AB INITIO STUDY OF RADII OF SIX-NUCLEON ISOBAR ANALOGUE STATES

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The matter and charge point-nucleon radii r_m and r_p are among the most significant observables characterizing atomic nuclei.

For nuclei far from the stability band, the study of these quantities causes serious difficulties, which are gradually overcome with the development of methods for obtaining ever more intense beams of short-lived isotopes.

However, such experiments are still technically difficult and their results obtained for the same isotope often differ markedly from experiment to experiment.

Radius r_n is unavailable for measurements and therefore is calculated using the expression

$$Ar_m^2 = Zr_p^2 + Nr_n^2.$$

At the same time, it should be stressed that simplified approaches, such as the shell model with an inert core and, even more so, schemes that consider the core without taking into account its nucleon structure, encounter difficulties in describing long-range nucleon correlations, exchange effects, etc. and, therefore, give results of limited reliability. So, the use of ab initio approaches is one of few possible ways to solve this task.

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 applied.

5) As a result, using this approach one 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 without use a fit 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 possibilities to take into account clustering and, as a consequence, problems in calculating nuclear reactions.

In NCSM computations we use the universal approach, which makes it possible to calculate all three size parameters. After calculating the binding energy and wave function, we proceed for calculating matter, neutron and proton radii for point nucleons.

$$r^2_{m(n,p)} = (1/N_{A(N,Z)}) \sum_i (\vec{r}_{m(n,p),i} - \vec{r}_{cm})^2$$

$$\text{где } \vec{r}_{cm} = (1/N_A) \sum_i \vec{r}_{m,i}$$

Calculation of this characteristic can be expressed as combination of one-body and two-body operators:

$$\vec{r}^{\,2}_{m(n,p)} = -\frac{4}{N_A \cdot N_{A(N,Z)}} \langle \Psi_A | \sum_{i<i} \vec{r}_{m(n,p,i)} \vec{r}_{m,j} | \Psi_A \rangle + \langle \Psi_A | r^2_{cm} | \Psi_A \rangle + \frac{N_A - 2}{N_A \cdot N_{A(N,Z)}} \langle \Psi_A | \sum_i r^2_{m(n,p),i} | \Psi_A \rangle.$$

which can be expressed through one- and two-body transition densities

$$\langle \Psi_A | r^2_{cm} | \Psi_A \rangle = \frac{3(\hbar c)^2}{2mc^2 \hbar\omega N_A}, \quad \langle \Psi_A | \sum_i \vec{r_i}^{\,2} | \Psi_A \rangle = \frac{1}{\sqrt{2J+1}} \sum_{k_a, k_b} OBTD(k_a, k_b, \lambda = 0) \langle k_a || r^2 || k_b \rangle,$$

$$\langle \Psi_A | \sum_{i<j} \vec{r}_i \vec{r}_j | \Psi_A \rangle = \frac{1}{\sqrt{2J+1}} \sum_{k_a \le k_b, k_c \le k_d, J_0} \langle k_a k_b J_0 || \vec{r}_1 \vec{r}_2 || k_c k_d J_0 \rangle \cdot TBTD(k_a, k_b, k_c, k_d, J_0).$$

The one-body and two-body transition densities (OBTD) and (TBTD) included in these formulas are expressed in terms of the matrix elements of the products of fermion second quantization operators:

$$OBTD(k_a, k_b, \lambda = 0) = \langle \Psi_A ||[a^+_{k_a} \otimes \tilde{a}_{k_b}]^{\lambda=0} || \Psi_A \rangle. \quad TBTD(k_a, k_b, k_c, k_d, J_0) = \langle \Psi_A ||[[a^+_{k_a} \otimes a^+_{k_b}]_{J_0} \otimes [\tilde{a}_{k_c} \otimes \tilde{a}_{k_d}]_{J_0}]^{\lambda=0} || \Psi_A \rangle.$$

The results of calculation of total binding energies and radii of ground state of ^6He using the Daejeon16 interaction

Total binding energy

hw/N	8	10	12	14
7	-23.97494	-25.94097	-27.27443	-28.14070
7.5	-25.01714	-26.757	-27.871	-28.5505
8	-25.88517	-27.398	-28.309	-28.8296
9	-27.16779	-28.25818	-28.83912	-29.13451
10	-27.96993	-28.72505	-29.08645	-29.25761
11	-28.43821	-28.95961	-29.19379	-29.30251
12,5	-28.76355	-29.09333	-29.23953	-29.31324
15	-28.85941	-29.09351	-29.21041	-29.27924

