PROSPECTS OF THEORETICAL NUCLEAR SPECTROSCOPY OF LIGHT NUCLEI

Yu. M. Tchuvil'sky
Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia

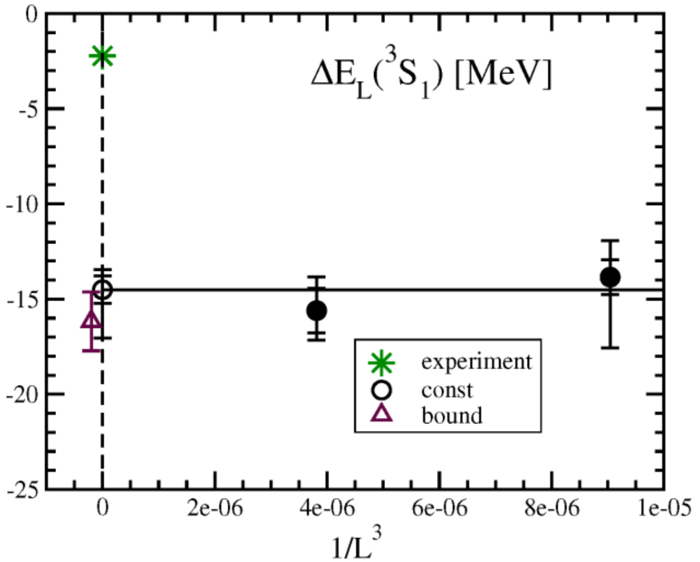
D. M. Rodkin
Dukhov Research Institute for Automatics, Moscow, Russia

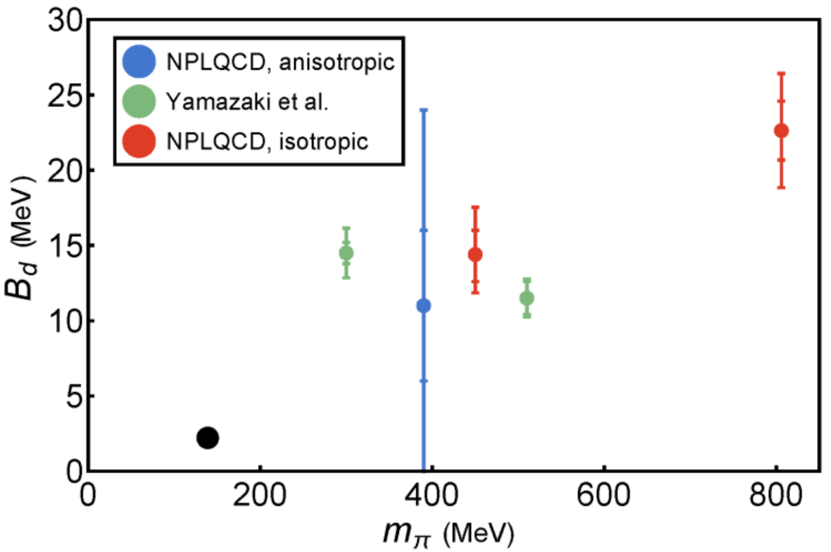
TERMINOLOGY USED

Microscopic approaches in nuclear theory are approaches in which the nucleus and / or a system of colliding (scattering) nuclear particles are considered as systems consisting of nucleons. For a quantitative description of such systems, interaction models are used that are characteristic of a given nucleus or a compact group of nuclei of the same type. Some of these models such as the shell model pretend to describe qualitatively a large bulk of nuclei.

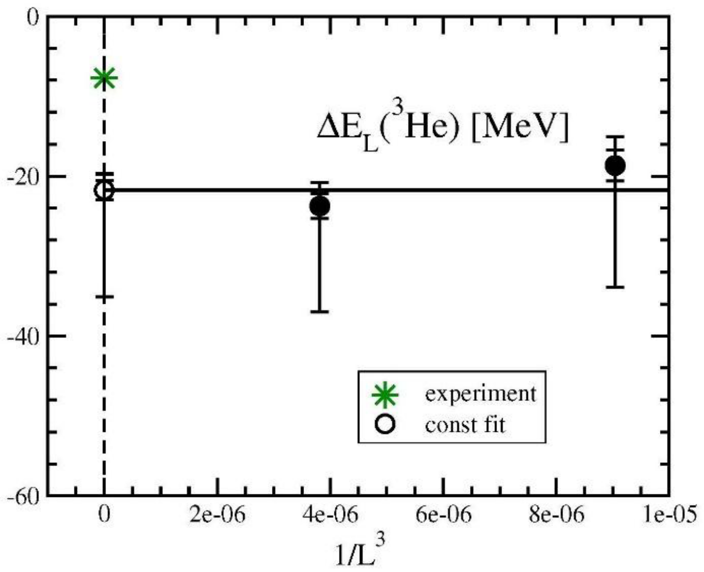
Ab initio approaches are the microscopic approaches based on an realistic theory of the interaction between nucleons (recently NN and NNN) which describes the NN-scattering, the properties of deuteron, etc. Approaches of this type are used to describe a fairly wide range of nuclei and processes with them. The NN and NNN interaction can vary from nucleus to nucleus, however, under the strict condition that the properties of the 2N- and 3N-sistem remain unchanged.

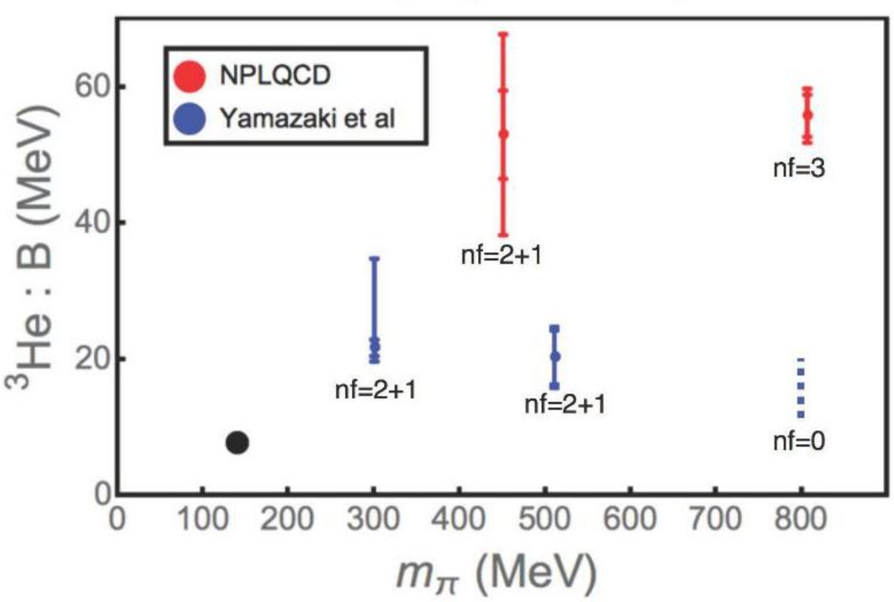
ARE AB INITIO SCHEMES BASED ON QCD?

