Study of neutron channels properties of light neutron-rich nuclei within the framework of ab initio approaches

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At present, light stable nuclei have been well studied experimentally. Their stable and resonance states and the partial and total decay widths into different decay channels are well known.

Thus, the focus of current researches has shifted towards studying the characteristics of unstable nuclei, in particular, light neutron-rich nuclei. Their properties are still mostly unknown.

In particular, only three lowest levels of the unstable ^{7}He nucleus are known.

E_x (MeV)	$J^\pi; T$	Γ_{cm}	Decay
g.s.	$(\frac{3}{2})^-; \frac{3}{2}$	150 ± 20 keV[a]	n
2.92 ± 0.09[a]	$(\frac{5}{2}^-); \frac{3}{2}$[a]	1990 ± 170 keV[a]	n
(5.8 ± 0.3)[a]		4 ± 1 MeV[a]	n

In this report, we use the theoretical method developed by us for studying the characteristics of neutron decay channels in unstable neutron-rich ^{7}He and ^{10}Li nuclei.

Methods for computation of light nuclei cluster characteristics

Traditional microscopic approaches:	Ab initio methods:
1) Phenomenological NN-potentials	1) Realistic NN-potentials, based on the data of nucleon-nucleon scattering and on chiral effective field theory
2) The use of free fitting parameters	2) Realistic description of nuclei and clusters wave functions
3) Wave functions of the nucleus and subsystems are described using minimal shell model configurations.	3) Due to extreme growth of Slater determinants basis there is a hard limit on mass of described nuclei
4) Possibility of accurate description of far asymptotic region.	

Current ab initio methods for describing the light nuclei structure and reactions with their participation have limited areas of applicability, which means that further work in this area is required. Most of the developed ab initio methods are based either on the No-Core Shell Model (NCSM) or on the Gamow Shell Model (GSM).

Main properties of NCSM model

The No-Core Shell Model approach is as follows:

1) The NCSM basis consists of A-nucleon Slater determinants:

$$\psi_i = \begin{vmatrix} \psi_{n_1 l_1 j_1 m_1}(r_1) & \dots & \psi_{n_A l_A j_A m_A}(r_1) \\ \dots & \dots & \dots \\ \psi_{n_1 l_1 j_1 m_1}(r_A) & \dots & \psi_{n_A l_A j_A m_A}(r_A) \end{vmatrix}. \qquad (1)$$

Basis restrictions are set by the condition $\sum_{k=1}^{A} 2n_k + l_k \le N_{\max}^{sum}$.

2) On this basis, the A-nucleon Schrödinger equation is solved

$$H\psi = E\psi, \psi = \sum_i c_i \psi_i, H = T + U$$

3) The solution to this equation is equivalent to the problem of finding the eigenvalues and eigenfunctions of the matrix

$$\begin{Vmatrix} \langle\psi_1|H|\psi_1\rangle & \dots & \langle\psi_N|H|\psi_1\rangle \\ \dots & \dots & \dots \\ \langle\psi_1|H|\psi_N\rangle & \dots & \langle\psi_N|H|\psi_N\rangle \end{Vmatrix}$$

On modern supercomputers, it is possible to achieve the dimension of the basis 10^{10}.

4) For calculating eigenvalues and eigenfunctions of this matrix, the iterative Lanczos algorithm is usually used.

