Ab initio calculation of neutron resonances of light nuclei

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STATEMENT OF THE GENERAL PROBLEM

A general strategy is formulated by K. Wildermuth and Y.C. Tang “A unified theory of the Nucleus” Veiweg, Braunschweig, 1977.

The goal is to build mathematical and computational methods making possible to describe various nuclear structures and nuclear processes simultaneously in a same microscopic(ab initio) manner.

Significant advances have been made towards the goal. 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.

ALGEBRAIC VERSION OF NCSMC

The line of attack of our approach is to build the algebraic version of the No-Core Shell Model with Continuum (AV NCSMC).

NCSMC → **AV NCSMC**

Unlikely NCSMC the use of cluster coefficients technique allows to obtain purely algebraic approach.

AV RGM formalism fits naturally into NCSM being based on the oscillator representation.

In following work formalism of AV NCSMC is discussed and results of calculation of neutron resonances of ^{5}He are demonstrated.

Ab initio calculation of light nuclei with NCSM

The basis model for ab initio calculation of light nuclei is No-Core Shell Model (NCSM).

Its essential elements are the following.

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

where $\psi_{n_1 l_1 j_1 m_1}(r_1)$ - single-particle oscillator function

The basis limits are $\sum_{k=1}^{A} 2n_k + l_k \le N_{\max}^{sum}, \quad N_{\max}^{sum} \approx 12$

2) A-nucleon equation $H\psi = E\psi, \psi = \sum_i c_i \psi_i, H = T + U$

3) The solution of the equation is equal to calculation of lowest eigenvalues of the following matrix

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

Dimension of the matrix is around $10^{7-9} \times 10^{7-9}$

4) Calculation method is iterative Lanczos algorithm for eigenvalues and eigenvectors

5)The results are total binding energies and wave functions of the ground and lower exited states of light nuclei obtained in ab initio calculations.

6) DISADVANTAGES: Difficulties in calculations of the asymptotic characteristics of various nucleon and cluster channels(it means difficulties with decay widths and cross sections).

Reason: The large average distance between the core and the halo nucleon or between clusters is a serious obstacle to the use of NCSM approach - even an extremely large NCSM basis is insufficient.

Construction of cluster terms of AV NCSMC basis

The cluster-channel terms are built in the form:

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

$A = A_1 + A_2$, $A -$ is the antisymmertizer,

Ψ_{A_i} – translationally-invariant WF of the fragment i,

$\varphi_{nlm}(\rho)$ – the WF of the relative motion.

For ab initio calculations the cluster-channel terms must be expressed as the superposition of Slater determinants $\Psi^{i}_{A} = \sum_{j=1}^{N_{size}} C^{i}_{j}\psi_{j}, N_{size} \approx N^{\max}_{NCSM}$

The algorithm for construction of the basis WF:

$\Phi^{A_i}_{000}(R_i)\Psi_{A_i}$ - NCSM solutions for individual clusters

$N_{N_i,L_i}(\mu^{\dagger})^{N_i-L_i}Y_{N_i,L_i}(\mu^{\dagger})\Phi^{A_i}_{000}(R_i)\Psi_{A_i}$ - WF of clusters with nonzero oscillations along the coordinate of the center of mass.

Talmi-Moshinsky transformation

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

Calculation of the total binding energies of the ground and lowest exited states in AV NCSMC

1)Construction of the basis of orthonormal WFs, which includes both the polarization terms ($\Psi^{(j)}_{pol}$) and the cluster WF of several channels ($\prod_{i=1,2}\Phi^{A_i}_{N_i,L_i,M_i}(R_i)\Psi_{A_i}$)

The corresponding WFs are obtained by matrix diagonalization

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

2) The solution of Schrödinger equation reduces to the finding the eigenvalues and eigenvectors of

