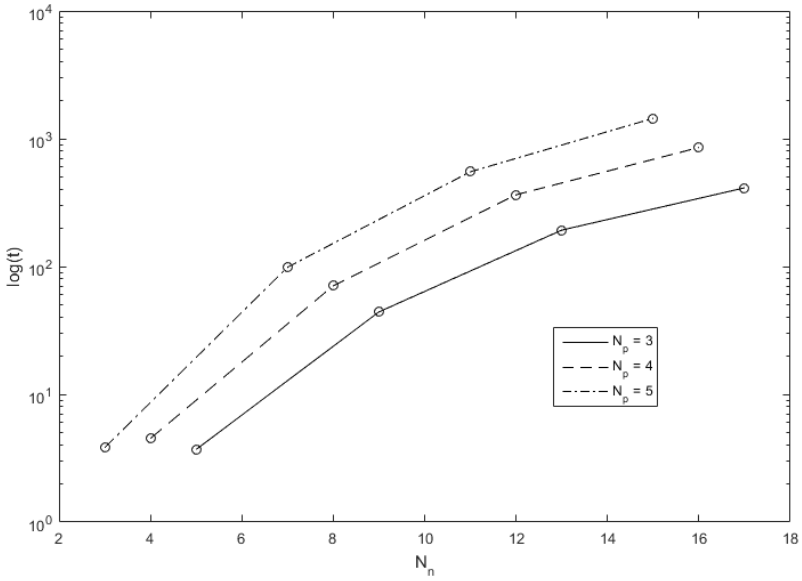

Figure 5. **The dependence of the processing time (in seconds) of the new algorithm on the asymmetry of neutron and proton subsystems**

In these calculations the number of protons in the nucleus N_p is fixed and the number of neutrons in the nucleus N_n varies. The obtained results show that for fixed number of one constituents of the nucleus, an increase in the number of other constituents exponentially increases the processing time

The proposed algorithm may be successfully used not only for light nuclei, but even for heavy nuclei. For example, we present the results of calculating proton and neutron distributions for the Uranium nucleus in Table 1.

Table 1. The characteristics of neutron and proton distributions in nuclear shells for the Uranium nucleus: 92 protons, 146 neutrons, E_{max} = 35

Shell index	N^{p}_{min}	N^{p}_{max}	N^{n}_{min}	N^{n}_{max}	N^{pn}_{min}	N^{pn}_{max}
1	0	2	0	2	0	4
2	0	6	0	6	4	12
3	1	12	4	12	13	24
4	3	20	9	20	23	43
5	3	30	13	30	33	60
6	0	42	14	42	29	84
7	0	28	0	56	0	69
8	0	17	0	34	0	34
9	0	11	0	17	0	17
10	0	8	0	11	0	11

Table 1 displays the characteristics of the distributions of neutrons and protons only for the 10 lower shells of the Uranium nucleus. The total number of shells in this problem amounts to 42 shells, and the processing time of the new algorithm is 4352 seconds.

Conclusions

In this paper the new algorithm for the protons and neutrons distributions in atomic nucleus shells calculation has been developed. Compared with the traditional approach, the method is based on the reformulation of iteration parameters in terms of particle energies instead of single-particle states. The advantage of this treatment results in implementation of very fast computation procedure, which significantly outperforms the traditional one. It should be noted, that the characteristic parameters of the distributions of protons and neutrons over nuclear shells produced by the proposed algorithm serve as input parameters and their calculation time is not critical for the contemporary computational challenges of *ab initio* NCSM *m*-scheme calculations. On the other hand, for heavily memory bound applications such as *ab initio* NCSM *m*-scheme codes, the bottleneck is not floating point operations, but aggregate memory and memory access. This is the reason for the restructuring of *ab initio* NCSM *m*-scheme codes in favor of calculating a large number of quantities at runtime, rather than their preliminary calculation (Maris et al., 2012). With the advancement of large-scale calculations of nuclear structure, a more efficient algorithm may be needed to calculate the distribution of protons and neutrons in atomic nuclei. The speedup of the new computation procedure not only covers the needs of the state-of-the-art

ab initio no-core shell model calculations of light atomic nuclei but even at the present time impossible *ab initio* no-core computations of heavy nuclei.