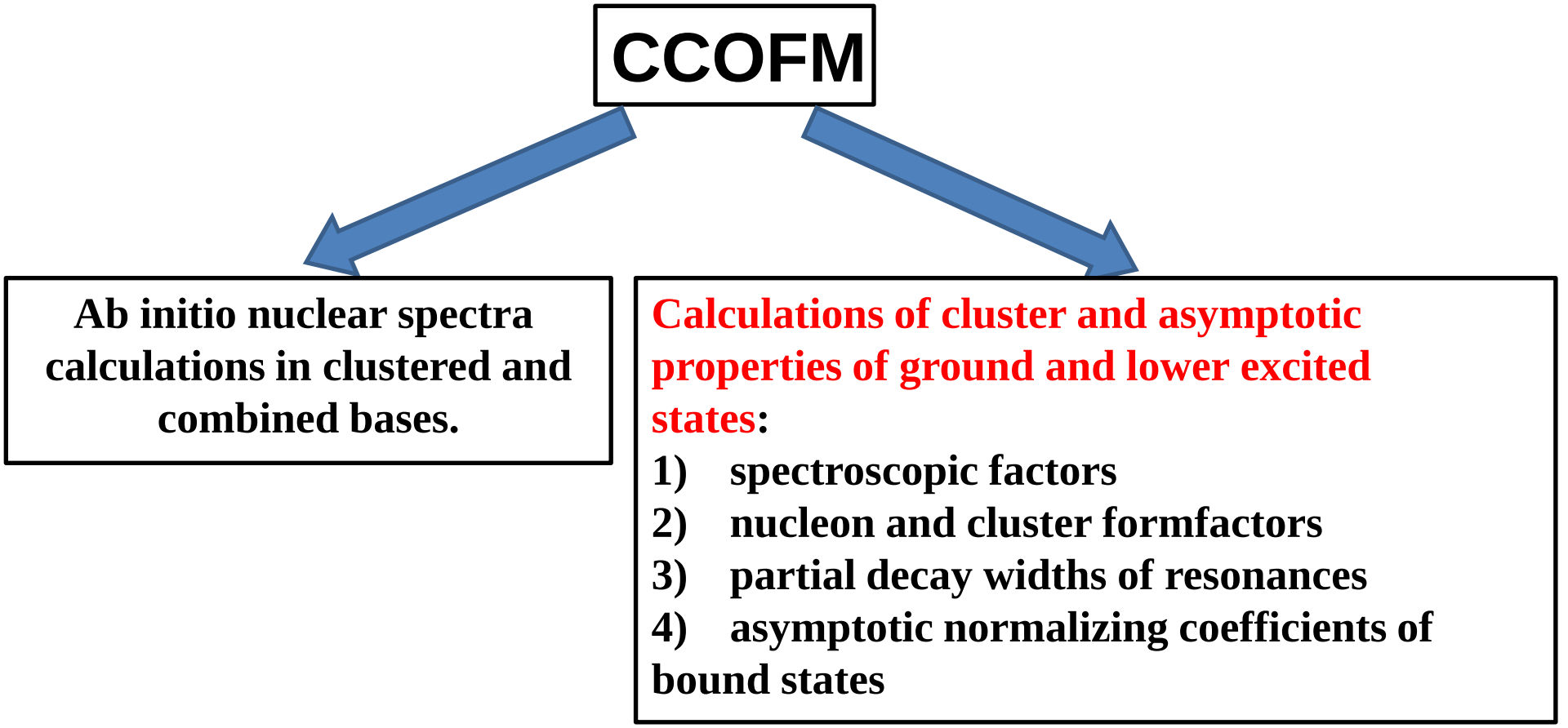
5) As a result, using this approach can perform ab initio calculations of the total binding energies, spectra, and wave functions of the ground and lower excited states of light nuclei.

6) Ab initio calculation of the light nuclei wave functions makes it possible to obtain the widths of electromagnetic transitions, beta decays, and the values of magnetic and quadrupole moments better than in other theoretical approaches.

DIFFICULTIES: The excessive growth of the Slater determinant basis in the description of mass-average nuclei or long-range asymptotics of light nuclei wave functions, limited methods for calculating cluster characteristics and, as a consequence, problems in calculating both nuclear reactions and characteristics like charge and material radii.

CCOFM Method

Cluster Channel Orthogonal Functions Method (CCOFM) can be used for ab initio calculations of various nuclear characteristics: :



Construction of cluster components of the CCOFM basis

The translation-invariant A-nucleon wave function is used as an element of the CCOFM cluster basis

$$\Psi^{i}_{A} = \frac{1}{W} A\{\Psi_{A_1,J_1}\Psi_{A_2,J_2}\varphi_{nl}(\rho)\}_{JM_J},$$

For ab initio calculations, the cluster basis WF should be represented as a superposition of Slater determinants (SD):

$$\Psi^{i}_{A} = \sum_{j=1}^{N_{size}} C^{i}_{j}\psi_{j}, N_{size} \approx N^{\max}_{NCSM}$$

The method for constructing the cluster basis WF:

$\Phi^{A_i}_{000}(R_i)\Psi_{A_i}$ -NCSM solutions for separate clusters with zero vibrations along the center of mass coordinate

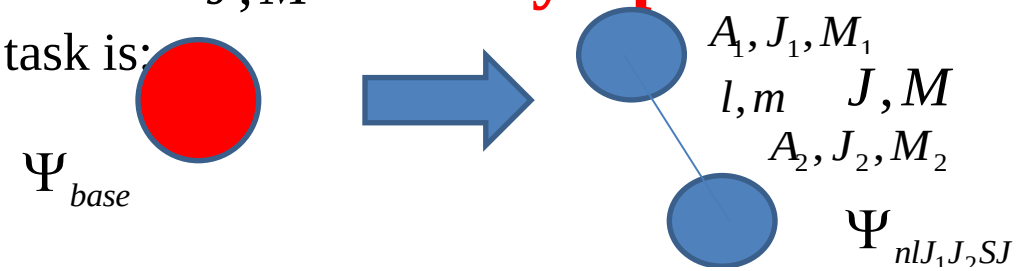
Obtaining the WF of clusters with non-zero vibrations along the center of mass coordinates $\Phi^{A_i}_{NLM}(R_i)\Psi_{A_i}$ as linear combinations of SD using the method of cluster coefficients

