STRUCTURE OF THE GROUND STATE OF SIX NUCLEON NUCLEI

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The optimal superposition of the harmonic oscillator shell model configurations for the six nucleon nuclei ground state description is obtained. It has been shown that only one such superposition is possible. This result is in the complete accordance with the experimental observations stating that in the six nucleon system there is only one bound state.

Keywords: six nucleon nuclei, translationally invariant shell model, density matrix

PACS: 21.60.Cs, 13.75.Cs, 21.10.Dr

1. Introduction

The nuclear shell model, years ago introduced as significant simplification of the atomic nuclei description, operates with some leading configuration, i. e. with a defined set of one-nucleon states and a simple wave function dependent on one-nucleon degrees of freedom. This picture of independent nucleons moving in some central field provides an easy way of the wave function antisymmetrization but currently can be considered only as some phenomenological tool for the heavy nuclei description, where microscopic approach based on the Schrödinger equation with some potential of the nucleon–nucleon (NN) interaction cannot be applied.

For few-nucleon systems or even for the lightest atomic nuclei this model gives unacceptable results. Moreover, it cannot describe even the simplest atomic nucleus – deuteron – due to the problems with translational invariance of the wave function and the nonzero quadrupole moment of this nucleus, asking for the D-state, i. e. the excited configuration, presence in the wave function expansion.

So, for the microscopic description of atomic nuclei it is necessary to apply the variational methods like Green function Monte-Carlo [1] or to take into account the huge amount of the excited shell-model configurations. In the last case the best for the wave function expansion is the basis of three-dimensional harmonic oscillator (HO) functions. This basis allows construction of the translationally invariant wave function taking into account the finite number of the basic states, produced by all allowed configurations at the given number of

the HO quanta [2, 3]. Sometimes this particular way of the lightest nuclei description is called the shell-model approach (to be more precise, 'no-core shell model'). However, even in this approach, operating with a huge amount of basic states, one again has to apply some phenomenological structures, defined as the effective potentials, due to extremely slow convergence of the expansions. The bare NN potentials require even more basic states for a more or less acceptable solution of the Schrödinger equation even for few-nucleon systems.

The goal of our paper is to find out how important for the ground and excited states' description is the starting wave function, by taking into account the complete set of the basic states of the minimal HO configuration for the reasons mentioned above. Our approach is based on the reduced Hamiltonian expansion for the energy of an atomic nucleus employing the translationally invariant wave function. This simple expression for the eigenvalue of a realistic nuclear Hamiltonian gives information about the role of different two nucleon channels in ensuring the stability of atomic nuclei.

Let us start our investigation with the nuclei consisting of six nucleons, because they are the lightest systems having a few more or less stable low-lying states with the well-defined quantum numbers [4] (Fig. 1). In five nucleon system there are no bound states at all. The nuclei consisting of a few nucleons (deuteron, tritium, and alpha particle) have no low-lying excited states. Therefore, the six nucleon systems are the best for verifying any new ideas of the atomic nuclei description [5].
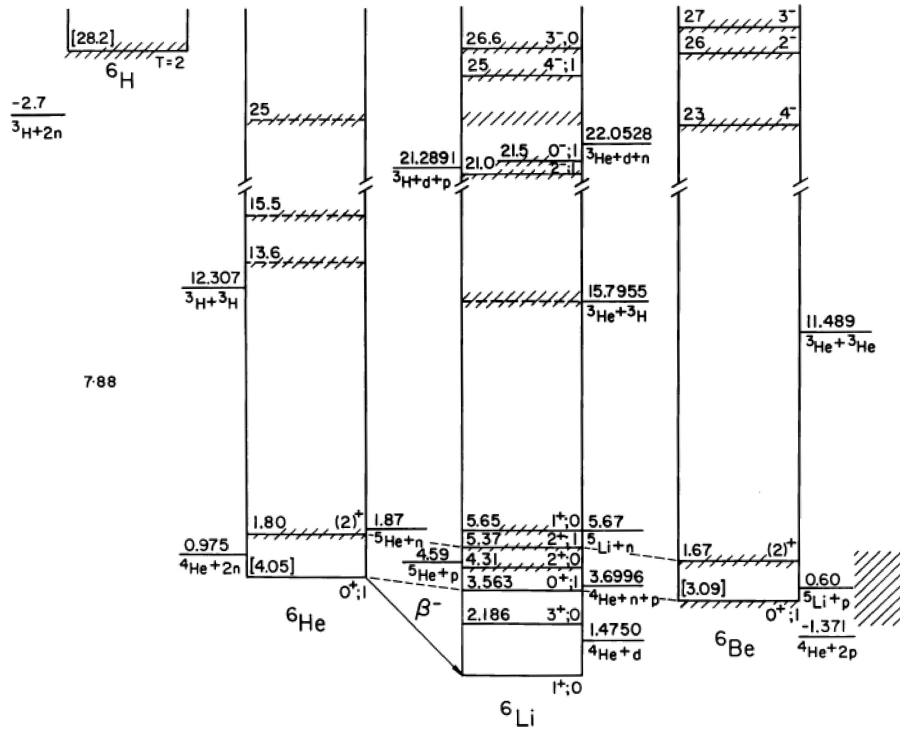
Fig. 1. Energy levels of the six nucleon nuclei [4].