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

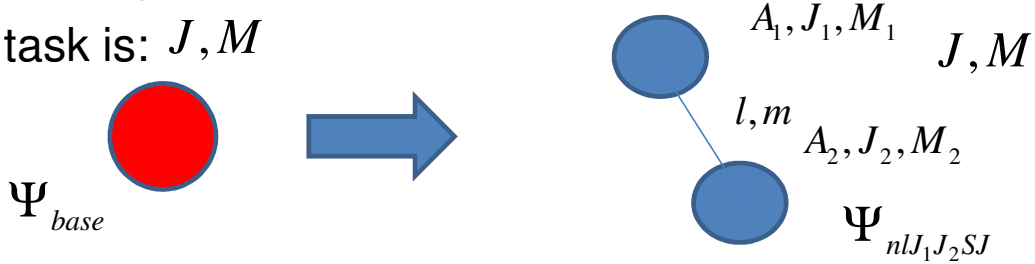
Eigenfunctions are presented in the form of

$$\psi = \sum_{i=1}^{N} c_i \psi_i, N \approx 10^2$$

3) The method of solution is direct diagonalization of the matrix

Decay width calculation of resonances

1)The task is: J, M



partial width for R-matrix theory is $\Gamma_n = 2k(F_l^2 + G_l^2)^{-1}_{r=R}\gamma^2$

2) Basis functions 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) Orthogonalization of WF 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 the initial wave function Ψ_{base} on a certain channel (calculation of the spectroscopic amplitude)

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

5) Determination of the cluster form factor

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

6) Calculations of partial width of neutron resonances

Results

For ab initio calculations of ^{5}He states as ^{4}He + n system realistic NN-potential **Daejeon16** (A.M. Shirokov, I.J. Shin, Y. Kim et al, PLB **761**, 87 (2016)) was used.

In the case of the ground state ^{4}He the experimental total binding energy is 28.296 MeV, for NCSM calculation with Daejeon16 potential when the basis is truncated at the level of $N^{(4)}_{max}$ = 6 total binding energy is E_b=28.22 MeV, when truncation level is $N^{(4)}_{max}$ = 4 E_b=28.12 MeV.

For NCSM calculation well-known shell code Antoine was used. For calculation of clustered terms of the discussed basis was created a code based on the algorithm described above.

Total binding energies of p-resonances of ^{5}He

3/2-, 1/2- states of ^{5}He were calculated. Calculations were carried out in NCSM, using cluster terms (^{4}He + n) and in AV NCSMC using Daejeon16 potential with oscillator parameter hw=22.5.

Table 1. Total binding energies of 3/2-, 1/2- states of ^{5}He

	NCSM	cluster terms (N_{He}=0)	cluster terms (N_{He}=2)	cluster terms (N_{He}=4)	*AV NCSMC* *(N_{He}=0)*	Exp.
3/2-	26.36	23.37	24.48	24.98	26.53	27.41
1/2-	22.52	19.87	20.50	20.39	23.00	23.41

The use of pure cluster terms in ab initio calculations shows large underestimation of the binding energy even in a strongly clustered system.

Calculation of decay width of 3/2- resonance of ^{5}He

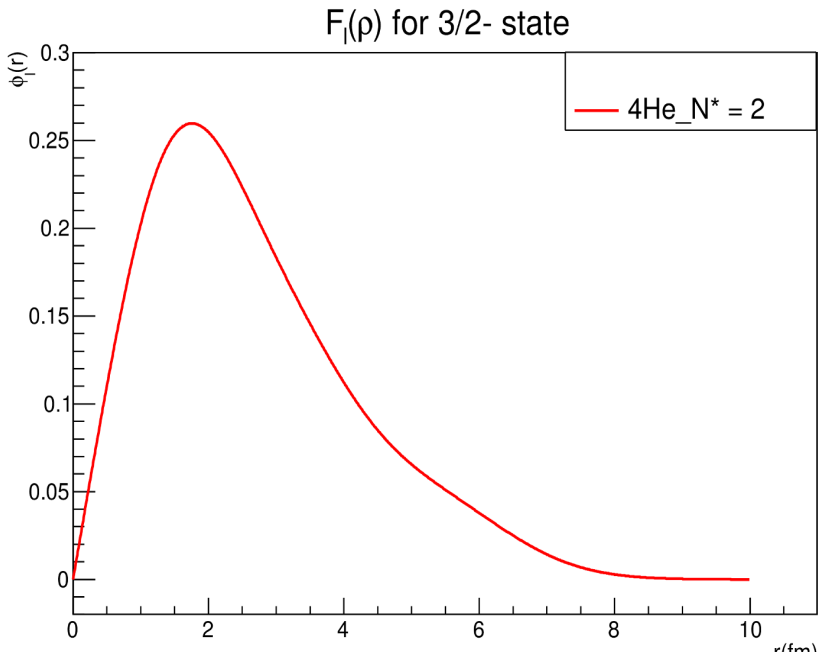
For ab initio calculation of decay width values of neutron spectroscopic factor and amplitudes of nucleon form factor are required. These values were calculated for 3/2- state of ^{5}He with total binding energy 26.530 MeV for ^{4}He with truncation level of $N^{max} = 2$. Total binding energy of ^{4}He is $E_{4He} = 27.259$ MeV.