Calculation of the cluster basis wavefunctions using the Talmi-Moshinsky transformation

$$\Psi^{i}_{A} = \frac{1}{W} A\left\{\sum_{N_1,L_1,M_1,N_2,L_2,M_2} \left\langle \begin{matrix} 000 \\ nlm \end{matrix} \middle| \begin{matrix} N_1,L_1,M_1 \\ N_2,L_2,M_2 \end{matrix} \right\rangle \Phi^{A_1}_{N_1,L_1,M_1}(R_1)\Psi_{A_1,J_1}\Phi^{A_2}_{N_2,L_2,M_2}(R_2)\Psi_{A_2,J_2}\right\}_{JM}.$$

Methodology of calculating cluster J, M and asymptotic characteristics

1)The task is:



2) Basis wavefunctions are $\Psi_A^{nlJ_1J_2SJ} = A\{\left\{\Psi_{A_1}^{J_1M_1}\Psi_{A_2}^{J_2M_2}\right\}_{SM_S}\varphi_{nlm}(\rho)\}_{JM_J}$,

3) Wavefunctions are orthogonalized separately for each channel

$$\Psi_A^i = \frac{1}{\sqrt{\varepsilon_i}} A\{\left\{\Psi_{A_1}^{J_1M_1}\Psi_{A_2}^{J_2M_2}\right\}_{SM_S}\varphi_{ilm}(\rho)\}_{JM_J},\ \varphi_{ilm}(\rho) = \sum_n B_n^i \varphi_{nlm}(\rho)$$

4) Projection of initial nuclei wavefunction Ψ_{base} into concrete decay channel (obtaining the spectroscopic amplitude)

$$C_{MDC}^{nl} = \left\langle \Psi_{base} \middle| \Psi_A^{nlJ_1J_2SJ} \right\rangle$$

5) Obtaining the cluster formfactor and spectroscopic factor as its normalization.

$$F_l(\rho) = \sum_n A_n^l \varphi_{nl}(\rho),\ A_n^l = \sum_{i,n'} (\varepsilon_i)^{-1/2} C_{MDC}^{n'l} B_{nl}^i B_{n'l}^i,\ S_l = \sum_n \left(A_n^l\right)^2.$$

Calculation of asymptotic characteristics of nuclei decay channels

1) Calculations of narrow neutron resonances

In this case, in a sufficiently wide sub-barrier region, the nuclear attraction is negligible.

For all points of this region, the relation $n_l(r) >> j_l(r)$ takes place.

This means that the contribution of the regular function can be neglected.

To determine the matching point R_{point} of ab initio WF with an asymptotic two-body solution, the following equation is used:

$$\frac{F'_l(r)}{F_l(r)} = \frac{n'_l(r)}{n_l(r)}$$

Then the partial width of the neutron resonance of this channel is

$$\Gamma = \frac{h^2}{\mu k}\left(\frac{F_l(R_{point})}{n_l(R_{point})}\right)^2$$

2) Calculations of cluster and proton resonances decay width

For cluster and proton channels, the Coulomb functions are used instead of the Bessel and Neumann functions.

3) Calculations of asymptotic normalizing coefficients (ANC) of bound states

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

4) Calculations of the wide or high-lying resonances widths

For high-lying resonances in the matching region, the contribution of the regular function $j_l(r)$ cannot be neglected, and the width is calculated within the framework ot one of the versions of the R-matrix theory, where the matching radius is determined by reaching the plateau of the value

$$\left(F_l^2(\rho_m)+G_l^2(\rho_m)\right)^{-1}\left(\Phi_A^{c_\kappa}(\rho_m)\right)^2$$

And the partial width, in turn, is equal to:

$$\Gamma = \frac{\hbar^2}{\mu k_0}\left(F_l^2(\rho_m)+G_l^2(\rho_m)\right)^{-1}\left(\Phi_A^{c_\kappa}(\rho_m)\right)^2$$

Application of the CCOFM method for calculating the asymptotic characteristics of light nuclei

The developed CCOFM method makes it possible to calculate both the values of the total binding energies and spectroscopic factors of light nuclei, and their asymptotic characteristics.

For an oscillatory basis, the range of distances, where the solutions of the Schrödinger equation are correctly described, expands proportionally to $[N^{max}_{tot}]^{1/2}$.