As mentioned earlier, the successful methods of microscopic description of the atomic nuclei operate with large arrays of basic states. This requires a lot of matrix elements for the Hamiltonian calculation. For the simplification of this process the basic states are presented in the simplest possible way. The main idea of our report is the recipe for construction of the best starting basic function of the minimal HO approximation that possesses the necessary set of quantum numbers. Applying such a function one can be sure that the centre of the mass of the nucleus is in the state with a minimal number of the oscillator quanta and will not combine (due to the translational invariance of the NN potential) with the spurious states (corresponding to the excited centre of mass) present in the set of the basic functions. As a result, the expansion of the final wave function will be free of admixture of such basic functions. Such a function dependent on single-nucleon variables is very simple in applications in comparison with a function dependent on translationally invariant (Jacobian) variables, but at the same time it will give the same result for the expectation values of any operator as the translationaly invariant one would. Moreover, the final function will have the same set of the exact quantum numbers as the starting one due to known symmetries of the NN potential, so one will not need to worry about these quantum numbers' projection.

2. Calculations and results

The relation between the nuclear shell model potential and the NN interaction is very complicated; therefore while applying the shell model picture it is hard to understand the dependence of the calculated nuclear characteristics on the NN potential.

However, there exists a well-known expression for the binding energies of the ground and excited states of the atomic nucleus in terms of the nucleon–nucleon potential characteristics, given by the corresponding reduced Hamiltonian (RH) operator [6]. This expression is

$$E_{J^\Pi T} = \sum_{nj^\pi t} \varepsilon_{nj^\pi t} \omega_{nj^\pi t}(J^\Pi T), \qquad (1)$$

where the set of quantum numbers $J^\Pi T$ defines the nuclear state under investigation, $\varepsilon_{nj^\pi t}$ is the nth eigenvalue of the RH operator in the two nucleon channel $j^\pi t$, and $\omega_{nj^\pi t}(J^\Pi T)$ is the diagonal element of the intrinsic density matrix, defining the probability of the given state $(nj^\pi t)$ of the RH operator in the wave function expansion.

Let us study the diagonal elements of the intrinsic density matrix of six nucleon system [7], given in Table 1. The configuration for this nucleus, recommended by the shell model, is $(00\frac{1}{2})^4(11\frac{3}{2})^2$. This configuration creates four states of the six nucleon system: $J^\Pi T = 1^+0, 3^+0, 0^+1, 2^+1$. All these states

Table 1. Diagonal elements of density matrix of the six nucleon nuclei [7].

