

PECULIARITIES OF THE ENERGY SPECTRUM OF THE ^{12}C NUCLEUS IN A 3α MODEL

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E.M. Tursunov, I. Mazumdar *Phys. Atom Nucl.* **85** (2022), pp.160-166.

CONTENTS

- **Motivation, why to study ^{12}C spectrum in the 3-alpha model?**
- **Variational method on Gaussian basis**
- **Results with the Ali-Bodmer alpha-alpha potential with a repulsive core**
- **Results with the Buck-Friedrich-Wheatley alpha-alpha potential using OPP method**
- **Results with the direct orthogonalization method**
- **Conclusions**

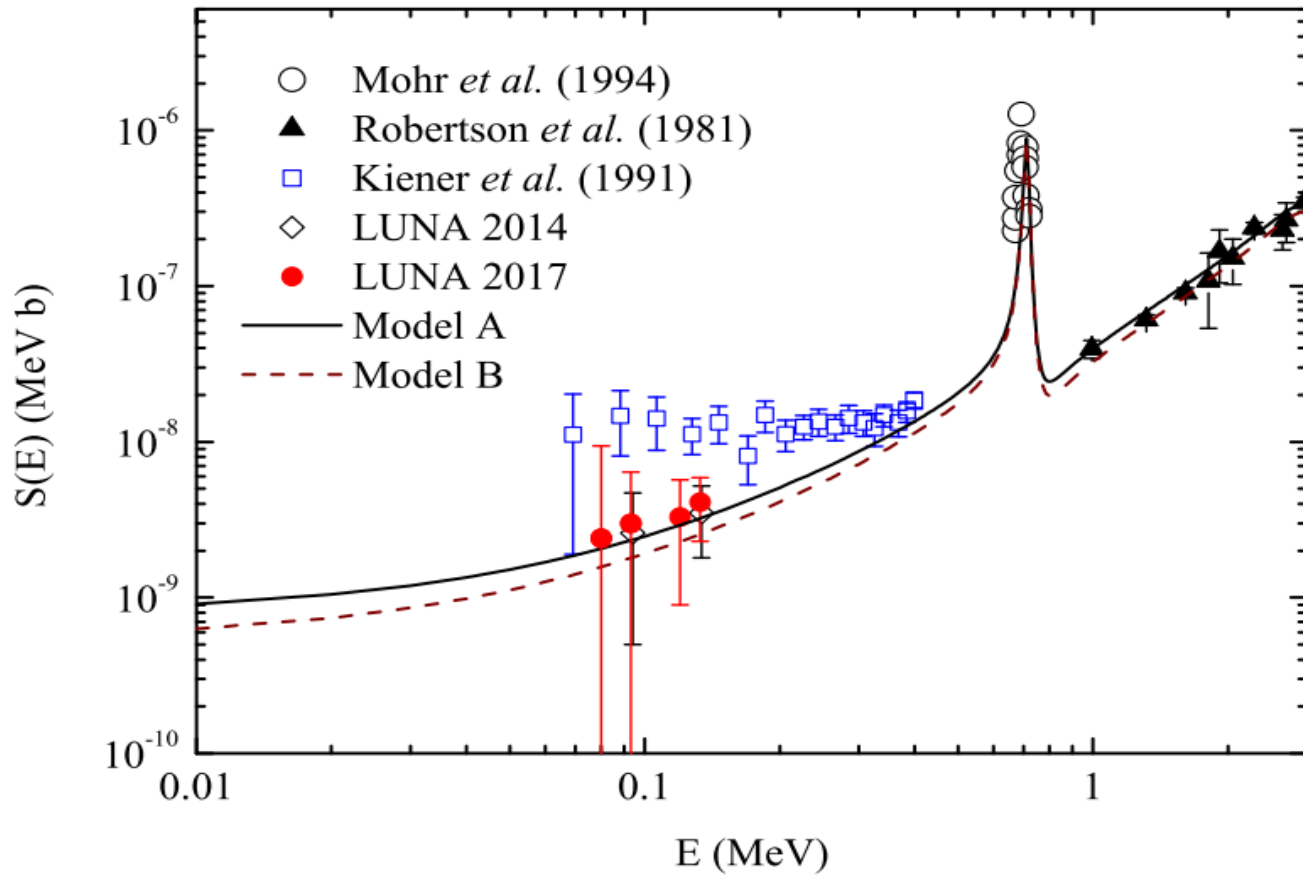
Motivation

Three-body models for systems with a single α particle



work very well. αN and NN potentials describing 2-body data (phase shifts and binding energy of the deuteron) with small additional 3-body potentials yield energies of the three-body systems and reaction cross sections.