In this regard, the microscopic description of cluster channels at distances where the asymptotic representation is valid requires an extremely high-dimensional basis.

Therefore, the cutoff parameter (the maximum total number of oscillatory quanta of the Slater determinant used in the basis) for the ^{7}He nucleus and positive parity states is 16, and the corresponding SD basis is $2.2 * 10^{7}$, and for the ^{10}Li nucleus and negative parity states, respectively, 16 and $6.5 * 10^{8}$.

Application of extrapolation methods to refine the total binding energies of nuclear levels

The calculations of the ^{7}He and ^{10}Li spectra were carried out on the NCSM bases of large dimensions, but the complete convergence of the total binding energies of the levels has not yet been achieved. It should also be noted that the values of the partial decay widths depend on the value of the penetrability function at the convergence radius:

$$P_l(\rho_m) = (\mathrm{F}_l^2(\rho_m) + \mathrm{G}_l^2(\rho_m))^{-1/2}.$$

For unstable nuclei, it is difficult to accurately determine the energies of resonance levels by experimental methods; therefore, it is necessary to refine the results of theoretical calculations, which is done using extrapolation methods. The extrapolation function for the total binding energy depends on five free parameters $E_\infty, a, c, d, k_\infty$ and additional parameters:

$$b = \sqrt{\hbar / m\omega}, \quad \Lambda_i = b^{-1}\sqrt{2\left(N_{tot,i}^{*\max} + 3/2\right)}, \; L_i = b\sqrt{2\left(N_{tot,i}^{*\max} + 3/2\right)},$$

$$L_t = L_i + 0.54437 \cdot b \cdot (\mathrm{L}_{i=0}/\mathrm{b})^{-1/3}.$$

$$E_{state}(\mathrm{N}_{tot,i}^{*\max}, \hbar\omega) = \mathrm{E}_\infty + a \cdot \exp(-\mathrm{c}\,\Lambda_i^2) + \mathrm{d} \cdot \exp(-2\,\mathrm{k}_\infty \mathrm{L}_t).$$

Experimentally-known levels of ^{7}He and ^{10}Li nuclei

E_x (MeV)	$J^\pi; T$	Γ_{cm}	Decay
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2.92 ± 0.09[a]	$(\frac{5}{2}^-); \frac{3}{2}$[a]	1990 ± 170 keV[a]	n
(5.8 ± 0.3)[a]		4 ± 1 MeV[a]	n

Experimentally-known levels of ^{7}He

E_{res} [b] (MeV)	Γ_{lab} (MeV)	J^π [c]
0.24 ± 0.04	0.10 ± 0.07	(1^+)
0.53 ± 0.06	0.35 ± 0.08	(2^+)
1.40 ± 0.08	0.20 ± 0.07	$(2^- + 1^-)$
2.35 ± 0.10	1.2 ± 0.4	$(1^+, 3^+)$
2.85 ± 0.07	0.3 ± 0.2	$(1^-, 2^+)$
4.19 ± 0.10	0.12 ± 0.08	
4.64 ± 0.10	0.2 ± 0.1	$(3^-, 2^+)$
5.7 ± 0.1	0.2 ± 0.1	

Experimentally-known levels of ^{10}Li

E_{res} [a] (MeV)	Γ_{res} (MeV)	Reaction	Reference	J^π
≤ 0.05		$^{nat}C(^{11}Be, ^{9}Li + n)X$	(1995ZI03)	
≤ 0.05		$^{9}Be(^{18}O, ^{9}Li + n)X$	(1999TH01)	
≤ 0.05		$^{9}Be(^{11}Be, X)^{10}Li$	(2001CH31)	
≤ 0.05		$^{9}Be(^{11}Be, X)^{10}Li$	(2001CH46)	
< 0.1	< 0.23	$^{11}B(^{7}Li, ^{8}B)^{10}Li$	(1994YO01)	
0.1 ± 0.1	0.4 ± 0.1	$^{11}B(\pi^-, p)^{10}Li$	(1998GO30)	(1^-)
0.15 ± 0.15	< 0.4	$^{11}B(\pi^-, p)^{10}Li$	(1990AM05)	
≤ 0.15		$^{nat}C(^{18}O, ^{9}Li)X$	(1993KR09)	
see [b,c]				
0.24 ± 0.04	0.10 ± 0.07	$^{10}Be(^{12}C, ^{12}N)^{10}Li$	(1999BO26)	1^+
(0.35 ± 0.11) [d]	< 0.32	$^{2}H(^{9}Li, p)^{10}Li$	(2003SA07)	

Different versions of the energies of the lowest resonances of ^{10}Li

Comparison of the theoretically calculated and experimentally obtained energies of the ^{6}He and ^{7}He levels