$J^\Pi T$	**1^+0**			**3^+0**	**0^+1**		**2^+0**	**2^+1**		**1^+1**
Configuration	$(\frac{3}{2})^2$	$(\frac{3}{2})(\frac{1}{2})$	$(\frac{1}{2})^2$	$(\frac{3}{2})^2$	$(\frac{3}{2})^2$	$(\frac{1}{2})^2$	$(\frac{3}{2})(\frac{1}{2})$	$(\frac{3}{2})(\frac{1}{2})$	$(\frac{3}{2})^2$	$(\frac{3}{2})(\frac{1}{2})$
RH state										
$^3S_1$	17/54	44/135	44/135	1/3	3/10	3/10	1/3	3/10	3/10	3/10
$^3S'_1$	1/81	8/405	1/810	0	0	0	0	0	0	0
$^1S_0$	3/10	3/10	3/10	3/10	29/90	14/45	3/10	29/90	14/45	3/10
$^1S'_0$	0	0	0	0	1/45	1/90	0	0	0	0
$^1P_1$	19/270	13/270	13/270	1/30	1/30	1/30	1/30	1/30	1/30	1/30
$^3P_0$	0	1/20	1/10	0	0	1/10	1/20	1/20	0	13/180
$^3P_1$	1/20	1/8	1/5	1/20	13/180	11/45	1/8	47/360	11/180	17/120
$^3P_2$	1/4	1/8	0	1/4	1/4	0	1/8	17/120	17/60	11/72
$^1D_2$	0	0	0	0	0	0	0	1/45	1/90	0
$^3D_1$	1/405	1/162	2/81	0	0	0	0	0	0	0
$^3D_2$	0	0	0	0	0	0	1/30	0	0	0
$^3D_3$	0	0	0	1/30	0	0	0	0	0	0

$^3S'_1$ and $^1S'_0$ are excited RH states.

are observed experimentally (Fig. 1): the ground state $J^\Pi T = 1^+0$, the first excited state $J^\Pi T = 3^+0$, the second excited state $J^\Pi T = 0^+1$ serving also as the ground state of ^{6}He and of ^{6}Be nuclei, and the fourth excited state of ^{6}Li nucleus $J^\Pi T = 2^+1$. The explanation of the two missing-on-the-list low-lying states $J^\Pi T = 1^+0, 2^+0$ requires more complex configurations. The first among them is the configuration $(00\frac{1}{2})^4(11\frac{3}{2})(11\frac{1}{2})$, giving the mentioned states as well as the states $J^\Pi T = 1^+1, 2^+1$ not yet identified experimentally. The complete set of configurations present in the minimal HO shell model consists of those mentioned and one additional configuration, $(00\frac{1}{2})^4(11\frac{1}{2})^2$, that yield two states: $J^\Pi T = 1^+0, 0^+1$. Thus the minimal HO shell model approximation contains three configurations and gives ten states, exceeding the number of experimentally observed levels by four.

Due to peculiarities of the realistic nucleon–nucleon potential the minimal value of the RH operator is in the channel $j^\pi t = 1^+0$ ($^3S_1$–$^3D_1$), playing the major role in accumulating the binding energy of nucleus [6]. This minimal RH eigenvalue requires the significant $^3D_1$ state admixture (not less than 30%, different for various realistic potentials) to the $^3S_1$ state. The diagonal entries of the intrinsic density matrix presented in Table 1 show that some admixture of this state can be found only in three 1^+0 ^{6}Li states, therefore at first glance it looks like the theory suggests that the ground and the first two excited states in the ^{6}Li nucleus should be the 1^+0 states. However, the experiment proves a different picture: one 1^+0 state appears as the ground

state, the second is the sixth in the row, and the third one is not found at all. It is thus obvious that the theoretical spectrum in minimal shell model approximation of the ^{6}Li nucleus is noticeably different from the one observed experimentally.

Is it possible to find out what linear combination of the mentioned three configurations would serve as the best starting function for describing the ground state $J^\Pi T = 1^+0$ of this nucleus? The answer is given by the intrinsic density matrix diagonalization.

The intrinsic density matrix in the reduced Hamiltonian state $^3D_1$ is

$$
\begin{pmatrix}
\dfrac{1}{405} & -\dfrac{1}{81\sqrt{10}} & -\dfrac{\sqrt{2}}{81\sqrt{5}} \\[2mm]
-\dfrac{1}{81\sqrt{10}} & \dfrac{1}{162} & \dfrac{1}{81} \\[2mm]
-\dfrac{\sqrt{2}}{81\sqrt{5}} & \dfrac{1}{81} & \dfrac{2}{81}
\end{pmatrix} . \qquad (2)
$$

It is the diagonal elements of this matrix that are given in Table 1. After the diagonalization of this density matrix the weight of the two nucleon state $^3D_1$ for one of the functions equals $1/30$, which is the maximum possible value, and the weights of this state in the diagonal density matrix of the remaining two states equals to zero (Table 2). The eigenvector corresponding to this

Table 2. Density matrix of the 1^+0 states of ^{6}Li after diagonalization.