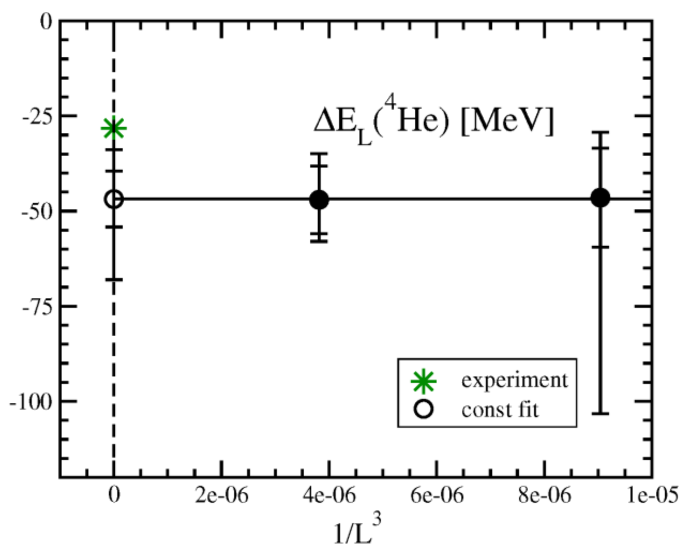




Binding energies of deuteron in QCD various calculations. L is the lattice size, a~0.1 fm – the lattice pitch, L~5 fm, Mπ= 300 - 800 MeV. The horizontal line is the result of the extrapolation to L → ∞. ∗ or ● - real values.







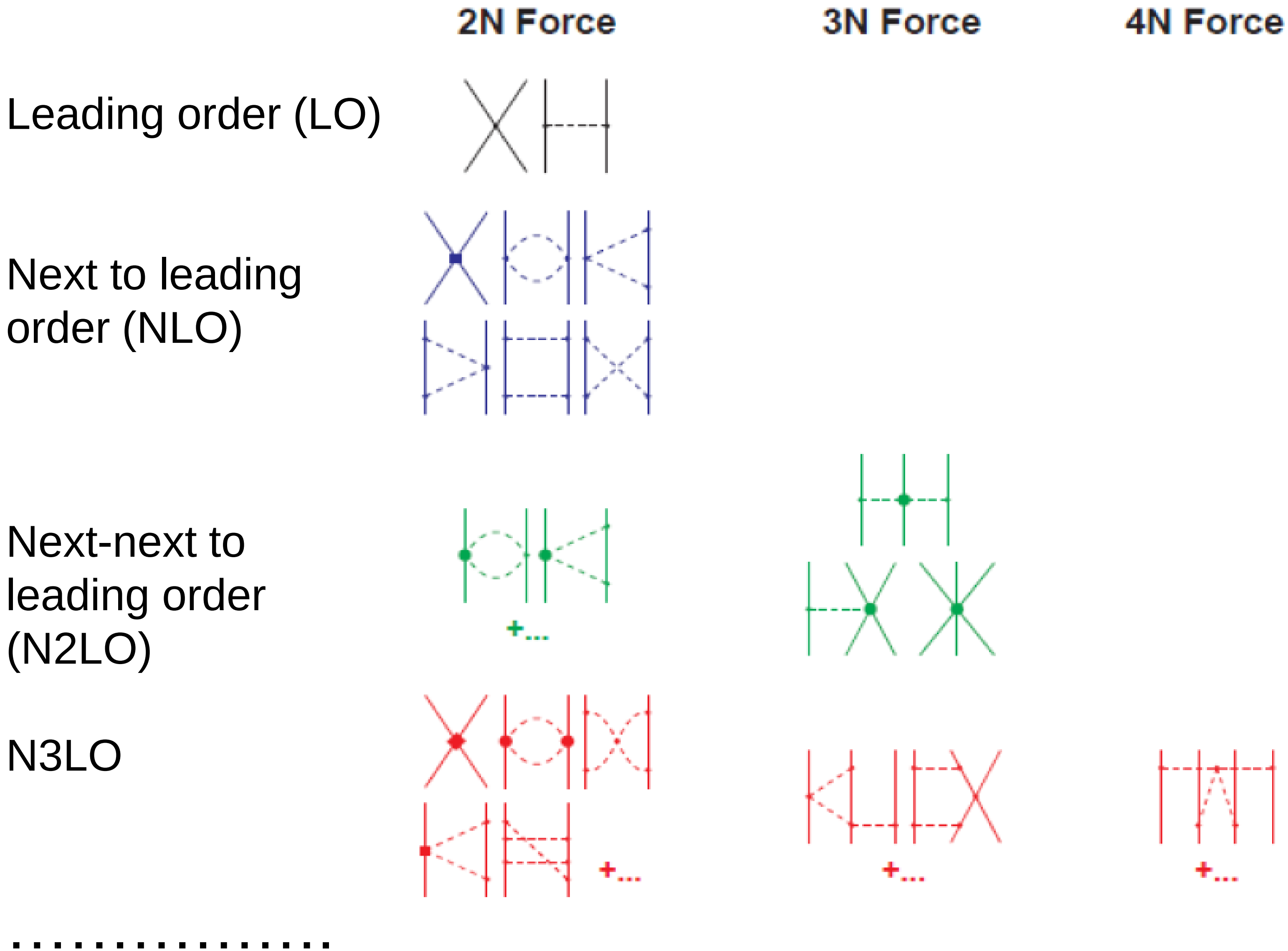
The same for 3He and 4He nuclei.

As a result, at the moment QCD-approaches cannot pretend to quantitatively describe nuclear systems.

REALISTIC POTENYIAL MODELS. CHIRAL EFFECTIVE FIELD THEORY

Well-known meason-exchange NN-potentials: Nijmegen-II, Argonn18, CD-Bonn, etc. qualify as realistic.