Matter radius

hw/N	8	10	12	14
7	2.60572	2.54793	2.50768	2.4821
7.5	2.53269	2.48541	2.4573	2.44303
8	2.47213	2.43556	2.41907	2.41608
9	2.38082	2.36766	2.37197	2.38648
10	2.32074	2.32865	2.3481	2.37178
11	2.28221	2.30591	2.33432	2.36197
12,5	2.24705	2.2842	2.3179	2.3476
15	2.20781	2.25163	2.28787	2.31818

Neutron radius

hw/N	8	10	12	14
7	2.8138	2.76039	2.72375	2.70146
7.5	2.73556	2.69322	2.66941	2.65938
8	2.67073	2.63993	2.62838	2.6305
9	2.57308	2.56716	2.57793	2.59866
10	2.50886	2.52532	2.55235	2.58274
11	2.46743	2.50066	2.53713	2.57172
12,5	2.42903	2.47624	2.51821	2.55474
15	2.38425	2.43799	2.48235	2.51947

Proton radius

hw/N	8	10	12	14
7	2.12939	2.05822	2.00691	1.97146
7.5	2.0681	2.00623	1.96556	1.93923
8	2.0171	1.96402	1.93363	1.91658
9	1.93998	1.90705	1.89399	1.89202
10	1.88909	1.87438	1.87395	1.88014
11	1.85714	1.85611	1.86363	1.87329
12,5	1.82957	1.84097	1.85343	1.86554
15	1.80387	1.82261	1.83818	1.85107

Application of extrapolation methods to refine the energies and radii of the lower state of ^{6}He

For refining the energy calculation, the well-known one-dimensional extrapolation method A5 is used:

$$E_{gs} = E_{\infty} + ae^{-c\Lambda_2^2} + E_{IR}(\lambda_t)\,,\; E_{IR}(\lambda_t) = de^{-2k_{\infty}/\lambda_t}\,.$$

E_{6He} = -29.374 MeV - for Daejeon16 potential.

E_{6He} = -29.126 MeV - for JISP16 potential.

To refine the calculation of the radii, the one-dimensional extrapolation method A3 is used:

$$r^2 = r_{\infty}^2\left[1 - (c_0\beta^3 + c_1\beta)e^{-\beta}\right]$$

Extrapolation violates the relationship between the matter, neutron and proton radii. In view of this, the introduced measure of the ratio violation is important for assessing the reliability of these results.

$$\Delta \;=\; 1 \,-\, [(Zr_p^2 + Nr_n^2)/Ar_m^2]^{1/2}$$

for Daejeon16 potential

r_m = 2.439 fm r_n = 2.643 fm r_p = 1.892 fm

In this case, the violation factor Δ is small and equal to 1.1 %.

for JISP16 potential

r_m = 2.369 fm r_n = 2.583 fm r_p = 1.858 fm

In this case, the violation factor Δ is equal to 0.5 %.

We also propose an alternative 2D extrapolation procedure. In this case, extrapolation is carried out according to the two-dimensional surface data (N^*_{max}, hw)

$$r^2_{m(n,p)}(\mathcal{N}^*_{max}, \hbar\omega) = r^2_{\infty,m(n,p)} + P_k(\hbar\omega)\exp(-\alpha\sqrt{\mathcal{N}^*_{max}})$$

where $P_k(x)$ – a polynomial of degree k whose coefficients are fitting parameters.

For Daejeon16 potential

$$r_m = 2.430(6)\ \mathrm{fm}, \qquad r_n = 2.663(3)\ \mathrm{fm}, \qquad r_p = 1.871(16)\ \mathrm{fm}.$$

In that case violation factor Δ is really small and it is equal to 0.09 %.

Radius of neutron halo is equal to $r_h = r_n - r_p = 0.792$ fm.

For JISP16 potential

$$r_m = 2.342(7)\ \mathrm{fm}, \qquad r_n = 2.582(3)\ \mathrm{fm}, \qquad r_p = 1.799(6)\ \mathrm{fm}.$$

For this calculation violation factor Δ is small and is equal to 0.36 %.

Radius of neutron halo in this case is equal to $r_h = r_n - r_p = 0.783$ fm.

Results of calculations of the total binding energy and radii of the ground state of ^{6}Li.