References

Barrett, Bruce; Navrátil, Petr; Vary, James (2013). „*Ab initio* no core shell model". Progress in Particle and Nuclear Physics, 69: 131–181.

Basdevant, Jean-Louis; Rich, James; Spiro, Michel (2004). Fundamentals in nuclear physics. New York: Springer-Verlag.

Caprio, Mark; Maris, Pieter; Vary, James (2012). „Coulomb-Sturmian basis for the nuclear many-body problem". Physical Review C, 86: 064301.

Dikmen, Erdal; Lisetskiy, Alexander; Barrett, Bruce; Maris, Pieter; Shirokov, Andrey; Vary, James (2015). „*Ab initio* effective interactions for *sd*-shell valence nucleons". Physical Review C, 91: 034312.

Fedurtsya, Anton; Deveikis, Algirdas (2011). „Neutronų ir protonų pasiskirstymo atomo branduolio sluoksniuose skaičiavimas". Informacinės technologijos (IVUS 2010): 37–40.

Heng, Taihua; Vary, James; Maris, Pieter (2017). „*Ab initio* no-core properties of ^{7}Li and ^{7}Be with the JISP16 and chiral NNLO$_{opt}$ interactions". Physical Review C, 95: 014306.

Maris, Pieter; Aktulga, Metin; Caprio, Mark; Çatalyürek, Ümit; Eg, Edmont; Oryspayev, Dossay; Potter, Hugh; Saule, Erik; Sosonkina, Masha; Vary, James; Yang, Chao; Zhou, Zheng (2012). „Large-scale *ab initio* configuration interaction calculations for light nuclei". Journal of Physics: Conference Series, 403, 1: 012019.

Navrátil, Petr; Vary, James; Barrett, Bruce (2000). „Large-basis *ab initio* no-core shell model and its application to ^{12}C". Physical Review C, 62: 054311.

Shin, Ik; Kim, Youngman; Maris, Pieter; Vary, James; Forssén, Christian; Rotureau, Jimmy; Michel, Nicolas (2017). „*Ab initio* no-core solutions for ^{6}Li". Journal of Physics G: Nuclear and Particle Physics, 44, 7: 075103.

Wang, XiaoBao; Dong, GuoXiang; Li, QingFeng; Shen, CaiWan; Yu, ShaoYing (2016). „An investigation of *ab initio* shell-model interactions derived by no-core shell model". Science China Physics, Mechanics & Astronomy, 59, 9: 692011.

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EFEKTYVUS PROTONŲ IR NEUTRONŲ PASKIRSTYMŲ ATOMO BRANDUOLIO SLUOKSNIUOSE SKAIČIAVIMO ALGORITMAS

Algirdas Deveikis

Santrauka

Straipsnyje siūlomas naujas neutronų ir protonų pasiskirstymų atomo branduolio sluoksniuose skaičiavimo algoritmas. Apskaičiuojamos algoritmu šių pasiskirstymų charakteristikos yra skirtos *ab initio* NCSM *m*-schemos atomo branduolio sluoksnių modelio skaičiavimams. Tradiciškai, tinkamo neutronų ir protonų pasiskirstymo atrankos kriterijai naudoja jų viendalelių būsenų kvantinius skaičius. Esant dideliems dalelių ir branduolio harmoninio osciliatoriaus sužadinimo kvantų skaičiams tokių parametrų skaičius gali būti pernelyg didelis pakankamam skaičiavimo efektyvumui pasiekti. Siūlomas efektyvesnis kriterijus pagrįstas atomo branduolio sluoksniuose esančių dalelių energijomis. Atlikti eksperimentiniai tyrimai su įvairiais neutronų ir protonų skaičiais bei branduolio harmoninio osciliatoriaus sužadinimo energijos kvantų skaičiais, demonstruoja pasiūlyto algoritmo pranašumą ir efektyvumą lyginant su tradiciniu metodu.

Pagrindiniai žodžiai: atomo branduolio sluoksnių modelis, harmoninio osciliatoriaus bazė, antisimetrinės daugiadalelės būsenos, kombinatorinė optimizacija.