Chiral Effective Field Theory is based on fundamental symmetries of QCD SU(2)×SU(2). Using this theory when constructing the NN-interaction, one takes into account a number of conditions imposed by the QCD. The theory allows, based on the same prerequisites, also receive three-, four- etc. -particle forces, thereby conducting computational experiments and determine the degree of need for accounting the corresponding effects. Recently NN- and NNN-forces are involved in calculations.

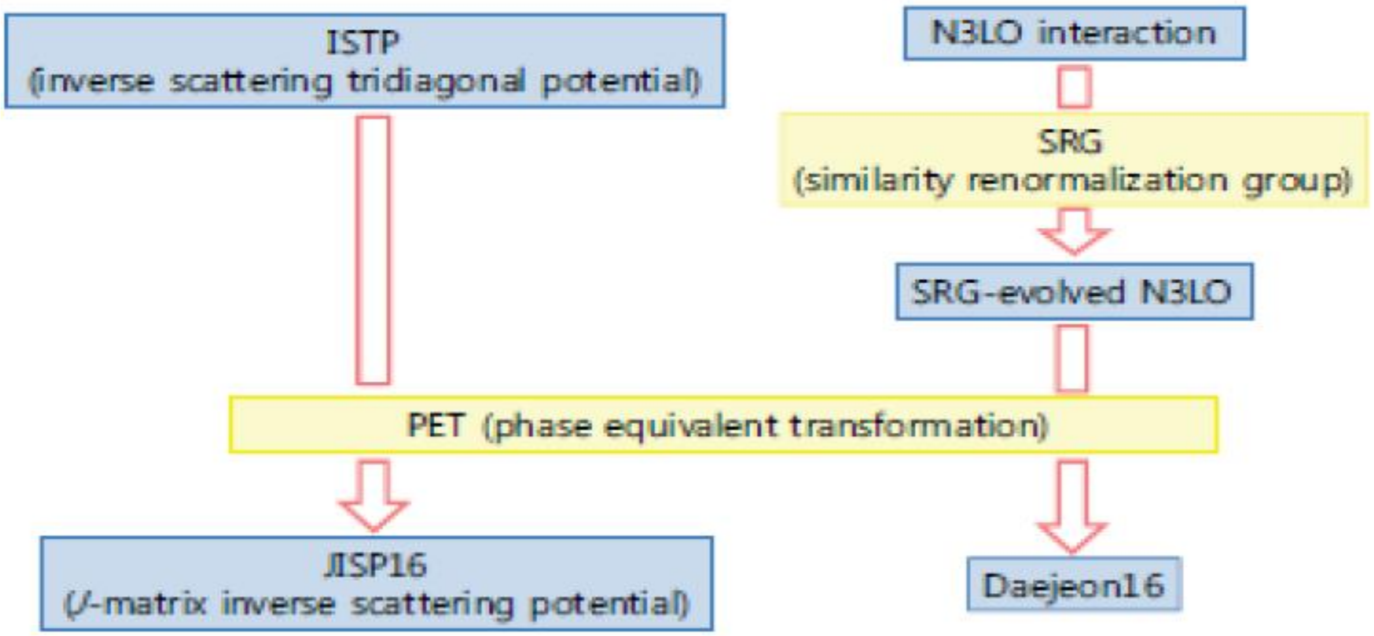


Diagrams of the effective chiral theory.

The constants determining the contribution of each of the diagrams to the potential are fixed in such a way as to correctly describe the two- and three-nucleon data.

A potential obtained in this way turns out to be too “high-momentum" and for multi-nucleon calculations requires a giant-size bases. For this reason, transformations: similarity renormalization group (SRG), or Lee-Suzuki are performed. The idea behind the transformations is that the physics of relatively low energies does not depend on the dynamics at high energies. These transformations do not affect the "two-nucleon" and “three-nucleon” data, but they drastically simplify the multiparticle calculations.

TYPICAL EXAMPLES



Obtaining procedure for potentials Daejeon16 (Shirokov A. M., Shin I. J., Kim Y. et al. PLB 761 87 (2016)) and JISP16 (Shirokov A. M., Kulikov V. A., Maris P. et al. EPJ Web Conf. 3 05015 (2010)) .

In both cases NN-forces only are presented. The transformation parameters are fitted on the basis of data on the energies of several ground and excited states of some light nuclei.