Total binding energy

hw/N	8	10	12	14
10	-30.4903	-31.310	-31.710	-31.898
12,5	-31.36396	-31.731	-31.895	-31.973
15	-31.49272	-31.748	-31.875	-31.946
17,5	-31.38032	-31.646	-31.795	-31.885
20	-31.13861	-31.471	-31.668	-31.791
22,5	-30.78201	-31.223	-31.490	-31.661

Matter radius

hw/N	8	10	12	14
7	2.61064	2.55543	2.5175	2.49126
7,5	2.54246	2.49727	2.47033	2.45502
10	2.34367	2.35028	2.36838	2.38929
12,5	2.27199	2.30702	2.3398	2.36786
15	2.23284	2.27603	2.31199	2.34116
17,5	2.19428	2.24041	2.27826	2.30904

Neutron radius

hw/N	8	10	12	14
7	2.59989	2.54443	2.50706	2.48126
7,5	2.53219	2.48684	2.46014	2.44511
10	2.33483	2.34114	2.35904	2.37969
12,5	2.26359	2.29805	2.33051	2.35817
15	2.22476	2.2673	2.30284	2.33162
17,5	2.18654	2.23204	2.26943	2.29978

Proton radius

hw/N	8	10	12	14
7	2.62134	2.56638	2.52789	2.50123
7,5	2.55268	2.50767	2.48047	2.46488
10	2.35248	2.35939	2.37768	2.39885
12,5	2.28037	2.31596	2.34904	2.3775
15	2.2409	2.28473	2.3211	2.35067
17,5	2.202	2.24875	2.28705	2.31827

Results of calculations of the total binding energy and radii of the 0^+ T=1 state of ^{6}Li.

Total binding energy

hw/N	8	10	12	14
7,5	-24.230	-25.9557	-27.0572	-27.7281
10	-27.112	-27.869	-28.236	-28.414
12,5	-27.879	-28.224	-28.383	-28.467
15	-27.966	-28.216	-28.347	-28.427
17,5	-27.833	-28.098	-28.253	-28.352
20	-27.587	-27.913	-28.114	-28.245
22,5	-27.238	-27.662	-27.928	-28.104

Matter radius

hw/N	8	10	12	14
7	2.62826	2.57602	2.54288	2.52344
7,5	2.55486	2.51302	2.4915	2.48499
10	2.34102	2.35516	2.38124	2.4121
12,5	2.26554	2.30762	2.34693	2.38211
15	2.22331	2.27101	2.31145	2.3462
17,5	2.18151	2.2305	2.27174	2.30658
20	2.13723	2.18758	2.22997	2.26577

Neutron radius

hw/N	8	10	12	14
7	2.61444	2.56045	2.5263	2.50501
7,5	2.5415	2.49819	2.47507	2.46673
10	2.32951	2.34137	2.36544	2.39356
12,5	2.25458	2.29444	2.33145	2.36444
15	2.21307	2.25866	2.29722	2.33009
17,5	2.1721	2.2193	2.25896	2.2921
20	2.12871	2.17766	2.21868	2.25302

Proton radius

hw/N	8	10	12	14
7	2.64201	2.5915	2.55935	2.54174
7,5	2.56814	2.52776	2.50783	2.50311
10	2.35247	2.36887	2.39695	2.43049
12,5	2.27644	2.32073	2.3623	2.39966
15	2.23351	2.2833	2.3256	2.3622
17,5	2.19087	2.24165	2.28444	2.32097
20	2.14572	2.19745	2.2412	2.27845

Results of calculations of the total binding energy and radii of the ground state of ^6Be.

Total binding energy

hw/N	8	10	12	14
7,5	-22.914	-24.617	-25.7030	-26.3643
8	-23.732	-25.214	-26.107	-26.622
9	-24.934	-26.013	-26.596	-26.903
10	-25.681	-26.445	-26.825	-27.018
12,5	-26.406	-26.777	-26.959	-27.062
15	-26.467	-26.752	-26.909	-27.009

Matter radius

hw/N	8	10	12	14
6	2.86	2.80011	2.75712	2.72794
7	2.66359	2.622	2.60003	2.59572
7,5	2.58896	2.55828	2.54882	2.55626
8	2.5272	2.50778	2.51054	2.53026
9	2.43468	2.43909	2.463	2.49988
10	2.37367	2.39908	2.43728	2.48237
12,5	2.29522	2.34727	2.39653	2.4432

Neutron radius

hw/N	8	10	12	14
6	2.3024	2.222	2.16209	2.11817
7	2.14214	2.07931	2.03789	2.01377
7,5	2.08094	2.02764	1.99711	1.98271
8	2.03035	1.98614	1.96629	1.96091
9	1.95452	1.93022	1.9272	1.93606
10	1.90505	1.89838	1.90707	1.9228