J^π	$E_{exp.}$ [73]	$E_{th.}^{lim.}$	$E_{th.}^{extr.}$	$E_{exp.}^{*}$	$E_{th.}^{*lim.}$	$E_{th.}^{*extr.}$
0_1^+	29.269	29.239	29.397	0	0	0
2_1^+	27.472	27.199	27.533	1.797	2.040	1.864
2_2^+	23.7	24.161	25.856	5.6	5.087	3.541

Energies, spin, and parities of ^{6}He levels

J^π	$E_{exp.}$ [73]	$E_{th.}^{lim.}$	$E_{th.}^{extr.}$	$E_n^{extr.}$
$3/2_1^-$	28.83^a	28.625	28.850	547
$1/2_1^+$	—	26.057	27.701	1696
$1/2_1^-$	—	25.864	27.079	2318
$5/2_1^-$	25.91^b	24.743	25.960	3437
$3/2_1^+$	—	24.115	25.905	3492
$5/2_1^+$	—	23.937	25.833	3564
$3/2_2^-$	—	23.966	25.455	3921

a) – $E_n^{exp.}$=430 keV b) – $E_n^{exp.}$=3360 keV

Energies, spin, and parities of ^{7}He levels

Comparison of the theoretically calculated and experimentally obtained energies of the ^{9}Li and ^{10}Li states

J^π	$E_{exp.}$	$E_{th.}^{lim.}$	$E_{th.}^{extr.}$	$E_{exp.}^{*}$	$E_{th.}^{*lim.}$	$E_{th.}^{*extr.}$
$3/2_1^-$	44.559 (45.340)	44.699	45.084	0.0	0.0	0.0
$1/2_1^-$	41.868 (42.649)	41.274	41.886	2.691	3.425	3.198

Energies, spin, and parities of ^{9}Li levels

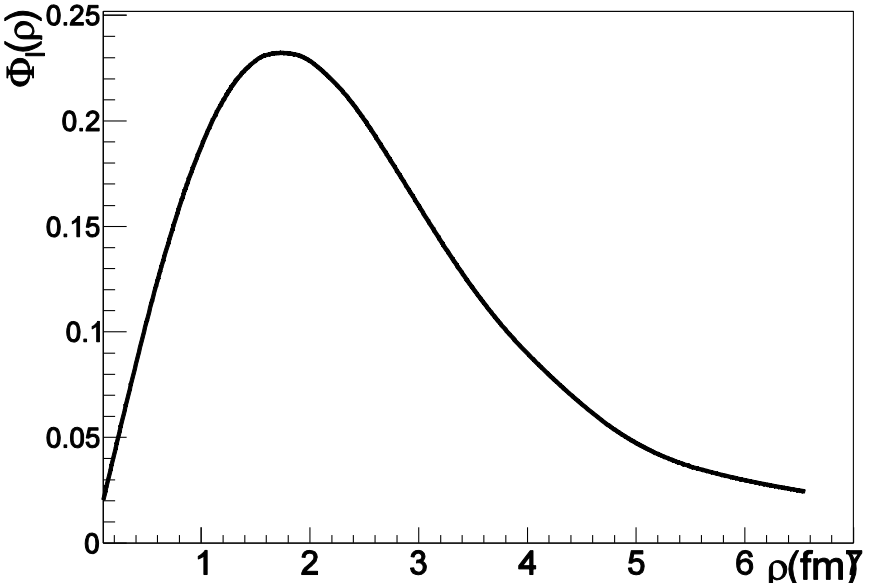
J^π	$E_{exp.}$	$E_{th.}^{lim.}$	$E_{th.}^{extr.}$	$E_{th.}^{n,extr.}$
1_1^+	44.139 (44.920)	43.166	44.133	0.951
2_1^-	—	41.622	43.697	1.387
2_1^+	43.840	42.614	43.660	1.424
1_1^-	—	40.696	43.111	1.973
0_1^+	—	40.178	42.445	2.639
1_2^-	—	38.981	41.788	3.296
2_2^+	—	37.941	41.064	4.020
1_2^+	—	38.511	40.883	4.201
4_1^-	—	38.802	40.790	4.294
0_1^-	—	38.248	40.782	4.302
3_1^+	—	37.725	40.495	4.589
2_2^-	—	37.195	40.133	4.951