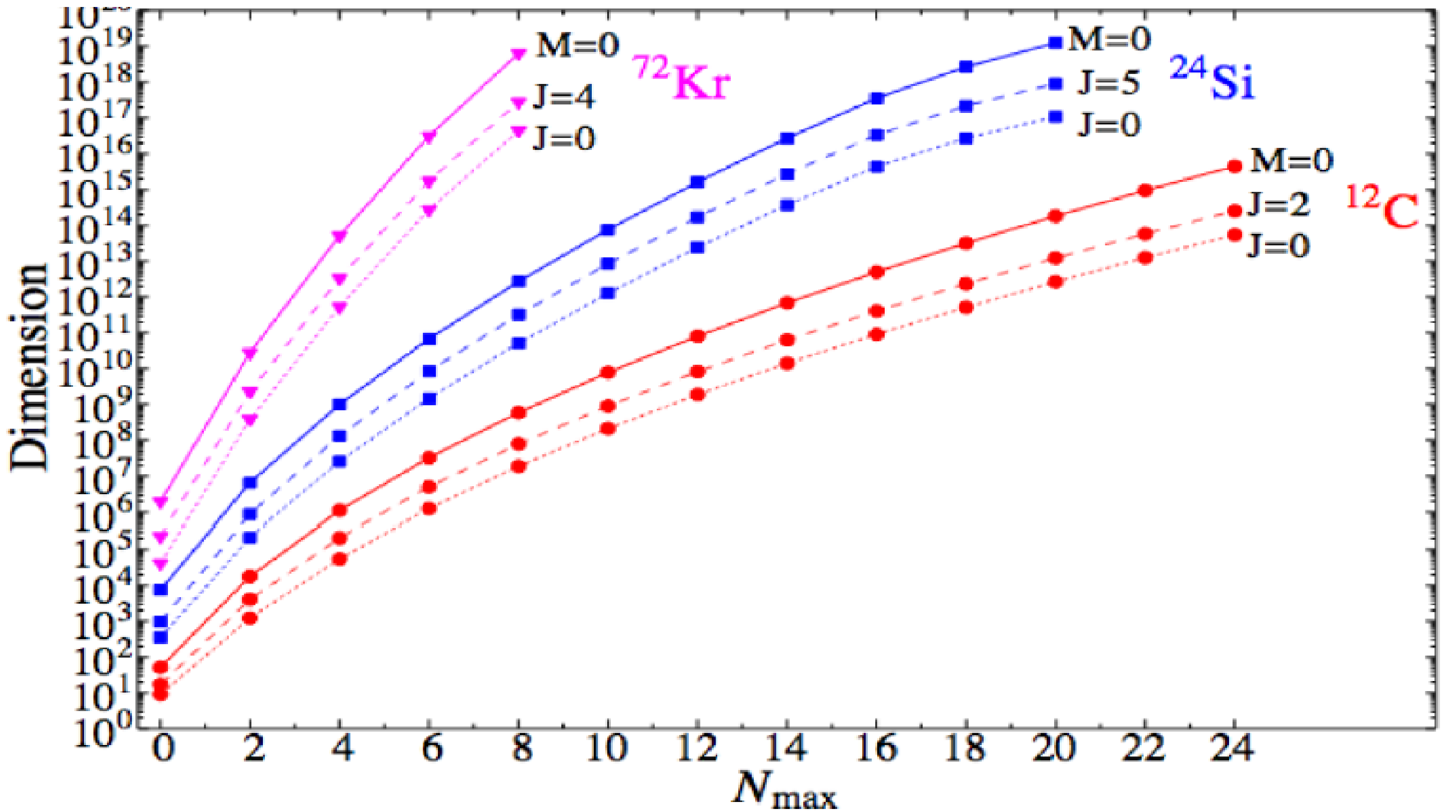
NO-CORE SHELL MODEL (NCSM) AS A GROUND OF AB INITIO APPROACHES

The dynamics of NCSM is described by A-nucleon Hamiltonian with realistic NN-interaction. The variational problem is solved by diagonalization of the Hamiltonian matrix on the basis of A-nucleon Slater determinants (so-called M-scheme is give as an example):

$$\Psi_i = \begin{vmatrix} \psi_{n_1 l_1 s_1 j_1 m_1}(r_1) & \dots & \psi_{n_A l_A s_A j_A m_A}(r_1) \\ \dots & \dots & \dots \\ \psi_{n_1 l_1 s_1 j_1 m_1}(r_A) & \dots & \psi_{n_A l_A s_A j_A m_A}(r_A) \end{vmatrix}. \quad N = \sum_{i=1}^{A} n_i \geq N_{\min} \qquad (1)$$

which, as a rule, consist of the spherical oscillator one-nucleon wave functions (oscillator in the most cases). All matrix elements are taken into account. Some of smaller ones may be neglected but after the calculation.

This basis is infinite, in real calculations, it is forced to truncate it at a certain level $N \le N_{\min} + N_{\max}$.



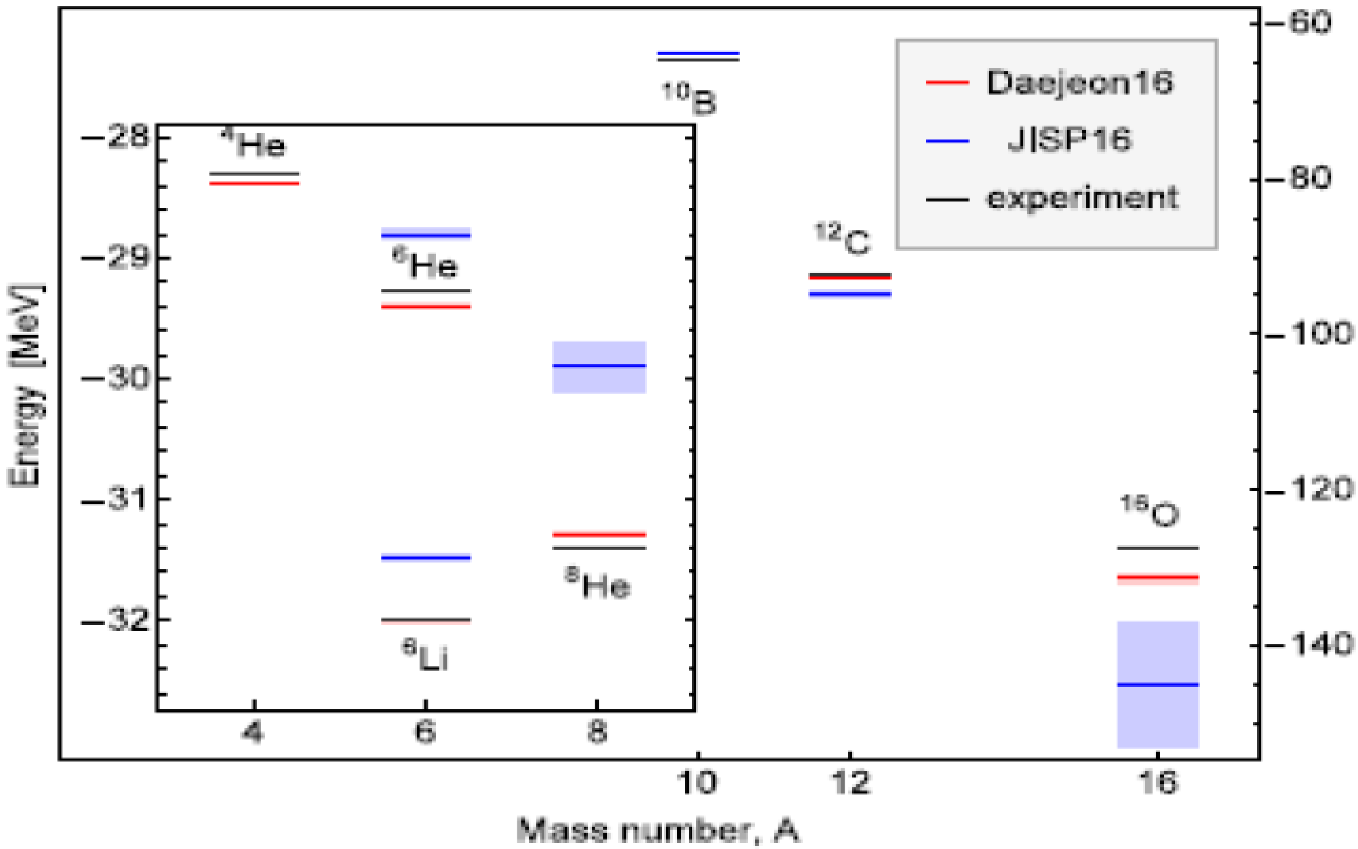
Dimensions of the M-scheme basis for 72Kr, 24Si and 12C nuclei.

Typical number of the nonzero matrix elements in a column – $10^2 \div 10^4$.