$J^\Pi T$	1^+0		
Configuration superposition RH states	ground state	excited state *1*	excited state *2*
$^3\mathrm{S}_1$	**1/3**	**23/70**	**32/105**
$^3\mathrm{S}'_1$	0	1/35	1/210
$^1\mathrm{S}_0$	3/10	3/10	3/10
$^1\mathrm{S}'_0$	0	0	0
$^1\mathrm{P}_1$	1/3	3/70	19/210
$^3\mathrm{P}_0$	1/12	1/70	11/210
$^3\mathrm{P}_1$	7/40	1/14	9/70
$^3\mathrm{P}_2$	1/24	3/14	5/42
$^1\mathrm{D}_2$	0	0	0
$^3\mathrm{D}_1$	**1/30**	**0**	**0**
$^3\mathrm{D}_2$	0	0	0
$^3\mathrm{D}_3$	0	0	0

maximal weight of the $^3\mathrm{D}_1$ state is

$$\begin{pmatrix} \dfrac{\sqrt{2}}{3\sqrt{3}} \\[2mm] -\dfrac{\sqrt{5}}{3\sqrt{3}} \\[2mm] -\dfrac{2\sqrt{5}}{3\sqrt{3}} \end{pmatrix}. \tag{3}$$

Obviously, this vector is equal to a superposition of the three mentioned configurations, giving the best starting approximation for description of the ground state of the ^{6}Li nucleus. Using the same orthogonal matrix we diagonalize the density matrices in all the other channels and obtain new ones for ^{6}Li, presented in Table 2.

The diagonal entries of the new matrices are the elements of the density matrix of translationally invariant shell model. After the diagonalization the second and the third 1^+0 states in the ^{6}Li nucleus become equivalent to all the other states of minimal approximation, i. e. they contain no $^3\mathrm{D}_1$ admixture. Thus, after the diagonalization, only one of the independent configuration superpositions having the maximal $^3\mathrm{D}_1$ state admixture corresponds to the best approximation for the ^{6}Li ground energy level description.

3. Discussion and conclusions

The obtained zero approximation for the ^{6}Li ground state wave function expansion in the translationally invariant shell model basis provides very interesting con-

clusions. Firstly, this result states that only one combination of the configurations in the minimal HO shell-model approximation has nonzero D-state admixture in the two-nucleon reduced Hamiltonian channel. The experimental situation corresponds to this result in the best possible way, because actually in the six-nucleon system there exists only one bound state – the ground state of the ^{6}Li nucleus. Some excited states are long-lived ones, but not completely bound. The second interesting result is that the obtained optimal superposition of configurations has the maximal weight equal to 20/27 of the configuration $(00\frac{1}{2})^4(11\frac{1}{2})^2$, while the configuration recommended by the HO shell-model $(00\frac{1}{2})^4(11\frac{3}{2})^2$ has ten times lower weight, equal to 2/27. The missing 5/27 is the weight of the last configuration $(00\frac{1}{2})^4(11\frac{3}{2})(11\frac{1}{2})$.

It is obvious that this component is a very important part of the complete wave function, but not the only one. The next terms in the expansion, corresponding to the superposition of the $E_{\min} + 2$ and the higher oscillator quanta configurations, are able to minimize the energy of the state to such an extent (as mentioned, in the RH channel $^3\mathrm{S}_1$–$^3\mathrm{D}_1$ the ground state requires approximately 30% of the $^3\mathrm{D}_1$ channel admixture, while the data in Table 2 show that the $^3\mathrm{D}_1$ probability makes up only 10% in comparison with the weight of the $^3\mathrm{S}_1$ state).

The problem with the negative quadrupole moment of the atomic nucleus ^{6}Li cannot be solved in this approximation, giving positive value, but it is this optimal zero approximation that makes it possible to obtain the negative value of the quadrupole moment taking into account the proper admixture of functions corresponding to the excited HO shell-model configurations.

Finally, this procedure does not ensure the minimization of the total energy and for a proper description of the six nucleon nuclei the admixtures of the excited shell model states in the wave functions expansion is necessary. These admixtures are unavoidable for the binding energy as well as for the negative value of the quadrupole moment in the description of the ground state of ^{6}Li nucleus.

References

[1] B.S. Pudliner, V.R. Pandharipande, J. Carlson, S.C. Pieper, and R.B. Wiringa, Quantum Monte Carlo calculations of nuclei with $A \le 7$, Phys. Rev. C **56**, 1720 (1997).