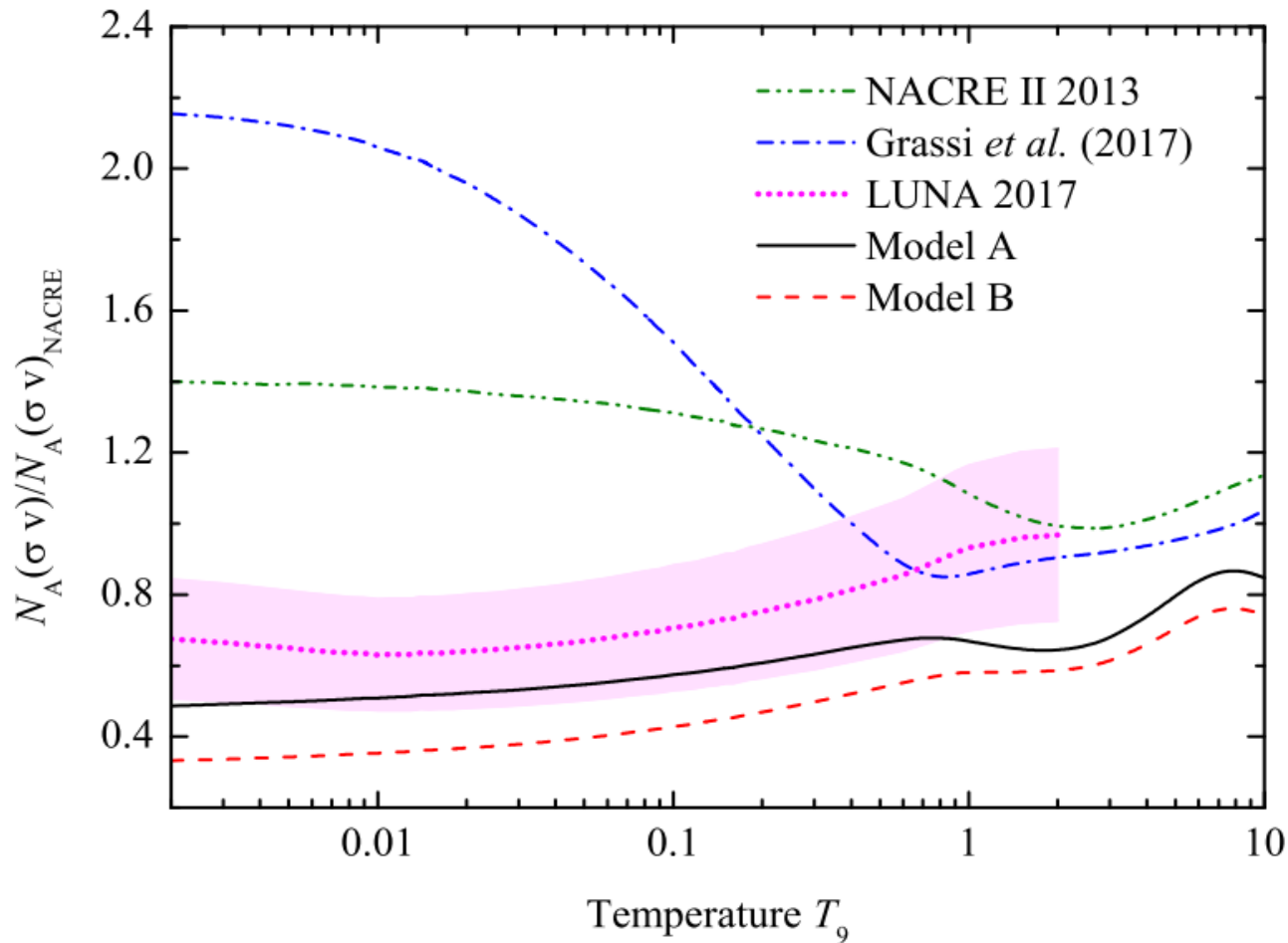
Astrophysical S-factor for the $\alpha(d, \gamma)^6\text{Li}$ capture process