Proton radius

hw/N	8	10	12	14
6	3.10142	3.04833	3.01086	2.9865
7	2.88924	2.85491	2.83967	2.84236
7,5	2.80873	2.78596	2.78397	2.79931
8	2.74208	2.7315	2.74246	2.77141
9	2.64224	2.65723	2.69119	2.73861
10	2.57621	2.61371	2.66309	2.71931
12,5	2.49014	2.55544	2.61638	2.67344

To refine the energy values in NCSM calculations using the Daejeon16 potential of the ^{6}Be, ^{6}He and ^{6}Li states, the A5 extrapolation method is used:

$E_{6He\ 0+}$ = -29.3747 MeV

$E_{6Li\ 1+}$ = -32.064 MeV

$E_{6Be\ 0+}$ = -27.039 MeV

$E_{6Li\ 0+}$ = -28.702 MeV

The experimental data are as follows:

$E_{6He\ 0+}$ = -29.269 MeV

$E_{6Li\ 1+}$ = -31.995 MeV

$E_{6Be\ 0+}$ = -26.826 MeV

$E_{6Li\ 0+}$ = -28.433 MeV

To refine the calculation of the ^{6}Be, ^{6}He and ^{6}Li radii, the A3 extrapolation method is used:

$r_{m\ 6He}$ = 2.439 fm | $r_{n\ 6He}$ = 2.643 fm | $r_{p\ 6He}$ = 1.890 fm

$r_{m\ 6Li\ 0+}$ = 2.491 fm | $r_{n\ 6Li\ 0+}$ = 2.477 fm | $r_{p\ 6Li\ 0+}$ = 2.502 fm

$r_{m\ 6Li\ 1+}$ = 2.457 fm | $r_{n\ 6Li\ 1+}$ = 2.444 fm | $r_{p\ 6Li\ 1+}$ = 2.466 fm

$r_{m\ 6Be\ 0+}$ = 2.598 fm | $r_{n\ 6Be\ 0+}$ = 1.970 fm | $r_{p\ 6Be\ 0+}$ = 2.876 fm

To refine the energy values in NCSM calculations using the JISP16 potential of the ^{6}Be, ^{6}He and ^{6}Li states, the A5 extrapolation method is used:

$E_{6He\ 0+}$ = -29.126 MeV

$E_{6Li\ 1+}$ = -31.639 MeV

$E_{6Be\ 0+}$ = -26.652 MeV

$E_{6Li\ 0+}$ = -27.969 MeV

The experimental data are as follows:

$E_{6He\ 0+}$ = -29.269 MeV

$E_{6Li\ 1+}$ = -31.995 MeV

$E_{6Be\ 0+}$ = -26.826 MeV

$E_{6Li\ 0+}$ = -28.433 MeV

To refine the calculation of the ^{6}Be, ^{6}He and ^{6}Li radii, the A3 extrapolation method is used:

$r_{m\ 6He}$ = 2.369 fm	$r_{n\ 6He}$ = 2.583 fm	$r_{p\ 6He}$ = 1.858 fm
$r_{m\ 6Li\ 0+}$ = 2.462 fm	$r_{n\ 6Li\ 0+}$ = 2.437 fm	$r_{p\ 6Li\ 0+}$ = 2.509 fm
$r_{m\ 6Li\ 1+}$ = 2.435 fm	$r_{n\ 6Li\ 1+}$ = 2.421 fm	$r_{p\ 6Li\ 1+}$ = 2.449 fm
$r_{m\ 6Be\ 0+}$ = 2.562 fm	$r_{n\ 6Be\ 0+}$ = 1.996 fm	$r_{p\ 6Be\ 0+}$ = 2.826 fm

Main results and conclusions

I. The matter, neutron, and proton radii of the ground and the isobar analogue states of ^{6}He, ^{6}Li, and ^{6}Be were calculated. The results cannot clearly confirm the existence of a neutron-proton halo around He core in the 0^+ state of the ^{6}Li nucleus, because the radius of the 0^+ state of ^{6}Li does not differ significantly from the radius of the ground state of 1^+.

II. Calculations have shown that the ^{6}He halo has a large size - 0.7-0.8 fm. These results confirm the neutron halo measurement data presented in Phys. Rev. C 92, 034608 (2015).

III. A new two-dimensional procedure for the extrapolation of the values of matter, neutron, and proton radii obtained in no-core shell model calculations, using various harmonic oscillator bases characterized by different parameters of N_{max} and hw to infinite basis size is proposed. It gives results that are in good agreement with experiment and, in fact, makes it possible to get rid of the violation of the relationship between matter, charge, and neutron radii.

THANK YOU FOR YOUR ATTENTION!