[2] G.P. Kamuntavičius, Root-mean-square radii of light atomic nuclei: Neutron skin, Phys. Rev. C **56**, 191 (1997).

[3] P. Navrátil, G.P. Kamuntavičius, and B.R. Barrett, Few-nucleon systems in a translationally invariant harmonic oscillator basis, Phys. Rev. C **61**, 044001 (2000).

[4] F. Ajzenberg-Selove, Energy levels of light nuclei $A = 5$–10, Nucl. Phys. A **490**, 1 (1988).

[5] P. Navrátil, J.P. Vary, W.E. Ormand, and B.R. Barrett, Six-nucleon spectroscopy from a realistic nonlocal

Hamiltonian, Phys. Rev. Lett. **87**, 172502 (2001).

[6] G.P. Kamuntavičius, The reduced Hamiltonian method in the identical particle systems bound state theory, Sov. J. Part. Nuclei **20**, 261 (1989).

[7] A. Deveikis and G.P. Kamuntavičius, Intrinsic density matrices of the nuclear shell model, Lithuanian J. Phys. **36**, 83 (1996).

ŠEŠIŲ NUKLEONŲ BRANDUOLIŲ PAGRINDINĖS BŪSENOS SANDARA

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Santrauka

Teoriškai nagrinėjamos šešių nukleonų branduolių aprašymo minimaliame harmoninio osciliatoriaus sluoksnių modelio artutinume galimybės. Pagrindinis šios šeimos branduolys yra ^{6}Li – lengviausias branduolys, turintis palyginus turtingą spektrą: vieną suruštą ir dar penkias gana ilgai gyvuojančias energetines būsenas su gerai apibrėžtais kvantiniais skaičiais.

Tradicinis sluoksnių modelis, kai apsiribojama tik rekomenduojama pagrindine konfigūracija $(00\frac{1}{2})^4(11\frac{3}{2})^2$, nusako tik keturias tų stebimų būsenų. Jeigu imamos visos trys įmanomos šio modelio konfigūracijos, tokių būsenų atsiranda dešimt. Taigi, modelis susiduria su principiniais sunkumais aprašant jau patį pirmąjį branduolį, turintį šiek tiek turtingesnį spektrą.

Ši seniai žinoma problema darbe sprendžiama pasinaudojant sluoksnių modelio modifikacija, paremta redukuotinio hamiltoniano operatoriumi ir užtikrinančia banginių funkcijų transliacinį invariantiškumą. Ši modifikacija leidžia bet kokios branduolio būsenos energiją išreikšti redukuotinio hamiltoniano tikrinėmis vertėmis, padaugintomis iš atitinkamų tikimybių. Seniai žinoma, kad

pagrindinis vaidmuo užtikrinant atomų branduolių stabilumą tenka redukuotinio hamiltoniano kanalui ^{3}S$_1$–^{3}D$_1$, – tam pačiam, kuris aprašo deuterono pagrindinę būseną. Optimali bet kurios branduolio būsenos energija užtikrinama minimizuojant šio kanalo redukuotinio hamiltoniano pagrindinės būsenos energiją. Šis procesas reikalauja tam tikros, lengvai gaunamos iš skaičiavimų ir kiek skirtingos skirtingiems realistiniams potencialams, ^{3}D$_1$ būsenos priemaišos. Atomų branduolių būsenos, kuriose šios redukuotinio hamiltoniano priemaišos tikimybė lygi nuliui, turi nedaug galimybių būti surištosios.

Sukonstravę šešių nukleonų branduolių tankio matricą ir ją diagonalizavę gavome, kad tik viena būsena iš dešimties turi nelygią nuliui šią tikimybę. Taigi, ji ir yra pagrindinė pretendentė aprašyti ^{6}Li branduolio pagrindinę būseną $J^\Pi T = 1^+0$. Tai gerai atitinka eksperimente stebimus rezultatus. Nelaukta išvada, kuri seka iš mūsų tyrimų, yra ta, kad pagrindinį svorį gautoje optimalioje nulinio artinio banginėje funkcijoje turi ne sluoksnių modelio rekomenduojama, o kita konfigūracija, būtent, $(00\frac{1}{2})^4(11\frac{1}{2})^2$.