D. Baye, E. [Tursunov](#), [J. Phys. G: Nucl. Part. Phys.](#) 2018, 45(8), 085102;

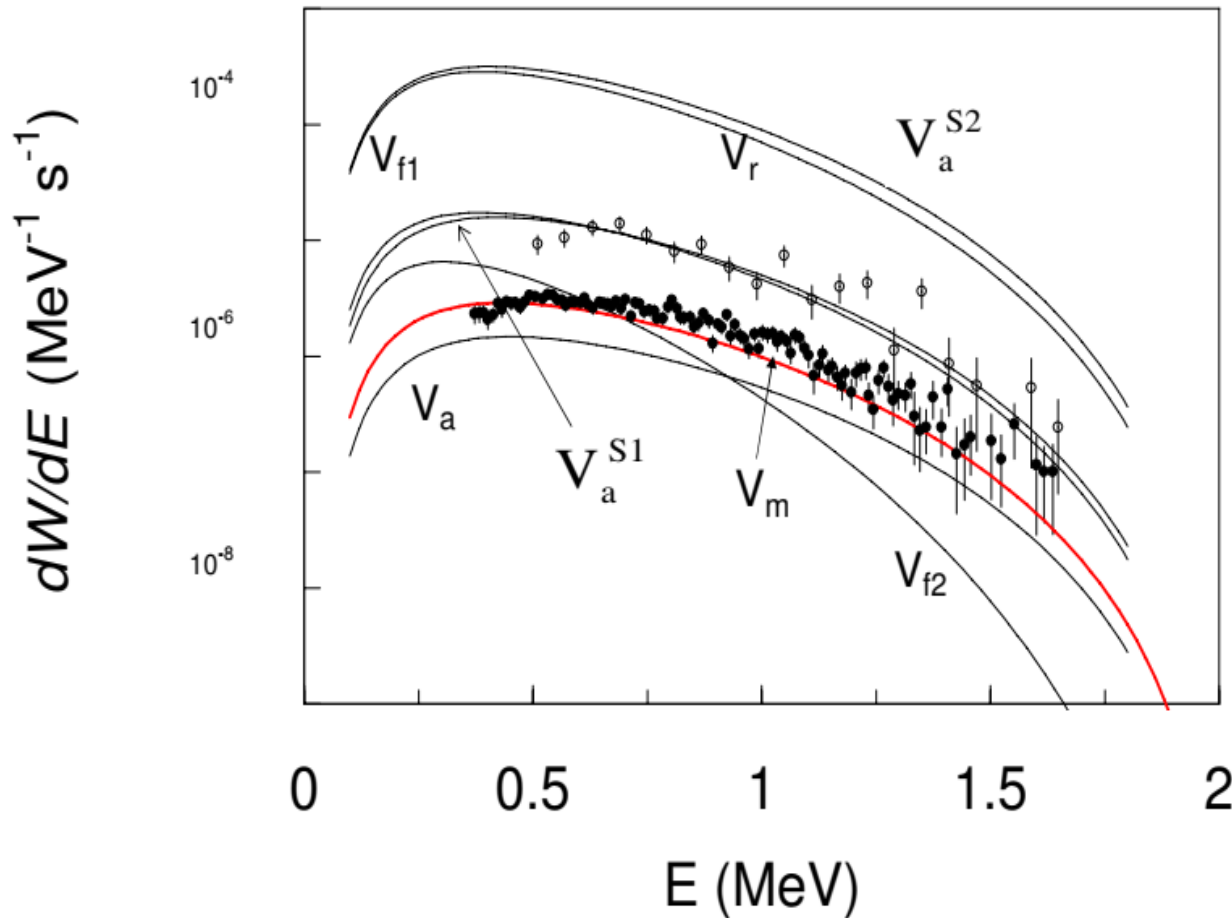
E. [Tursunov et al.](#), [Phys. Rev.C](#), 2018, 98(5), 055803

Reaction rates of the $\alpha(d, \gamma)^6\text{Li}$ astrophysical synthesis process



E. [Tursunov](#)
et al.
[Physical](#)
[Review C](#),
2018, 98(5),
055803

Transition probability per time and energy units dW/dE of the ${}^6\text{He}$ beta decay into the $\alpha+d$ continuum for different $\alpha+d$ potentials



[E.M. Tursunov](#), D. Baye,
P. [Descouvemont](#),
Phys. Rev. C, 2006,
73(1), 014303

But, there is a big problem in the $^{12}\text{C}=3\alpha$ model

a) Potential ABd0 with a repulsive core

[S. Ali, A.R. Bodmer,](#)

[Nucl. Phys. A80](#)

(1966) 99

$$V_{AB}(r) = V_1 \exp(-\eta_1 r^2) + V_2 \exp(-\eta_2 r^2) + V_{coul}(r),$$

$$V_1 = 500 \text{ MeV}, \quad \eta_1 = 0.49 \text{ fm}^{-2} \quad V_{Coul}(r) = 4e^2 \text{erf}(br)/r$$

$$V_2 = -130 \text{ MeV}, \quad \eta_2 = 0.225625 \text{ fm}^{-2} \quad b=0.75 \text{ fm}^{-1}$$

b) l-dependent potential ABd with a repulsive core

$$V_1 = 320 \text{ MeV for } l = 2, \quad V_1 = 0 \text{ for } l > 2 \quad b = \sqrt{3}/2.88 \text{ fm}^{-1}$$

Energies of the $^{12}\text{C}(0^+)$ states in a 3α model with potentials with a repulsive core

(J^π, T)	LMM	ABd ₀ (l-indep.) HHM	VGM	
$(0_1^+, 0)$	-0.58427008	-0.58407	-0.584266	with Coulomb
$(0_1^+, 0)$	-5.122093595	-5.122	-5.1220936	no Coulomb
$(0_2^+, 0)$	-1.3606	-1.2	-1.36062	
$(0_3^+, 0)$	-1.338	-0.8	-1.33873	
$(2_1^+, 0)$		-1.15	-1.3398	
		ABd (l-dep.)		
$(0_1^+, 0)$		-1.523	-1.523	with Coulomb
$(0_1^+, 0)$		-6.423	-6.423	no Coulomb
$(0_2^+, 0)$		-1.92	-1.934	

Exp.