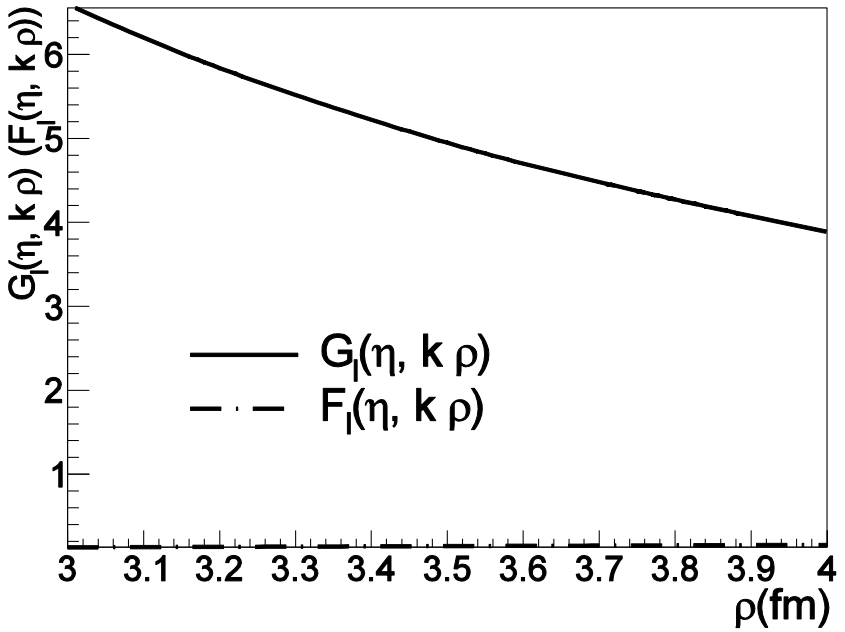
Energies, spin, and parities of ^{10}Li levels

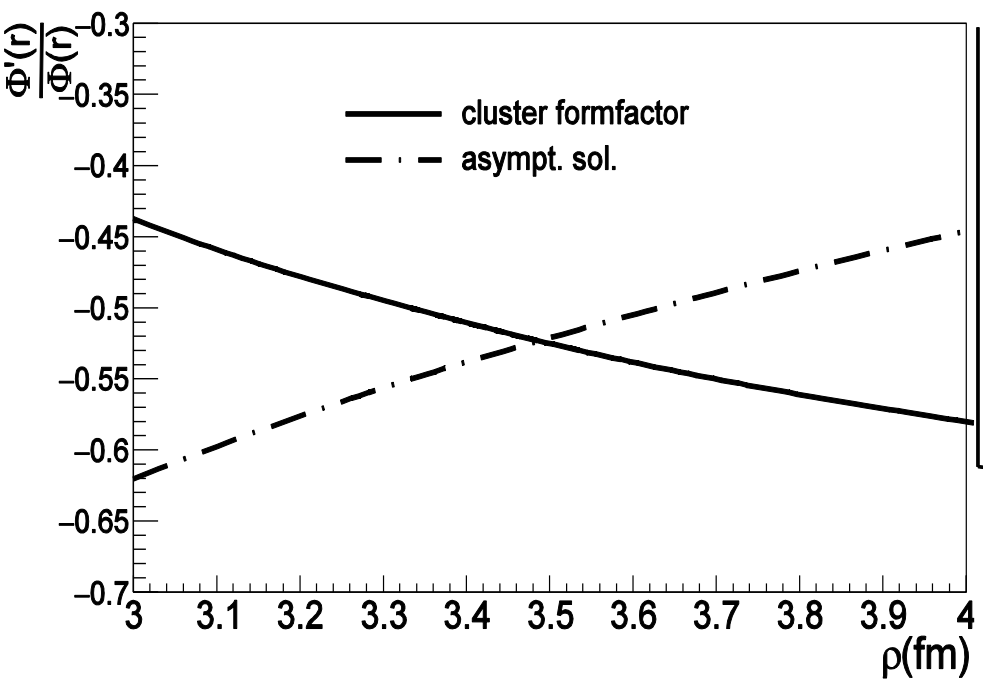
Method for obtaining of the asymptotic characteristics on the example of the lowest state ^{10}Li