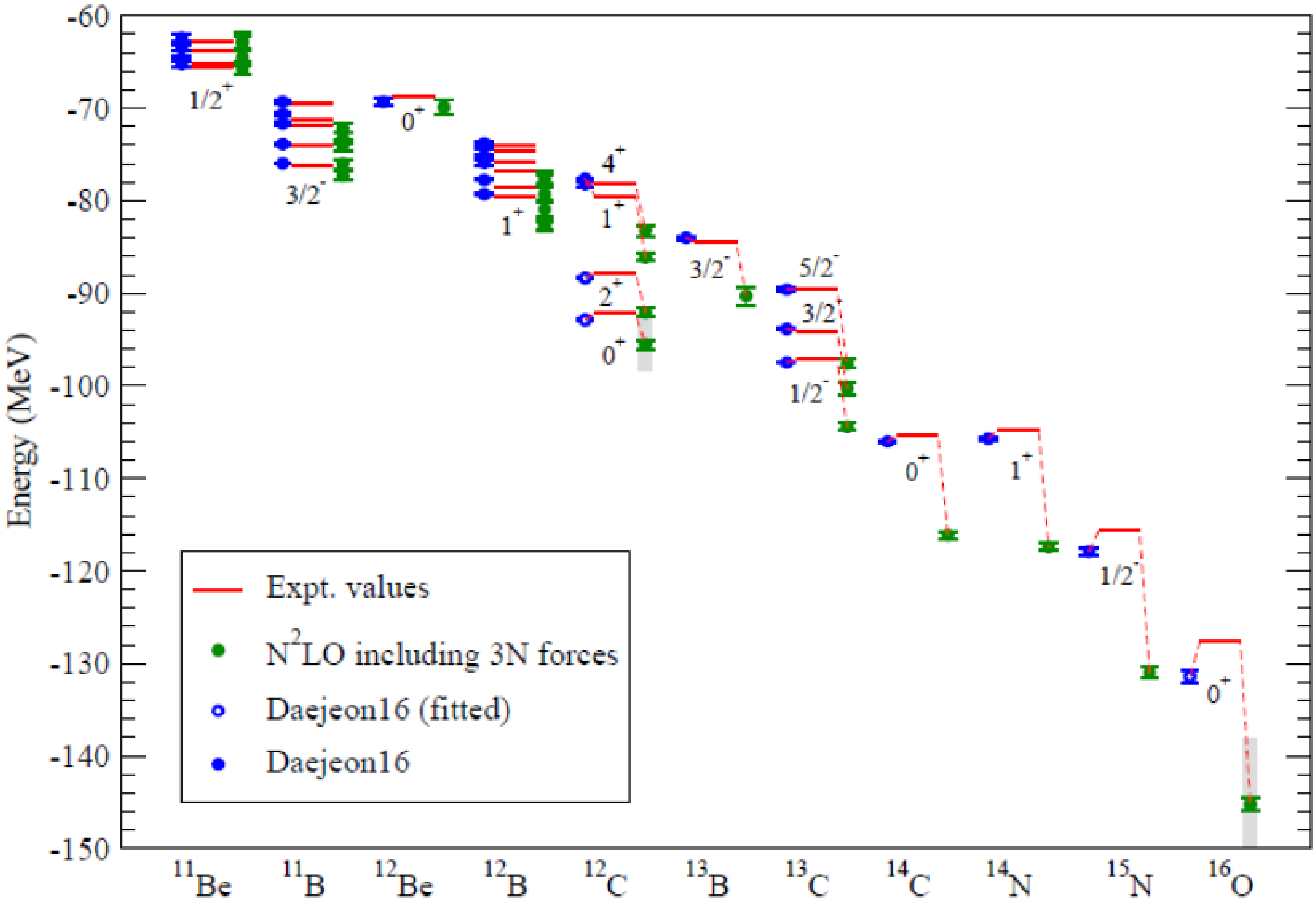
An interesting strategy is to get rid of at least a part of inessential matrix elements before a calculation. This strategy was also progressed and significant advances have been made in realization of it. Namely the SU(3)-NCSM, which uses natural symmetries of a nuclear system (Dreyfuss A. C., Launey K. D., Dytrych T. et al. PRC 95 044312 (2017)) and No-Core Monte-Carlo Shell Model (NCMCSM) (Abe T., Maris P., Otsuka T. et al. PRC 86 05430, (2012)) were created.

Another goal is to study continuous spectrum. The No-Core Shell Model / Resonating Group Model (NCSM / RGM) and No-Core Shell Model with Continuum (NCSMC) were created by P. Navratil, S Quaglioni, R. Roth, G. Hupin S., Baroni et al. (a lot of papers) for these purposes. However the area of applicability of these models is the lightest nuclei and decay channels with light clusters A≤3. Another approach of such a type (SS-HORSE) was presented by V. Kulikov at this conference.

Nevertheless, the canonical NCSM remains the basic tool for ab initio studies.



Total binding energies of nuclei calculated using JISP16 and Daejeon16 potentials.



Spectra of low-laying states of nuclei.

Thus, the calculations within the NCSM with accurately calibrated potentials reproduce quite well the most important experimental data: the total binding energies of nuclei and excitation energies of their lower levels. A number of the procedures, extrapolating the results of the calculations of the total binding energies to infinite basis were proposed (an example is contained in the presentation by D. Rodkin). These procedures provide very good reproduction of the experimental data. As a result, for unmeasured levels and transitions, one can reasonably use these theoretical data. Calculations of the probabilities of beta transitions in the NCSM are planned by ab initio community and good quality results can be expected for allowed transitions.

The ab initio approaches reproduce the magnrtic moments of nuclei and the probabilities of electromagnetic M1-transitions well.

On the other hand the NCSM calculations of quadrupole moments and probabilities of E2 and especially E1 electromagnetic transitions are not so advantageous as the just mentioned.

The situation with the calculation of core sizes in NCSM seems to be interesting. The capabilities of modern supercomputers are not enough to achieve complete convergence of results for nuclei with the mass A > 4. Nevertheless the radii of heavier nuclei obtained in this way often seem more reliable than experimental ones (see the analysis presented by I.A. Mitropolsky).

So, in some areas of nuclear spectroscopy, ab initio calculations are already becoming competitive with experiment.

NUCLAR DECAY WITH THE EMISSION OF NUCLEONS OR CLUSTERS

Decays into nucleon and cluster channels play a role in nuclear spectroscopy of light nuclei comparable with the role of electromagnetic transitions. Alpha, neutron, deuteron, proton and triton (from the unknown state of the 11Be nucleus formed in the process of beta decay of 11Li) decays were observed. The theoretical description of these processes is more or less uniform. It is based on the theory of cluster channels.