$(0_1^+, 0)$	-7.275
$(0_2^+, 0)$	0.3796
$(2_1^+, 0)$	-2.836

[E. Tursunov,](#)
[D. Baye,](#)
[P. Descouvemont,](#)
[Nucl. Phys. A723](#)
 (2003), 365–374

$\alpha\alpha$ - potential of BFW with forbidden states in S and D waves

$$V(r) = V_0 \exp(-\eta r^2) + 4e^2 \operatorname{erf}(br) / r,$$

$$V_0 = -122.6225 \text{ MeV}, \eta = 0.22 \text{ fm}^{-2}$$

$$b = 0.75 \text{ fm}^{-1}$$

B. Buck, H. Friedrich,
C. Wheatley. Nucl. Phys.
A275 (1977) 246

Very good description of the experimental phase shifts $\delta_L(E)$ for the $\alpha\alpha$ -elastic scattering in the partial waves $L = 0, 2, 4$ within the energy range up to $E=40$ MeV and the energy positions and widths of the ^8Be resonances.

Pauli forbidden states in the S wave with energies $E1 = -72.6257$ MeV and $E2 = -25.6186$ MeV, and a single forbidden state in the D wave with $E3 = -22.0005$ MeV.

A) Method orthogonalising pseudopotentials (OPP) for removing Pauli forbidden states in the 3-body system within variational approach on Gaussian basis (V. I. Kukulin and V. N. Pomerantsev, Ann. Phys. (N.Y.) **111, 330 (1978))**

$$\tilde{H} = H_0 + \tilde{V}(r_{12}) + \tilde{V}(r_{23}) + \tilde{V}(r_{31}) \quad \text{- Hamiltonian.}$$

$$\tilde{V}(r_{ij}) = V(r_{ij}) + \sum_f \lambda_f \hat{\Gamma}_{ij}^{(f)}.$$

- pseudopotentials.

$$\Psi_s^{JM} = \sum_{\gamma j} c_j^{(\lambda, l)} \varphi_{\gamma j}^s,$$

- expansion on symmetrized Gaussian basis.

$$\varphi_{\gamma j}^s = \varphi_{\gamma j}(1; 2, 3) + \varphi_{\gamma j}(2; 3, 1) + \varphi_{\gamma j}(3; 1, 2),$$

$$\varphi_{\gamma j}(k; l, m) = N_j^{(\lambda l)} x_k^\lambda y_k^l \exp(-\alpha_{\lambda j} x_k^2 - \beta_{l j} y_k^2) \times \mathcal{F}_{\lambda l}^{JM}(\mathbf{x}_k, \mathbf{y}_k).$$

$$\mathbf{x}_k = \frac{\sqrt{\mu}}{\hbar} (\mathbf{r}_l - \mathbf{r}_m) \equiv \tau^{-1} \mathbf{r}_{l,m}$$

- Jacobi coordinates

$$\mathbf{y}_k = \frac{2\sqrt{\mu}}{\sqrt{3}\hbar} \left(\frac{\mathbf{r}_l + \mathbf{r}_m}{2} - \mathbf{r}_k \right) \equiv \tau_1^{-1} \boldsymbol{\rho}_k$$

$$\alpha_{\lambda j} = \alpha_0 \tan \left(\frac{2j-1}{2N_\lambda} \frac{\pi}{2} \right), \quad j = 1, 2, \dots, N_\lambda$$

$$\beta_{lj} = \beta_0 \tan \left(\frac{2j-1}{2N_l} \frac{\pi}{2} \right), \quad j = 1, 2, \dots, N_l,$$

- Chebishev
grid

$$\mathcal{F}_{\lambda l}^{JM} (\widehat{\mathbf{x}}_k, \widehat{\mathbf{y}}_k)$$

$$= \{Y_\lambda (\widehat{\mathbf{x}}_k) \otimes Y_l (\widehat{\mathbf{y}}_k)\}_{JM} \phi(1) \phi(2) \phi(3)$$

- angular part of the
basis w.f.

$$\hat{H} = -\frac{\partial^2}{\partial \mathbf{x}_k^2} - \frac{\partial^2}{\partial \mathbf{y}_k^2}$$

- kinetic energy operator

Projector on the fixed f -wave in the i -two-body system:

$$\hat{\Gamma}_i^{(f)} = \frac{1}{2f+1} \times \sum_{m_f} |\varphi_{fm_f}(\mathbf{x}_i)\rangle \langle \varphi_{fm_f}(\mathbf{x}'_i)| \delta(\mathbf{y}_i - \mathbf{y}'_i)$$

