AB INITIO STUDY 0F CLUSTERING, RESONANCE AND HALO EFFECTS IN LIGHT NUCLEI

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CHIRAL EFFECTIVE FIELD THEORY HAMILTONIAN

Diagrams of the chiral effective theory. $k=1$ $(k) + \sum U(k, l) + \sum U(k, l, m) + \ldots$ *A k k l k l m* = $H = \sum T(k) + \sum U(k, l) + \sum U(k, l, m) +$

3

The weights of amplitudes of all chosen diagrams are fitted to all known two- and three-nucleon systems data. The Similarity Renormalization Group transformation that preserves two- and three-nucleon data is used to tune the Hamiltonian used in multiparticle calculations. This Hamiltonian is exployted in large-scale variational calculations.

Descriptive ability of such method is good. Predictive power is also good.

The approach is workable to study nuclei with the masses $A \leq 16$.

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

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

$$
\Psi_{i} = \begin{vmatrix} \psi_{n_{1}l_{1}s_{1}j_{1}m_{1}}(r_{1}) & \dots & \psi_{n_{A}l_{A}s_{A}j_{A}m_{A}}(r_{1}) \\ \dots & \dots & \dots \\ \psi_{n_{1}l_{1}s_{1}j_{1}m_{1}}(r_{A}) & \dots & \psi_{n_{A}l_{A}s_{A}j_{A}m_{A}}(r_{A}) \end{vmatrix} . \quad N = \sum_{i=1}^{A} n_{i} \ge N_{\min}
$$
 (1)

which, as a rule, consist of the spherical oscillator onenucleon wave functions. All matrix elements are taken into account.

NCSM-BASED REFINED APPROACHES

An interesting strategy is to get rid of at least a part of inessential matrix elements before a calculation.

For these purposes the SU(3)-NCSM, which uses natural symmetries of a nuclear system (Dreyfuss A. C., Launey K. D., Dytrych T. PRC 95 044312 (2017)), No-Core Monte-Carlo Shell Model (NCMCSM) (Abe T., Maris P., Otsuka T. et al. PRC 86 05430, (2012)), etc. were created.

Various extrapolating procedures are used to refine the results.

Recently the maximal bases om canonical NCSM may be 2⋅10¹⁰ × 2⋅10¹⁰

NCSM, NUCLEAR PROPERTIES AND GAMMA-TRANSITIONS

Calculations within the NCSM with accurately calibrated potentials reproduce quite well not only the total binding energies of nuclei up to 16O and excitation energies of their lower levels. The magnetic moments of nuclei and the probabilities of M1-transitions are also reproduced well. The accuracy of NCSM calculations of nuclear radii, quadrupole moments and probabilities of E2 and E1 transitions is slightly lower, but, nevertheless, satisfactory. As a result, for undetected levels and loosely measured transitions, it looks reasonable to base on these theoretical data. So, in some areas of nuclear spectra, ab initio calculations are already becoming competitive with measurments of the same observables.

PROBLEM OF CLUSTERING (STRUCTURING)

How to state the problem of substructures (clusters) in two- (or few-) cluster system taking into account indistingvishibility of identical fermions?

STRUCTURING OF MOLECULES

SHELL MODEL VERSUS CLUSTER MODEL. 8Be EXAMPLE

Let Ψ_{α} and Ψ_{8Be} be translationally-invariant wave functions of the alpha particle and 8Be nucleus in the lowest shell model configurations. Then:

$$
\Psi_{8Be} \equiv [1/\Phi_{00}(R)] | s^4 p^4 L = 0S = 0T = 0 \rangle \equiv
$$

(1/Q) $\hat{A} \{ \Psi_{\alpha_1} \Psi_{\alpha_2} \varphi_{n=4, l=0}(\vec{\rho}) \},$

K. Wildermuth and T. Kannelopulos

NCSM AND NUCLAR DECAY WITH THE EMISSION OF NUCLEONS OR CLUSTERS

Decays into nucleon and cluster channels (spontaneous or induced be resonance reactions) play a role in nuclear spectroscopy of light nuclei which is comparable or even superior with the role of electromagnetic transitions.