Table 2. Values of neutron spectrofactor and amplitudes of neutron form factor for 3/2- state of ^{5}He.

	n=0	n=1	n=2	n=3	n=4	n=5	*SF*
^{4}He 3/2-	0.856	-0.365	0.257	-0.171	0.0965	-0.0439	0.9713

This state is strongly clustered.

Neutron form factor of 3/2- state of ^{5}He

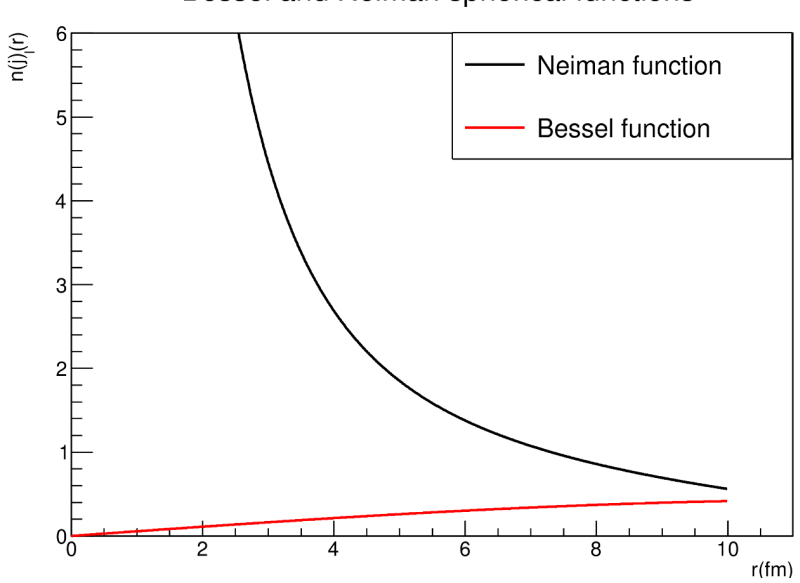


For calculated value of neutron resonance energy (0.729 MeV) in significant area for r coordinate

$$n_l(\mathrm{r}) >> \mathrm{j}_l(\mathrm{r})$$

In this case

$$P_l(r) = (\mathrm{G}_l^2(\mathrm{r}) + \mathrm{F}_l^2(\mathrm{r}))^{-1} \approx (\mathrm{kr})^{-2}(n_l(r))^{-2}$$



For calculation of the matching point of ab initio WF of 3/2- resonance with 2-body solution we use the following equation

$$\frac{F'_l(r)}{F_l(r)} = \frac{n'_l(r)}{n_l(r)} \qquad R_{point} = 3.55 \text{ fm}$$