Complete 3-body projector, proven: $\text{kernel}(\hat{\Gamma}) = \text{kernel}(\hat{P})$

$$\hat{P}_i = \sum_f \hat{\Gamma}_i^{(f)}$$

$$\hat{P} = \sum_{i=1}^3 \hat{P}_i,$$

$$\begin{aligned} \hat{\Gamma} &= \sum_{i=1}^3 \hat{P}_i - \sum_{i \neq j=1}^3 \hat{P}_i \hat{P}_j \\ &+ \sum_{i \neq j \neq k=1}^3 \hat{P}_i \hat{P}_j \hat{P}_k - \dots \end{aligned}$$

In the OPP method with $\lambda \rightarrow +\infty$ the Pauli forbidden states should be removed from the solution of the 3-body Schroedinger equation.

The energy spectrum of the ^{12}C nucleus with $(J\pi; T) = (0+; 0)$ in MeV at several values of the projecting constant

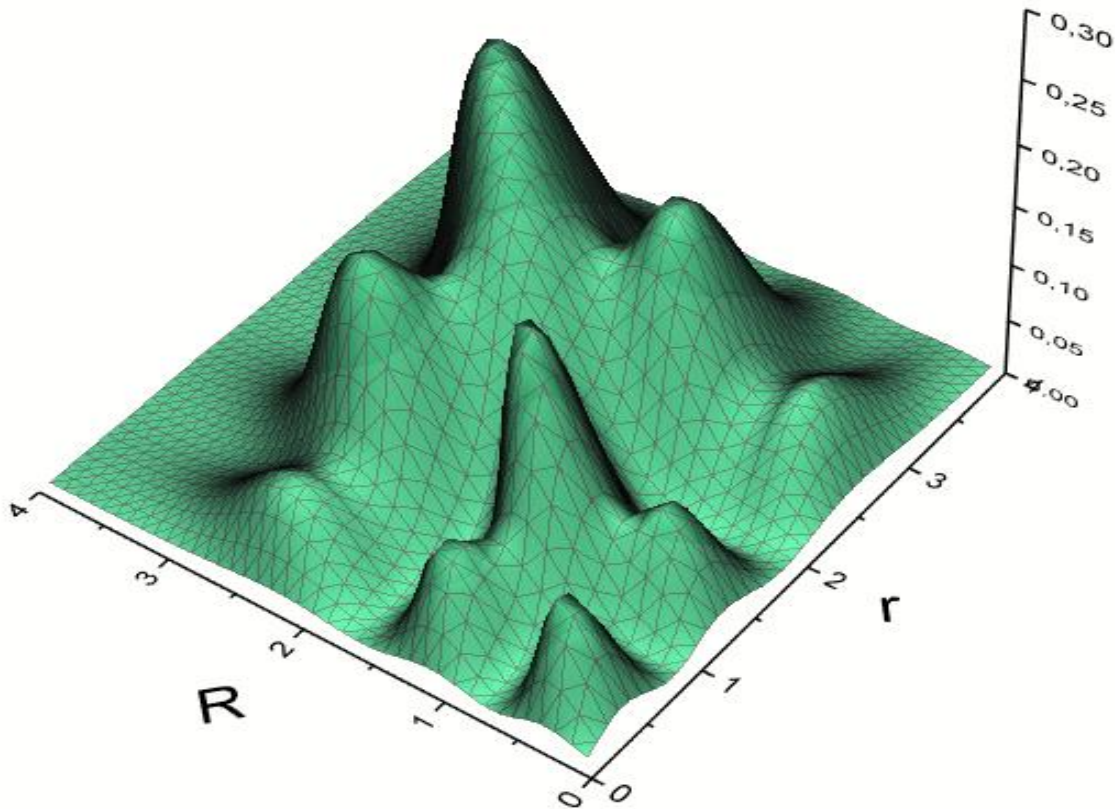
λ (MeV)	10	10^2	10^3	10^4	10^5	10^6	10^7	10^8
E_1	-210.69	-44.207	-20.15	-16.106	-8.830	-0.435	-0.307	-0.283
E_2	-150.32	-17.585	-0.531	-0.422	1.353	1.407	1.513	1.551
E_3	-109.32	-15.310	+1.334	1.353	+3.019	3.316	4.038	4.055
$\langle P \rangle$	29.95	28.92	1.130	3.777	0.721	8.76E-2	2.3E-2	4.7E-3