CLUSTERING IN AB INITIO APPROACHES

Two-fragment clustering in bound and resonance states is considered. To take the effect into account cluster channel orthogonal functions method (CCOFM) is proposed.

The cluster-channel terms of CCOFM basis are built in the form:

$$\Psi_A = \frac{1}{W} \hat{A}\{\Psi_{A_1} \Psi_{A_2} \varphi_{nlm}(\vec{\rho})\}_{JM_J}, \qquad (2)$$

$A = A_1 + A_2$, $\hat{A}$ is the antisymmertizer, Ψ_{A_i}

– translationally-invariant WF of the fragment; $\varphi_{nlm}(\vec{\rho})$

– the oscillator WF of the relative motion.

A technique has been developed for transforming such functions to superpositions of Slater determinants.

The basis may be exploited itself or being added to a certain number of shell-model WF (polarization terms). In the latter case a hybrid basis appears. Projecting of an eigenvector on the states of this basis will define the cluster characteristics of a nuclear state (an eigenvector of the Hamiltonian).

However some problems remain. In general case WFs (2) are not orthogonal one to another and to the shell-model components.
Moreover the basis of cluster-channel terms (2) incorporating all channels of a certain fragmentation A1 + A2 (a complete set of internal states of each cluster) is complete but this basis is overload and even linear dependent.

Thus, the next step in creationg of a basis is to build orthonormalized WFs including the cluster terms of several channels and the polarization terms. The WFs are obtained by diagonalization of the overlap matrix

$$\left\| \begin{matrix} [1] & \left\langle \Psi^{(j)}_{pol} \middle| \hat{A} \middle| \prod_{i=1,2} \Phi^{A_i}_{N_i,L_i,M_i}(\vec{R}_i)\Psi_{A_i} \right\rangle \\ \left\langle \Psi^{(j)}_{pol} \middle| \hat{A} \middle| \prod_{i=1,2} \Phi^{A_i}_{N_i,L_i,M_i}(\vec{R}_i)\Psi'_{A_i} \right\rangle & \left\langle \prod_{i=1,2} \Phi^{A_i}_{N'_i,L'_i,M'_i}(\vec{R}_i)\Psi'_{A_i} \middle| \hat{A}^2 \middle| \prod_{i=1,2} \Phi^{A_i}_{N_i,L_i,M_i}(\vec{R}_i)\Psi_{A_i} \right\rangle \end{matrix} \right\| \quad (4)$$

in which the terms of the products are expressed in the form of superpositions of SDs.

Eigenvectors of the matrix normalized by its eigenvalues shape the desirable basis of CCOFM taking the form of SD linear combinations.

CLUSTER FORM FACTORS AND SPECTROSCOPIC FACTORS

The value CFF of the channel $A_1 + A_2$ is defined as:

$$F_l(r) = \left\langle \Psi_{base} \middle| N^{-1/2} \hat{A}\{\Psi_{A_1} \frac{1}{\rho^2} \delta(\rho - \rho')Y_{lm}(\Omega_{\rho'})\Psi_{A_2}\} \right\rangle.$$

where the norm (overlap) kernel takes the form:

$$N(\rho', \rho'') = \left\langle \hat{A}\{\Psi_{A_1} \frac{1}{\rho^2} \delta(\rho - \rho'')Y_{lm}(\Omega_{\rho''})\Psi_{A_2}\} \middle| \hat{A}\{\Psi_{A_1} \frac{1}{\rho^2} \delta(\rho - \rho')Y_{lm}(\Omega_{\rho'})\Psi_{A_2}\} \right\rangle.$$

Let us denote its eigenvalues and eigenfunctions

$\varepsilon_k \equiv EV_k[N(\rho, \rho')]$ and $f_l^k(\rho) \equiv EF[N(\rho, \rho')]$ respectively.

By representing of the delta function as

$$\delta(\rho - \rho') = \sum_n \left| \varphi_{nl}(\rho') \right\rangle \left\langle \varphi_{nl}(\rho) \right|$$

the eigenfunctions turn out to be expressed through the oscillator wave functions

$$f_l^k(\rho) = \sum_n B_{nl}^k \phi_{nl}(\rho).$$

And the eigenvalues take the form:

$$\varepsilon_k =< \hat{A}\{\Psi_{A_1} \; f_l^k(\vec{\rho})\Psi_{A_2}\} | \hat{1} | \hat{A}\{\Psi_{A_1} \; f_l^k(\vec{\rho})\Psi_{A_2}\} >;$$

Thus the final forms of CFF and SF are the following:

$$\Phi_l(\rho) == \sum_k \varepsilon_k^{-1/2} \sum_{nk} C_{AA_1A_2}^{nl} \, f_l^k(\rho);$$

$$S_{AA_1A_1(l)} \equiv \int |\Phi_l(\rho)|^2 \, \rho^2 d\rho = \sum_k \varepsilon_k^{-1} \sum_{nn'} C_{AA_1A_2}^{nl} C_{AA_1A_2}^{n'l} B_{nl}^k \; B_{n'l}^k. \quad (5)$$

where

$$C_{AA_1A_2}^{nl} = \left\langle \Psi_{base} \middle| \hat{A}\{\Psi_{A_1} \frac{1}{\rho^2} \varphi_{nl}(\rho) Y_{lm}(\Omega_{\rho'}) \Psi_{A_2}\} \right\rangle$$