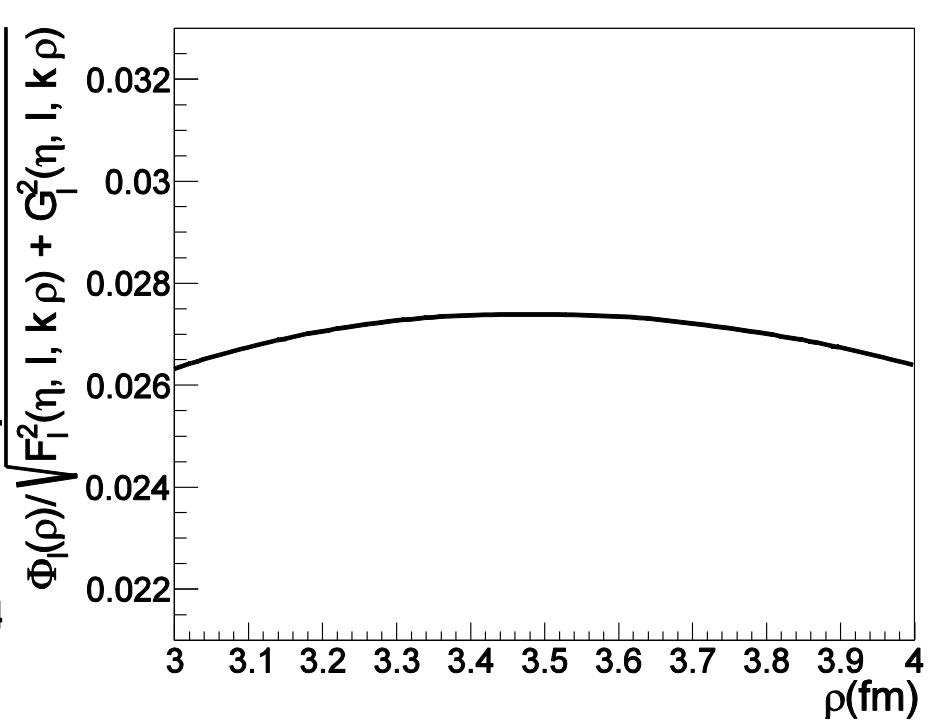
The calculation of the asymptotic characteristics is carried out by the matching of the ab initio calculated formfactor with an asymptotic two-body solution. The upper figure shows the CFF of the lowest resonance of ^{10}Li- 1^{+}.

This resonance is narrow and the regular asymptotic solution can be neglected in the vicinity of the matching point.



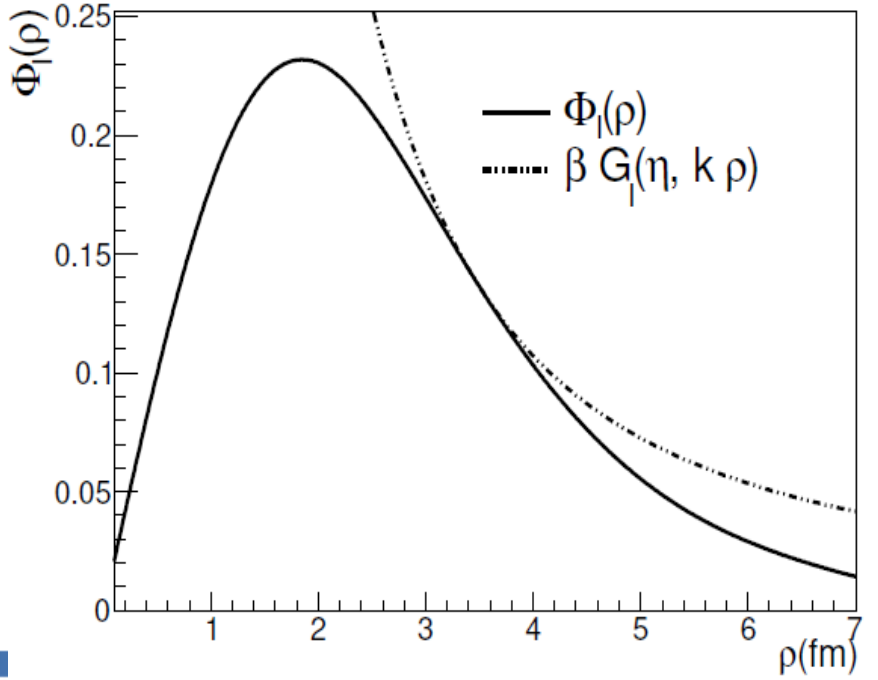






The matching radius for the given neutron resonance is 3.48 fm.

The relationship between the CFF and the asymptotic solution in the vicinity of the matching point is stable, which ensures the stability of the solution with respect to fluctuations in the matching radius value.