E. M. Tursunov, J. Phys. G: Nucl. Part. Phys. **27**, 1381 (2001).

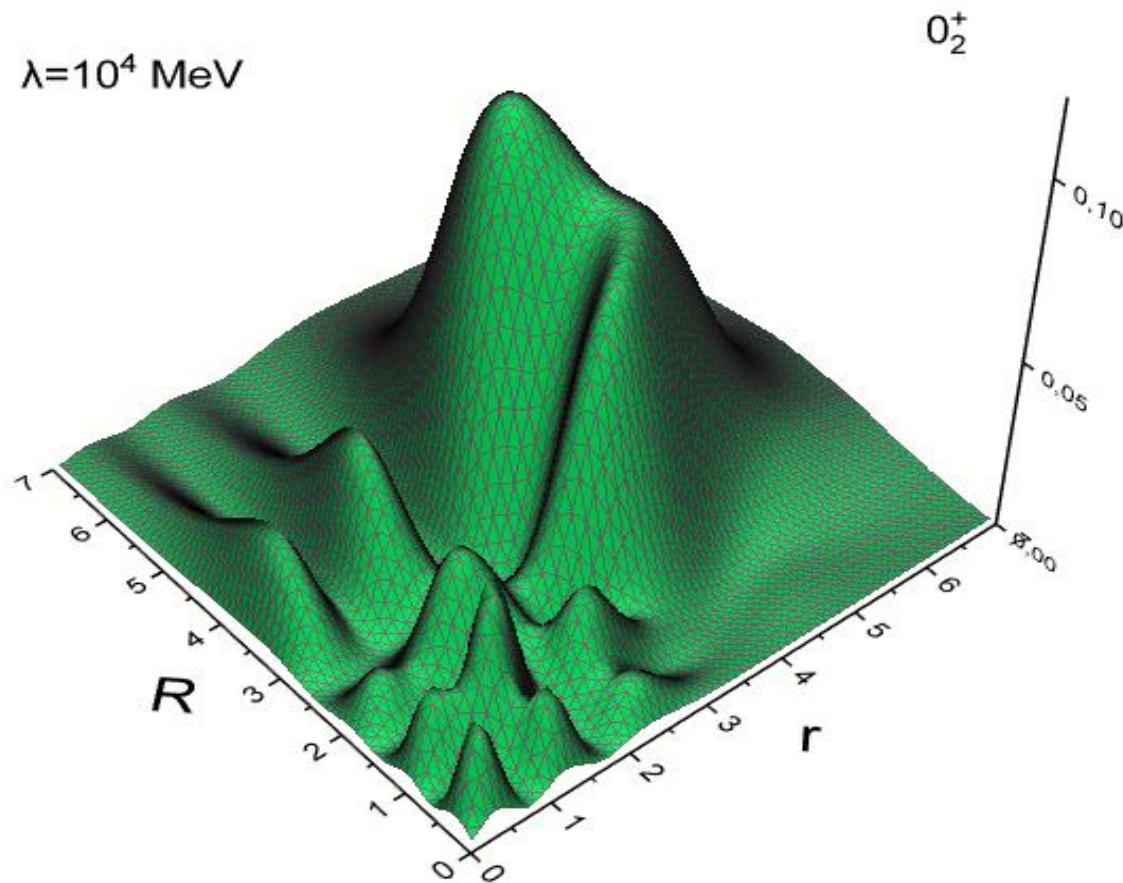
Probability density function of matter for the $^{12}\text{C}(0^+)$ g.s.

$\lambda=10^3$ MeV

$$P(x, y) = \int d\hat{x}_1 d\hat{y}_1 \Psi^*(\vec{x}_1, \vec{y}_1) \Psi(\vec{x}_1, \vec{y}_1)$$



Probability density function of matter for the $^{12}\text{C}(0_2^+)$ (Hoyle) state



Contributions of 3-body partial waves to the energy of the ground and Hoyle states of the ^{12}C nucleus

λ	l	$N_\alpha N_\beta$	Contribution to g.s. (%)
0	0	14*12	28.777
2	2	14*12	35.722
4	4	16*14	34.885
6	6	16*14	0.606
8	8	16*14	0.010

$^{12}\text{C} (0_1^+)$
g.s.

λ	l	$N_\alpha N_\beta$	Contribution (%)
0	0	14*12	55.012
2	2	14*12	24.120
4	4	16*14	17.008
6	6	16*14	3.418
8	8	16*14	0.442

$^{12}\text{C}(0_2^+)$
Hoyle s.

The energy spectrum of the ^{12}C nucleus with $(J\pi; T) = (2+; 0)$ in MeV at several values of the projecting constant

λ (MeV)	10^3	10^4	10^5	10^6	10^7	10^8
E_1	-17.361	-15.649	-8.243	1.042	1.086	1.162
E_2	1.030	1.032	1.034	1.475	2.524	2.643
$\langle P \rangle$	1.062	1.127	5.974	1.2E-2	3.1E-2	2.7E-2

Lowest 0^+ (g.s.) and 2_1^+ states go to the continuum when $\lambda \rightarrow +\infty$.