So the next problem is to build theoretical nuclear spectroscopy of resonances and their decays, i. e. to create more or less universal (suitable for a lot of resonances and decay channels) schemes of the theoretical description of these processes. Naturally these schemes are based on the theory of cluster channels.

AB INITIO STUDIES OF CONTINUOUS SPECTRUM AND RESONANCES

The No-Core Shell Model / Resonating Group Model (NCSM / RGM) and No-Core Shell Model with Continuum (NCSMC) P. Navratil et al – a lot of papers.

Another approach is Fermionic Molecular Dynamics (T. Neff and H. Feldmeier, Int. J. Mod. Phys. E 17, 2005 (2008)).

The combination of NCSM and SS-HORSE methods (A.M. Shirokov, A.I. Mazur, I.A. Mazur et al. Phys. Rev. C. 94, 064320 (2016)) also looks an interesting scheme to explore this problem.

CLUSTER CHANNEL ORTHOGONAL FUNCTIONS METHOD

Two-fragment clustering in bound and decay of resonance states is considered in this talk. To describe the virtual or real decay so-called Cluster Channel Orthogonal Functions Method (CCOFM) was proposed. The cluster-channel terms of CCOFM basis are built in the formof the following wave functions (WFs): **RTHOD**

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d decay

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mof the fo
 ${}_{1}\Psi_{A_{2}}\varphi_{nlm}(\bar{\rho})$

rtizer, ${}_{1}\Psi_{A}$

fragment; $\frac{1}{\sqrt{2}}\hat{A}\{\Psi_{A}^{\dagger},\Psi_{A}^{\dagger},\varphi_{nlm}(\vec{\rho})\}.$ **IONS METHOGONAL**
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 W ¹¹¹² A_1 ² A_2 ^{*P*} n lm</sub> \vee ^{*P*} \n *J* M_J ²

 $1 \t1 \t2$, $1 \t1$ ˆ $A = A₁ + A₂$, *A* is the antisymmertizer, Ψ_{A_i} Ψ ,

– translationally-invariant WF of the fragment; () *nlm*

– the oscillator WF of the relative motion.

A technique has been developed for transforming such WFs to superpositions of Slater determinants (SDs).

Projecting of an eigenvector of ab initio Hamiltonian on the functions of the cluster basis defines the cluster characteristics of the corresponding nuclear state.

However some problems appear. In general case WFs (2) are not orthogonal one to another and to the shellmodel components.

Thus, the next step in creating of a basis is to build orthonormalized WFs. The WFs are obtained by diagonalization of the overlap matrix

$$
\left\|\left\langle\Psi^{(j)}_{pol}\right|\hat{A}\left|\prod_{i=1,2}\Phi^{A_i}_{N_i,L_i,M_i}(\vec{R}_i)\Psi^{*}_{A_i}\right\rangle\right\|\left\langle\prod_{i=1,2}\Phi^{A_i}_{N_i,L_i,M_i}(\vec{R}_i)\Psi^{*}_{A_i}\right\|\hat{A}^2\left|\prod_{i=1,2}\Phi^{A_i}_{N_i,L_i,M_i}(\vec{R}_i)\Psi^{}_{A_i}\right\rangle\right\|
$$

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 measure of clustering is called cluster form factor. The value CFF of the channel $A_1 + A_2$ is defined as:

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

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

By representing of the delta function as the oscillator expansion $\delta(\rho - \rho') = \sum |\varphi_{nl}(\rho')\rangle \langle \varphi_{nl}(\rho)|$

ions also turn out t
 l cillator wave funct
 l $\int_{l}^{k} (\rho) = \sum_{n} B_{nl}^{k} \phi_{nl}(\rho)$.

values take the form
 $\int_{l}^{k} (\vec{\rho}) \Psi_{A_2} \} | \hat{1} | \hat{A} \{ \Psi_{A_1} f_{A_2} \} |$

s of CFF and its no the eigenfunctions also turn out to be expressed through the oscillator wave functions