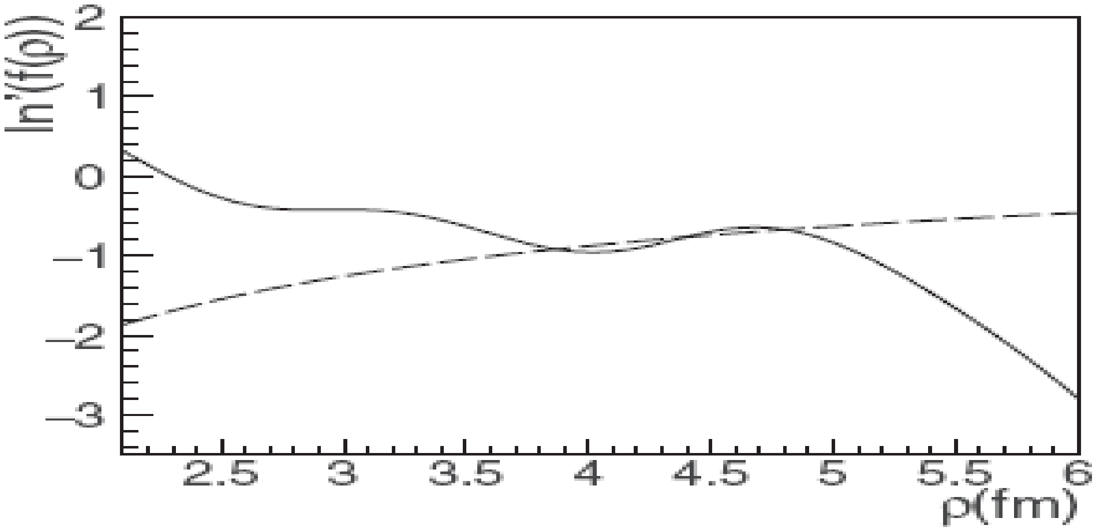
This definition of CFF and SF plays an important role in the theory of nuclear reactions. The authors of the idea (T. Fliessbach, and H. J. Mang, Nucl. Phys. A **263** 75 (1976)) called the values “new” CFF and SF.

ASYMPTOTIC CHARACTERISTICS (ANC, PARTIAL AND TOTAL Γ)

The asymptotic characteristics are deduced using the matching procedure and various R-matrix approaches.

To determine the position of the matching point R_p of the CFF and the asymptotic WF, the condition of equality of the logarithmic derivatives is used:

$$\frac{F'_l(r)}{F_l(r)} = \frac{W'_{-\eta_0,l+1/2}(2kr)}{W_{-\eta_0,l+1/2}(2kr)} \quad \text{or} \quad \frac{F'_l(r)}{F_l(r)} = \frac{G'_l(\eta,r)}{G_l(\eta,r)} \qquad \frac{F_l(\eta,r)}{G_l(\eta,r)} = P_l(r_>) \ll 1$$



Logarithmic derivatives of CFF *(solid line) and* function $G_l(\rho)$ *(dashed line) for 7/2⁻ state of* 7Li nucleus for 4He+3H channel.

Therefore, the decay width of this resonance is given by the expression:

$$ANC = \frac{rF_l(R_p)}{W_{-\eta,l+1/2}(2kR_p)}$$

$$\Gamma_l = \frac{\hbar^2}{\mu k}\left(\frac{F_l(R_p)}{G_l(\eta,R_p)}\right)^2$$

If the resonance is wide, then the partial width is calculated using the standard R-matrix theory

$$\Gamma_\alpha = \frac{\hbar^2}{\mu k}(F_l(\eta,r)^2 + G_l(\eta,r)^2)^{-1}_{r=R_p} F_l(R_p)^2$$

For determining the decay width of subthreshold resonance, we used the formulation of (Mukhamedzhanov and Tribble,1999):

$$\Gamma_{subth}(E) = \frac{\hbar^2}{\mu_{ab}} kR_p(F_l(\eta,r)^2 + G_l(\eta,r)^2)^{-1}_{r=R_p} \frac{W^2_{-\eta_0,l+1/2}(2k_0P_p)}{R_p}\left|ANC_{ab}\right|^2$$

RESULTS AND DISCUSSION

The results of all calculations presented bellow are obtained by use of NN-potential **Daejeon16** which is built starting from N3LO forces (A.M. Shirokov, I.J. Shin, Y. Kim et al, PLB **761** 87 (2016)} are explored. The potential are well-tested in the calculations of A-nucleon systems (A≤16). Potential JISP16 is sometimes used too.

Code Bigstick is used for shell-model computing of the polarization terms and the internal WFs of clusters.

Strongly clustered systems 7Li and 8Be are considered.

The matrix of the Hamiltonian has the dimension about $10^{8.5} \times 10^{8.5}$.

SPECTRUM OF 7Li NUCLEUS

J^π	E_{expt}	E_{theor}	$E^{expt}_{\alpha+t}$	$E^{theor}_{\alpha+t}$	ANC_α [66]	ANC_α theor.	E^{expt}_n	E^{theor}_n	l	J_n	ANC_n theor.	ANC_n [78]
$3/2^-$	39.245	39.110	−2.467	−2.529	3.57 ± 0.15	3.44	−7.25	−7.639	1	1/2	−1.618	1.652
									1	3/2	1.317	1.890
$1/2^-$	38.768	38.279	−1.99	−1.69	3.0 ± 0.15	2.95	−6.77	−6.81	1	1/2	−0.531	−0.540
									1	3/2	1.979	−2.540

J^π	E_{expt}	E_{theor}	$E^{expt}_{\alpha+t}$	$E^{theor}_{\alpha+t}$	Γ_α [74]	Γ_α theor.	E^{expt}_n	E^{theor}_n	Γ_n [67]	l	J_c	$\Gamma_n(ANC_n)$ theor.	Γ theor. [42]
$7/2^-$	34.593	34.409	2.195	2.172	0.069	0.065	−2.59	−2.938		3	1/2	0.013[a]	$\Gamma_\alpha = 0.214$
$1/2^+$	32.804	28.921	3.984	7.66	3.15 [67]	7.4	−0.81 [67]	2.55	0.295 keV[b]	0	1/2	0.54 keV[b]	
$5/2^-$	32.641	31.610	4.147	4.971	0.918[c]	0.564	−0.65	−0.139		1	3/2	0.199[a]	$\Gamma_\alpha = 0.785$
$5/2^-$	31.791	30.816	4.997	5.765	0.033 [67]	0.797	0.2	0.655	0.058	1	3/2	0.053	$\Gamma_n = 0.210$
										1	1/2	0.088	
$3/2^-$	30.495	28.175	6.293	8.406	4.7[c]	0.873	1.5	3.296	0.867 [79]	1	3/2	1.0	$\Gamma_n = 1.70$
										1	1/2	0.23	
$1/2^-$	30.155	27.280	6.633	9.301	2.7[c]	0.282	1.84	4.191		1	3/2	1.0	$\Gamma_n = 2.44$
													$\Gamma_\alpha = 0.435$
$7/2^-$	29.675	28.489	7.133	8.092	0.437[c]	0.453	2.32	2.982		3	1/2	0.72 keV	$\Gamma_n = 0.039$
$3/2^-$		27.047		9.60		1.25		4.424		1	1/2	0.785	

[a] ANCs ($fm^{-1/2}$).

[b] Γ ($E_n = 1$ eV).

[c] Total decay width.