E. M. Tursunov, J. Phys. G: Nucl. Part. Phys. **27**, 1381 (2001).

B) DIRECT orthogonalization method (H. Matsumura, M. Orabi, Y. Suzuki, and Y. Fujiwara, Nucl. Phys. A **776**, 1 (2006)).

$$\hat{\Gamma}_i^{(f)} = \frac{1}{2f+1} \times \sum_{m_f} |\varphi_{fm_f}(\mathbf{x}_i)\rangle \langle \varphi_{fm_f}(\mathbf{x}'_i)| \delta(\mathbf{y}_i - \mathbf{y}'_i)$$

$$\hat{P} = \sum_{i=1}^3 \hat{P}_i,$$

$$\hat{P}_i = \sum_f \hat{\Gamma}_i^{(f)}$$

The direct orthogonalization method is based on the separation of the complete Hilbert functional space into two parts. The first subspace L_Q , which we call **allowed subspace**, is defined by the *kernel of the complete three-body projector*. The rest subspace L_P contains 3α states forbidden by the Pauli principle. After the separation of the complete Hilbert functional space of 3α states into the L_Q (allowed) and L_P (**forbidden**) subspaces, at next step we solve the three-body Schrodinger equation in L_Q .

The allowed subspace L_Q is defined by the eigen states of the operator P , corresponding to its zero eigen value: $P\Phi = 0$.

1 step: Separation of $L_Q = \text{kern}(P)$.

2-step: Solution of the Schroedinger equation in L_Q .

As in mentioned work, there are two eigen states of the operator P among other eigen states, which play a *decisive role* for the structure of the $12\text{C}(0+)$ lowest states. *Special (kritical) eigen states*

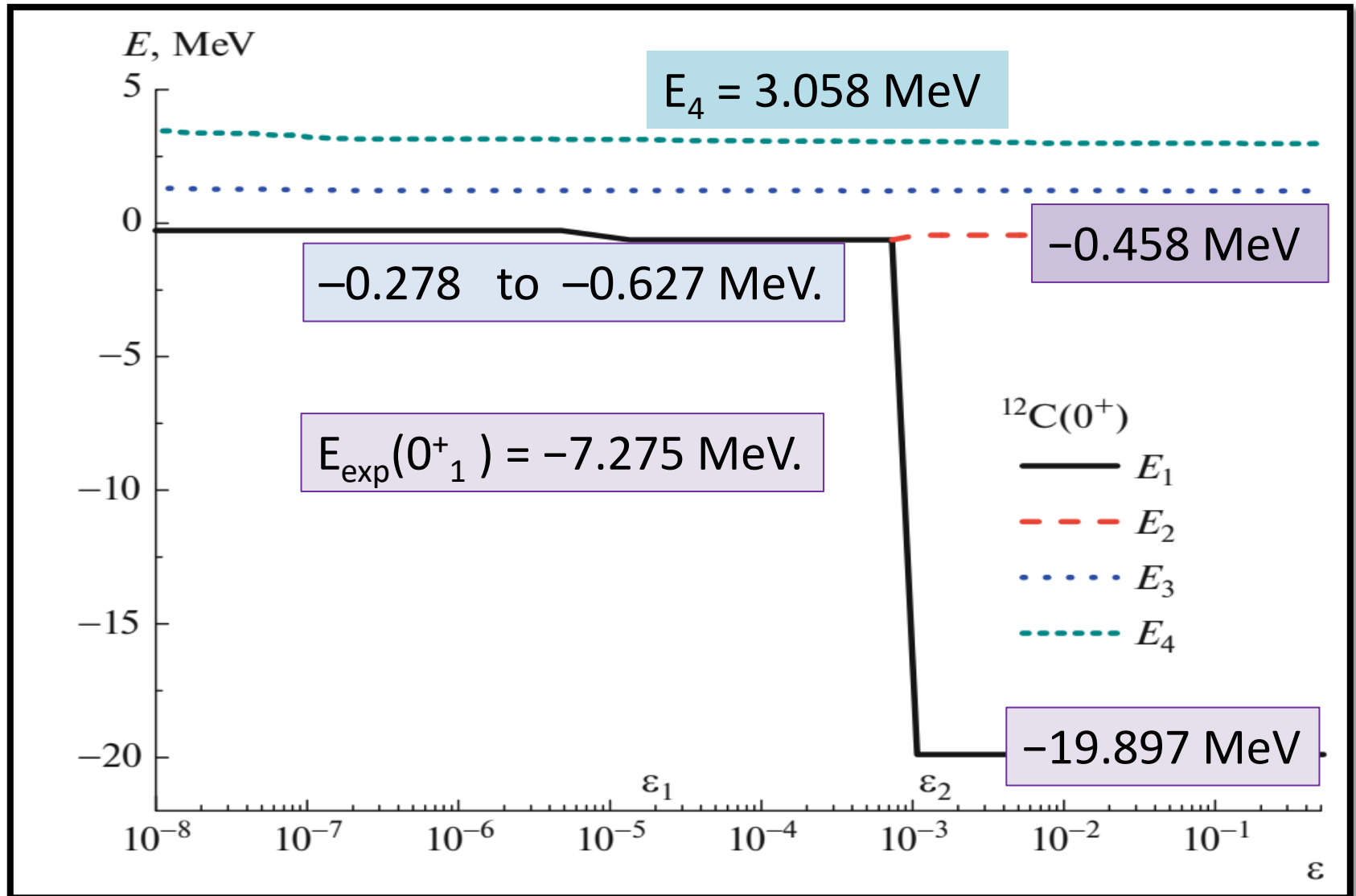
$$\Phi_1: \quad \varepsilon_1 = 1.35333 \times 10^{-5}$$