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

n And the eigenvalues take the form:

$$
\varepsilon_{k} = <\hat{A} \{ \Psi_{A_{1}} f_{l}^{k}(\vec{\rho}) \Psi_{A_{2}} \} | \hat{1} | \hat{A} \{ \Psi_{A_{1}} f_{l}^{k}(\vec{\rho}) \Psi_{A_{2}} \} >;
$$

The final forms of CFF and its norm – spectroscopic factor (SF) are the following: $I_l(\rho) = \sum_{i} \varepsilon_k^{-1/2} \sum_{i} C_{AA_1A_2}^{nl} f_l^k(\rho);$ $\Phi_{I}(\rho) = \sum \varepsilon_{k}^{-1/2} \sum C_{AA,A}^{n} f_{I}^{k}(\rho);$ he eigenfunctions also turn out to be expressed

hrough the oscillator wave functions
 $f_l^k(\rho) = \sum_n B_{nl}^k \phi_{nl}(\rho)$.

And the eigenvalues take the form:
 $\varepsilon_k = < \hat{A} \{ \Psi_{A_1} f_l^k(\vec{\rho}) \Psi_{A_2} \} | \hat{1} | \hat{A} \{ \Psi_{A_1} f_l^k(\vec{\rho$ tions also turn out to be expressed

scillator wave functions
 $f_l^k(\rho) = \sum_{n} B_{nl}^k \phi_{nl}(\rho)$.

walues take the form:
 $k(\vec{\rho}) \Psi_{A_2} | |\hat{1}| \hat{A} {\Psi_{A_1}} f_l^k(\vec{\rho}) \Psi_{A_2} \rangle$ >;

s of CFF and its norm – spectroscopic factor

p

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

where

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

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 WIDTHS)

The asymptotic characteristics are deduced using the matching procedure described in textbooks on quantum mechanics. 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:

Therefore, the asymptotic normalization coefficient (ANC) the decay width of this resonance is given by the expression: $\sqrt{2}$

$$
ANC = \frac{rF_l(R_p)}{W_{-\eta, l+1/2}(2kR_p)} \qquad \qquad \Gamma_l = \frac{\hbar^2}{\mu k} \left(\frac{F_l(R_p)}{G_l(\eta, R_p)} \right)
$$

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

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

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

$$
\Gamma_{subth}(E) = \frac{\hbar^2}{\mu_{ab}} k R_p (F_l(\eta, r)^2 + G_l(\eta, r)^2)_{r=R_p}^{-1} \frac{W^2_{-\eta_0, l+1/2} (2k_0 P_p)}{R_p} |ANC_{ab}|^2
$$

Our ab initio approach is in fact the sole allows one to obtain the partial decay widths in multy-channel cases.

METHOD OF CALCULATIONS

The results of all calculations of the total binding energies and excitation energies of nuclear levels presented bellow are obtained by use of advanced NNpotential **Daejeon16**. It is built starting from N3LO forces of the Effective Field Theory and then softened with the Similarity Renormalization Group flow parameter $\lambda = 1.5$ fm⁻¹. The novel is that various phase equivalent transformations are apply to it (A.M. Shirokov, I.J. Shin, Y. Kim et al, PLB **761** 87 (2016)}.

The Daejeon16 interaction is well-tested. The set of parameters of it is obtained by the fit to binding energies of 3H, 4He, 6Li, 8He, 10B, 12C and 16O nuclei and to excitation energies of a few narrow excited states: the two lowest excited states $(3+, 0)$ and $(0+, 1)$ in 6Li, the first excited state (1+, 0) in 10B, and (2+, 0) in 12C.

Code Bigstick is used for shell-model computing of the energies and WFs of decaying nuclear states and fragments.

For the analysis of dense spectra step by step tracing of each level with the grows of the basis size is required. The overlap of the WF with $N_{\text{max}}+2$ with each of the WFs with N_{max} is a criterion.

So-called A5 extrapolation procedure is applied to determine the values of level energies for infinite basis.