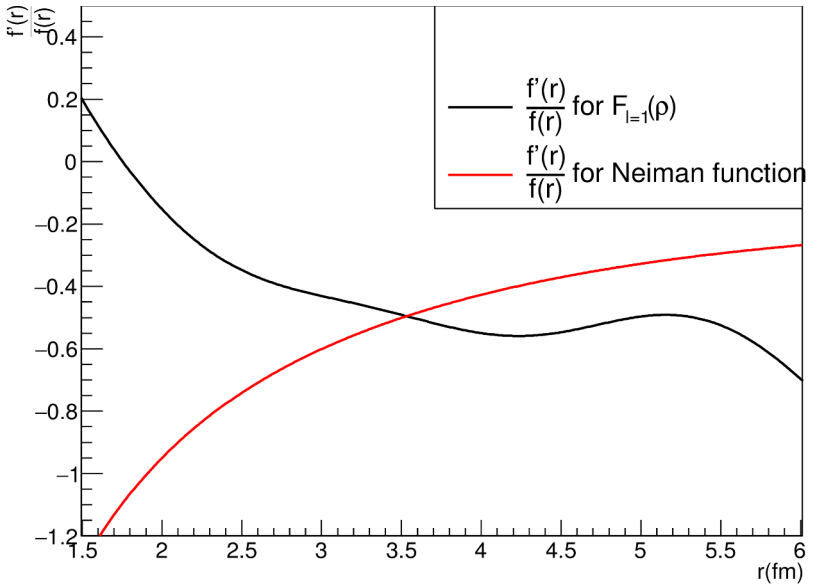
For the matching point $\frac{F_l(r)}{n_l(r)} = -0.043$

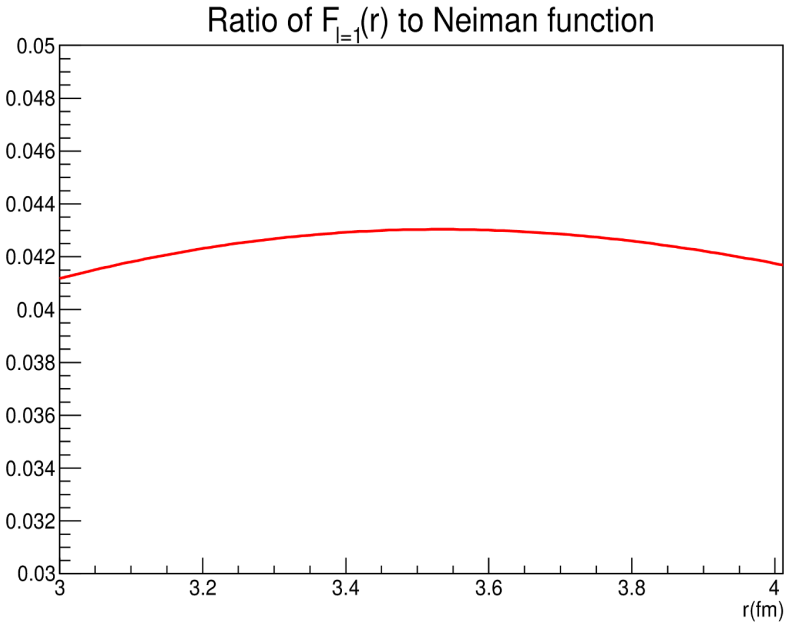
$$\Gamma_{3/2-} = \frac{\hbar^2}{\mu k}\left(\frac{F_l(r)}{n_l(r)}\right)^2 = 572 \text{ keV}$$

For the 3/2- resonance $\frac{F_l(r)}{n_l(r)} \cong const$

in the vicinity of the matching point.

Consequently the asymptotic region is achieved in ab initio calculations





Total binding energies and decay width of 1/2- and 3/2+ states of ^{5}He

Calculation of total binding energy of these states were carried out in NCSM, calculation of spectrofactors were performed using ^{4}He with N* = 2.

Because of high energy of states $n_l(r) >> j_l(r)$ relation is invalid, so R-matrix theory approximation is used.

Table 3. Total binding energies (MeV) and decay widths (MeV) for high existed states of ^{5}He.

	E_{res}	E(exp.)	SF	$\Gamma(exp.)$	$\Gamma(th.)$
1/2-	4.25	4.0	0.9559	4.0(TOI 1996)	4.29
3/2+	10.23	----	0.885	----	8.13
3/2+	19.71	17.48	0.0181	0.076	0.14

Even in case of more general approach of R-matrix theory the decay widths show rather good agreement with the experimental values.