J^π	T	E_{expt}	E_{theor}	E_{He}^{expt}	E_{He}^{theor}	Γ_{tot} [74]	SF_{He}	$\Gamma_{He}(ANC_{He})$ theor.	$E_{Li^*}^{expt}$	$E_{Li^*}^{theor}$	SF_{Li^*}	$\Gamma_{Li^*}(ANC_{Li^*})$ theor.
$1/2^-$	1/2	30.155	27.280	−0.885	1.538		0.1465	0.343[a]	−1.727	0.638	0.0453	0.259[a]
$3/2^-$	3/2	28.005	27.247	1.265	1.571	0.260 ± 0.35	0.1638	0.111	0.433	0.671	0.3770	0.117

[a] ANCs ($fm^{-1/2}$).

The experience of investigating the states of the 7Li nucleus and, first of all, the channels of their neutron decay made it possible to extend the studies to exotic systems 7He and 10Li. Approximately 10 levels in each nucleus and a large number of widths of their neutron decay channels were predicted. The results are presented by D. Rodkin.

SPECTRUM of 8Be NUCLEUS (DAEJEON16)

$J^\pi, \bar{T}$	E_{bind} MeV	E^*_{dae} MeV	E^*_{exp}MeV(T)	SF	Γ_{th} MeV	Γ_{exp} MeV
0^+_1,0	56.25	0.0	0.0 (0)	0.879	7.29 eV	5.57 (6.8)* eV
2^+_1,0	52.85	3.40	3.03±0.01 (0)	0.849	1.17	1.513
4^+_1,0	44.63	11.62	11.35±0.15 (0)	0.792	2.41	3.5
$\mathbf{0^+_2}$,0	44.54	**11.71**	—	**0.813**	**8.86**	—
$\mathbf{2^+_2}$,0.001	42.09	**14.16**	—	**0.715**	**3.57**	—
2^+_3,0.971	39.65	16.59	16.626±0.003 (0+1)	0.0025	0.019	0.108
2^+_4,0.078	39.05	17.19	16.922±0.003 (0+1)	0.354	0.416	0.074
$\mathbf{4^+_2}$,0.001	37.48	**18.76**	—	**0.288**	**3.39**	—
2^+_5,0.065	35.02	21.22	20.1±0.01 (0)	0.0459	0.434	0.8 (1.1)
0^+_3,0.852	35.01	21.23	20.2±0.01 (0)	0.0208	0.056	0.7 (≤1)
0^+_4,0.315	34.44	21.80	—	0.0610	0.092	—
2^+_6,0.966	34.27	21.97	—	0.0039	0.002	—
4^+_3,0.007	34.24	22.00	19.86±0.05 (0)	0.441	5.13	0.7
2^+_7,0.028	33.57	22.70	22.2 (0)	0.059	0.135	0.8
2^+_8,0.996	33.22	23.02	—	0.001	0.004	—
0^+_5,0.017	32.91	23.33	—	0.215	1.71	—
4^+_4,0.997	32.69	23.55	—	0.0009	0.009	—

SPECTRUM of 8Be NUCLEUS (JISP16)

J^π,T	E_{bind} MeV	E^*_{th} MeV	$E^*_{exp} MeV(T)$	SF	Γ_{th} MeV	Γ_{exp} MeV
$0^+,0$	53.766	0.0	0.0 (0)	0.841	6.72 eV	5.57 (6.8)* eV
$2^+,0$	50.112	3.663	3.03±0.01 (0)	0.803	1.08	1.513
$4^+,0$	41.277	12.498	11.35±0.15 (0)	0.729	1.65	3.5
$2^+,0.987$	37.113	16.663	.16.626±0.003 (0+1)	0.0003	0.005	0.108
$2^+,0.038$	36.4457	17330	16.922±0.003 (0+1)	0.018	0.305	0.074
$0^+,0.002$	34.797	18.978		0.698	10.45	
$4^+,0.002$	33.866	19.909	19.86±0.05 (0)	0.022	0.249	0.7
$2^+,0.008$	33.060	20.715	20.1±0.01 (0)	0.166	2.91	0.8 (1.1)
$2^+,0.995$	31.871	21.904		0.0045	0.079	
$0^+,0.986$	31.550	22.226	20.2±0.01 (0)	0.0086	0.110	0.7 (≤1)
$2^+,0.005$	31.447	22.329	22.2 (0)	0.354	5.53	0.8
$2^+,0.999$	30.158	23.617		0.0008	0.0011	
$0^+,0.039$	30.136	23.640		0.3175	2.48	
$4^+,0.999$	29.416	24.359		0.00015	0.0026	
$2^+,0.004$	28.716	25.059		0.270	3.67	
$4^+,0.001$	27.579	26,196		0.216	3.74	

	E (MeV)	E*(MeV)	S_α	Γ (MeV)
0+	56.500	0.0	-----	6.8(5.6) эВ
2+	53.460	3.040	-----	1.5
4+	45.100	11.40	-----	3.5
0+	56.241	0.0	0.880	7.29 эВ
2+	52.840	3.401	0.849	1.31
4+	44.617	11.624	0.792	3.24
0+	53.776	0.0	0.841	6.72 эВ
2+	50.112	3.663	0.803	1.08
4+	41.277	12.498	0.729	1.65

Properties of the first rotational band of 8Be. Black-experiment, red – results of Jaejeon16 calculations, blue – results of JISP16 calculations.

	E (MeV)	E*(MeV)	S_α	Γ (MeV)
0+	44.54	11.71	0.813	8.86
2+	42.09	14.16	0.715	3.57
4+	37.48	18.76	0.288	3.39
0+	34.80	18.98	0.698	10.45
2+	31.45	22.33	0.354	5.53
4+	27.58	26.20	0.216	3.74

Properties of the predicted second rotational band of 8Be.
Red – results of Jaejeon16 calculations, blue – results of JISP16 calculations.

SUMMARY

1. The development of theoretical concepts designed to describe the structure of the atomic nuclei, computational methods and supercomputer technology has led to the present time to the creation of ab initio approaches with high predictive power.
2. For some types of spectroscopic data concerning light nuclei, using such approaches it is possible to obtain information that is not inferior, but sometimes even superior, in terms of its reliability, that the one provided by modern measuring methods.
3. As a result, from my point of view, a new situation has arisen at present in the area under discussion for conducting studies based on the synthesis of experiment and theory and enriching both of these areas of research work. This applies primarily to exotic nuclear systems and states.


THANK YOU FOR YOUR ATTENTION!