EVOLUTION OF LEVEL SQUENCE IN THE DENSE SPECTRUM OF ⁸Be

through the maximum value of the overlap of the WFs with N_{max} +2 with each of the WFs with N_{max} .

SPECTRUM OF 7Li NUCLEUS

 $^{\rm a}$ ANCs (fm^{-1/2}).

^b Γ ($E_n = 1$ eV).

"Total decay width.

SPECTRUM of 8Be NUCLEUS (positive parity)

NEGATIVE PARITY STATES of 8Be NUCLEUS AND 7Be(n,p)7Li REACTION

Another fit of 2-(1) state (Adahchour A., Descouvemont P.):

Гp= 1409 keV. Гn= 225.

SPECTRUM OF EXOTIC 7He NUCLEUS

Resonance energies, decay widths of open channels (keV), and channel spectroscopic factors of 7He nucleus states

CONCLUSION I

CCOFM in combination with NCSM calculations make it possible to obtain detailed spectroscopic information about the states of light nuclei over a wide range of excitation energies.

Almost all levels discovered so far are reproduced. With rare exceptions, the deviation of their energy values does not exceed ~1 MeV. The existence of a significant number of unknown levels is predicted

The abilities of the approach to compute the partial decay widths, their amplitudes with reliably determoined signs are unique.

The deviation of the absolute values of the decay widths is less than two times. The values of the asymptotic noralization coefficients evaluated from the reliable experiments tunrs out to be well-reproduced.

CALCULATION OF RESONANCE REACTION CROSS SECTIONS BASED ON THE RESULTS OF AB INITIO COMPUTATIONS

I present here the idea of a research strategy to expand as widely as possible the scope of the use of ab initio methods in the study of nuclear properties and nuclear processes and some results of its realization.

This strategy is often implemented at the cost of abandoning purely deductive schemes for calculating various characteristics of atomic nuclei and cross sections of nuclear reactions.

To calculate the cross section of resonant reaction the standard *R*-matrix theory is exploited. The spectroscopic data, obtained by ab initio computations are used as an input. Naturally, this "hybrid" theory does not belongs to the class of ab initio approaches.

LOW ENERGY 9Be (n,n) 9Be PROCESS

Spectral characteristics of 10Be and its 9Be + n decay channels. Symbol (-) denotes the sign of reduced partial width amplitude

Let me present the cross section for the elastic scattering 9Be(*n*, *n*)9Be calculated with three sets of the input data in comparison with various experimental data. In all variants, reduced partial width amplitudes of neutron and alpha-decay channels calculated with the CCOFM were used. The level energies were taken from existing experimental data (the solid and dotted lines) or from extrapolation calculations (the dashed line). The dotted line presents the calculations with ANCs obtained from experimental data.

The *R*-matrix code AZURE2 is used in our calculations. The basic formula reads:

$$
U_{cc'} = (U_{cc}^0 U_{c'c'}^0) \cdot \left(\delta_{cc'} + \frac{i\Gamma_{\lambda c}^{1/2} \times \Gamma_{\lambda c'}^{1/2}}{E_{\lambda} + \Delta_{\lambda} - E - \frac{i}{2}\Gamma_{\lambda}^{tot}} + O\left(\frac{\langle \Delta - \frac{i}{2}\Gamma^{tot} \rangle}{D}\right) \right)
$$

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CALCULATION OF CROSS SECTIONS FOR REONANCE REACTIONS SHAPING 8Be COMPOUND NUCLEUS

 7 Li (p, 4 He) 4 He

 4 He(4 He,p) 7 Li

⁷Be(n,⁴He)⁴He

⁴He(⁴He,n)⁷Be

Differential cross sections of ⁶Li(d,d)⁶Li elastic scattering at 125 -(a) and 170 - (b) scattering angles

Inclusive and exclusive total cross sections for 6 Li(d,p)⁷Li, 6 iLi(d,p)⁷Li* reactions.