Conclusion

I.A method adapted for describing the characteristics of neutron resonances of light nuclei basing at ab initio nucleon potentials has been developed.

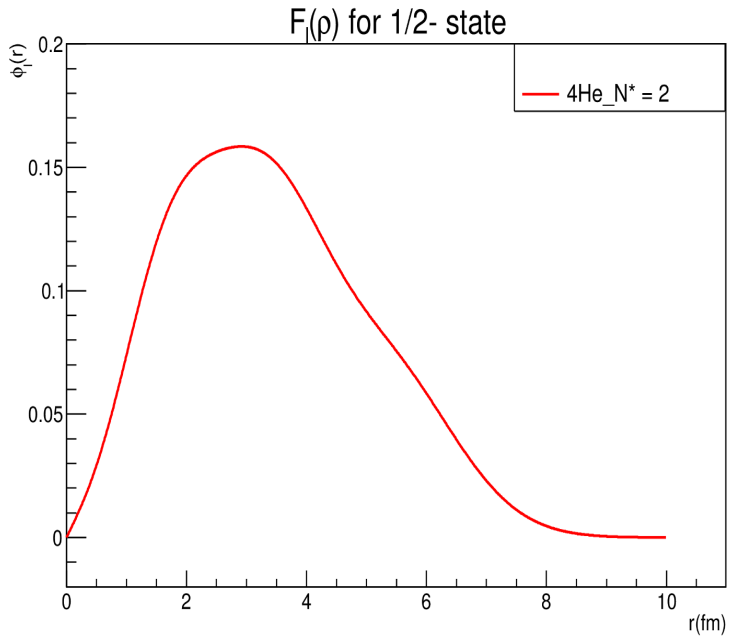
II. This method makes it possible to perform calculations both with effective and realistic nucleon-nucleon potentials, including two-, three-, etc. nucleon forces.

III. This method allows us to calculate both the energies of low-lying states and their decay width within the framework of the general ab initio approach.

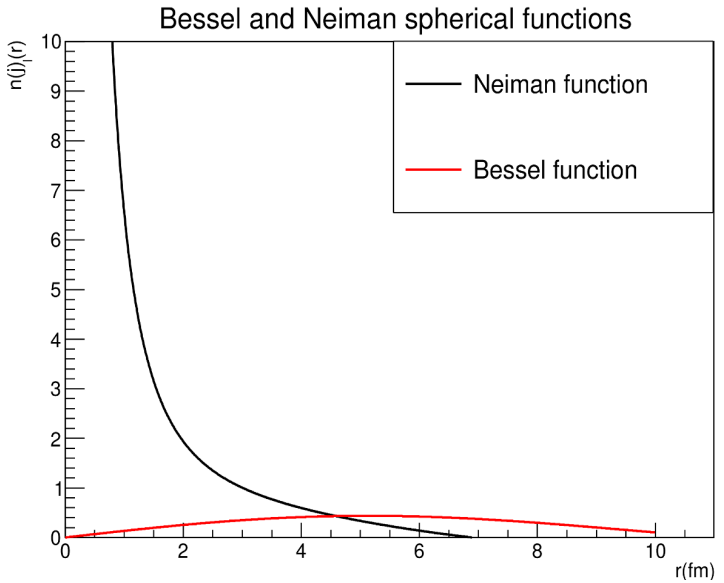
IV. Calculations of the p- and d-states of the 5He nucleus were carried out. The results of calculations of the resonance energies and the decay widths show rather good agreement with the experimental values.

THANK YOU FOR YOUR ATTENTION!

Neutron form factor of 1/2- state of ^{5}He



For calculated value of 1/2- state neutron energy (4.259 MeV) in significant area for r coordinate the approximation $n_l(\mathrm{r}) >> \mathrm{j}_l(\mathrm{r})$ couldn't be used



We define channel radius $R_{point} = 4.0$ fm

For this channel radius

$$\frac{F_l(r)}{\sqrt{n_l^2(r) + j_l^2(r)}} = -0.184$$

It means that

$$\Gamma_{1/2-} = 2kP_l\gamma^2 = 4.29 \quad \text{MeV}$$