The theoretically calculated widths of the ^{7}He resonances

J^π (^{7}He)	J^π (^{6}He)	$E_n^{lim.}$	$E_n^{extr.}$	l(S)	SF	$\Gamma^{lim.}$	$\Gamma_{11}^{extr.}$	$\Gamma_{13}^{extr.}$	Γ_{tot} [30]	Γ_{tot} [8]	Γ_{tot} [33]	$\Gamma_{tot}^{exp.}$
$3/2_1^-$	0_1^+	614	547	1(1/2)	0.730	387	336	334[a]	300	178	110	182
$1/2_1^+$	0_1^+	3184	1696	0(1/2)	0.844	3670	2670	2670	—	—	—	—
$1/2_1^-$	0_1^+	3375	2318	1(1/2)	0.814	2440	1940	1850	2890	—	4300	750[b]
	2_1^+	1335	454	1(3/2) 3(5/2)	0.509 $0.21\cdot10^{-3}$	812 —	253 0.47 eV	221 0.46 eV	—	—	—	—
$5/2_1^-$	0_1^+	4496	3437	3(1/2)	$0.37\cdot10^{-3}$	110 eV	56 eV	52 eV	—	—	—	—
	2_1^+	2606	1573	1(3/2) 1(5/2)	0.420 0.758	1366 1783	980 1200	881 1060	1070	2300	1360	1990
$3/2_1^+$	0_1^+	5124	3492	2(1/2)	0.041	125	84.4	83.4	—	—	—	—
	2_1^+	3084	1628	0(3/2) 2(3/2)	0.752 0.051	3430 58	2590 22.3	2490 17.9	—	—	4400	—
$5/2_1^+$	0_1^+	5302	3564	2(1/2)	0.126	382	285	258	—	—	—	—
	2_1^+	3262	1700	0(5/2) 2(5/2)	0.704 0.019	3100 29	2210 13.7	2240 11.1	—	—	5000	—
	2_2^+	224	23	0(5/2) 2(3/2)	0.001 0.012	9.3 38.6 eV	3.33 0.15 eV	2.98 0.14 eV	—	—	—	—

a) – for the experimental value of $3/2_1^-$ state resonance energy 430 keV computed value Γ =250 keV; b) – there are other experimental results: 2.0 MeV [75] and 10.0 MeV [76].

The theoreticallv calculated widths of the ^{10}Li resonances

J^π (^{10}Li)	$E^{extr.}_{^{10}Li}$	J^π (^{9}Li)	$E^{extr.}_{^{9}Li}$	$E^{extr.}_{n}$	l(S)	SF	$\Gamma^{extr.}$
1^+_1	44.133	$3/2^-_1$	45.084	0.951	1(1)	0.8031	718[a]
					1(2)	0.7985	679[b]
2^-_1	43.697	$3/2^-_1$	45.084	1.387	2(1)	0.0721	18
					2(2)	0.0702	19
					0(2)	0.741	$2.01*10^3$
2^+_1	43.660	$3/2^-_1$	45.084	1.424	1(1)	0.6871	908
					1(2)	0.8429	$1.15*10^3$
					3(1)	0.0004	$3.62*10^{-3}$
1^-_1	43.111	$3/2^-_1$	45.084	1.973	2(1)	0.0002	—
					2(2)	0.0386	34
					0(1)	0.789	$2.99*10^3$
0^+_1	42.445	$3/2^-_1$	45.084	2.639	1(1)	0.6871	$1.73*10^3$
1^-_2	41.788	$3/2^-_1$	45.084	3.296	2(1)	0.3902	521
					2(2)	0.1988	321
					0(1)	0.0545	243
		$1/2^-_1$	41.886	0.098	0(1)	0.3945	170
2^+_2	41.064	$3/2^-_1$	45.084	4.02	1(1)	0.08746	271
		$1/2^-_1$	41.886	0.822	1(1)	0.00778	5.68
1^+_2	40.883	$3/2^-_1$	45.084	4.201	1(1)	0.0311	135
					1(2)	0.0050	26.6
					3(2)	0.0081	5.2
		$1/2^-_1$	41.886	1.003	1(0)	0.4024	388
					1(1)	0.7325	676

Resonance energies, decay widths of open channels (keV), and channel spectroscopic factors of ^{10}Li nucleus states. For the experimental value of 1^+_1 state resonance energy 420 keV computed value Γ is a) in case of l(S) = 1(1) – 257 keV. b) in case of l(S) = 1(2) – 243 keV.

Main findings and conclusions

I. Within the framework of the cluster channels orthogonal functions method, the partial decay widths into all open neutron channels of resonance states of ^{7}He and ^{10}Li nuclei were calculated.

II. The results of these calculations showed good agreement with the known experimental data, are not inferior to them in accuracy and provide much more information.

III. The results of theoretical calculations of the ^{10}Li system show the absence of a low-lying narrow resonance 1-, whose presumptive existence is indicated by a number of experiments.

IV. The obtained theoretical spectra of ^{7}He and ^{10}Li nuclei can be useful for analyzing the results of experiments at FLNR JINR, since the cross sections for nuclear reactions in this energy range are approximated within the framework of the R-matrix theory, whose input parameters can also be the energies and reduced partial widths of resonances.

THANK YOU FOR YOUR ATTENTION!