Inclusive and exclusive total cross sections for ⁶Li(d,n)⁷Be, ⁶iLi(d,n)⁷Be* reactions

Partial expansion onto J of cross sections of 6 Li(d,n)⁷Be - (a) and 6 Li(d,n) 7 Be^{*} - (b) reactions

Cross section of 6 Li(d, 4 He) 4 He reaction - (A). Cross section of 6 Li(d, 3 H)X reaction - (B)

Total cross section of ⁷Be(n,p)7Li reaction - (a). Contribution of the set of 2⁻ resonances (b)

CONCLUSION II

1. The hybrid method allows one to determine cross sections and other characteristics, which can be interpreted as "theoretically estimated" for resonant processes for which experimental data on partial widths are absent, contradictory, unreliable, or obtained with large errors (such processes are numerous and are physically most interesting).

2. This method also makes it possible to strongly reduce the number of parameters used to fit experimental data with the *R*-matrix model.

Prospects for using the results of ab initioo methods in studies of direct nuclear reactions are also broad.

3. Ab initio theoretical approaches have become now an instrument of equal strength in the studies of spectroscopy of light nuclei and the reactions induced by their collisions.

WHAT ABOUT DRECT REACTIONS? Transfer reactions. Distorted-wave Born Approximation.

The matrix element is written in the form:

$$
T_{if} = \int d^3r \chi_f^{(-)}^*(k_f, r) \chi_f^{(+)}(k_i, r) G_{if}(r); G_{if}(r) = \int d^3r_2 \psi_f^{*}(r_2) V_2(r_2) \psi_i(r_2 - r).
$$

Usually WFs of bound clusternucleus states *ψi(f)(ρ)* are built as the eigenvalues of a phenomenological two-body Hamiltonian. They are normalized by the corresponding SFs. The SF mai be calculated initially. However a promising idea is the substitution cluster form factor $\Phi_{(f)}(\rho)$ in place of $\psi_{(f)}(\rho)$.

The effect looks as follows:

RADII OF LIGHT NUCLEI AND HALO EFFECT

HALO EFFECTS IN LIGHT NUCLEI

NUCLEAR RADII: MATTER, CHARGE, NEUTRON

**AR RADII: MATTER, CHARGE,
\n**NEUTRON**
\n
$$
\overline{r}_{m(p,n)}^2 = 1/N_{A(Z,N)} \sum_i (\overline{r}_{m(p,n)i} - \overline{r}_{cm})^2
$$
\n
$$
Ar_m^2 = Zr_p^2 + Nr_n^2.
$$
\nlational definition of the halo size:

\n
$$
\overline{r}_{halo} = \overline{r}_n - \overline{r}_p
$$**

Traditional definition of the halo size:

$$
\overline{r}_{halo} = \overline{r}_n - \overline{r}_p
$$

Measured values of 6He nucleus radii (fm), obtained using the radius of proton *R^p* from: [23] *a* and [24]. Results of direct computing of light nuclei radii turned out to be not satisfactory. Various extrapolation procedures were built in order to improve their description.

We proposed two-dimentional, so-called "twisted tape extrapolation" procedure for these purposes:

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

It contains an approximation polynomial P_k . The results presented bellow are obtained using simple version of the polynomial: $P_1(\hbar\omega) = A + B\hbar\omega$,

```
The extrapolation procedure has been performed
throughout the two-dimentional domains with:
the total range 6 - 17.5 MeV (D0);
the narrowed ranges:
6 - 15 MeV (D1),
7.5 - 15 MeV (D2),
and 7.5 – 12.5 MeV (D3).
```


Matter (a), neutron (b) and point-proton (c) radii of 6He nucleus for different $$ extrapolation domains in case of the use of the JISP16 potential.

Matter (a), neutron (b) and point-proton (c) radii of 6He nucleus for different *ħω* extrapolation domains in case of the use of the Daejeon16 potential.

NUMERRICAL RESULTS

A very unexpected result is almost complete coincidence of the size of the neutron. Indeed, this value is equal to 0.792 and 0.783 fm for JISP16 and Daejeon16 respectively.

THANK YOU FOR YOUR ATTENTION!