$$\Phi_2: \quad \varepsilon_2 = 1.07152 \times 10^{-3}$$

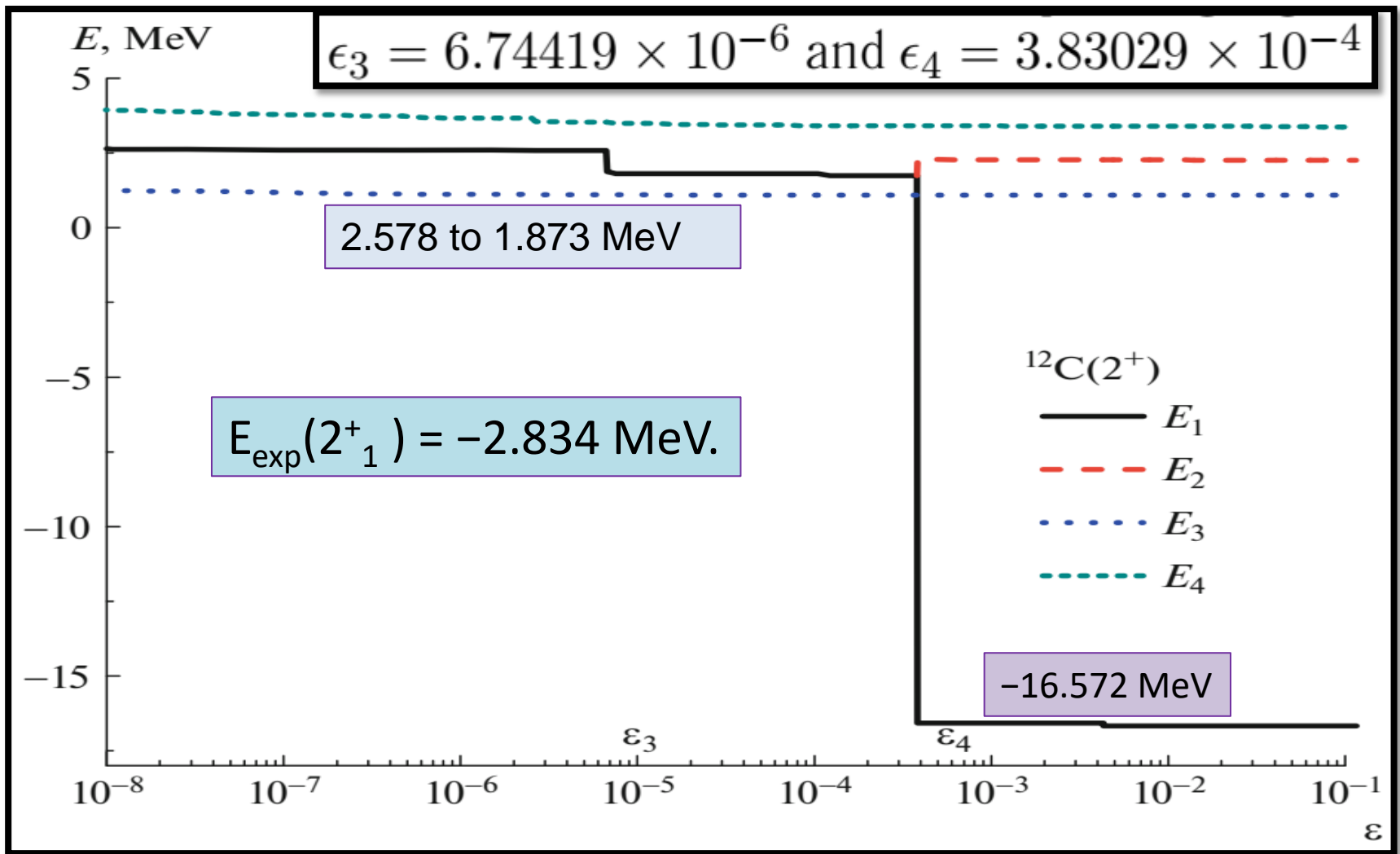
$$P \Phi_k = \varepsilon_k \Phi_k$$

In the paper of H. Matsumura et al they are called “almost forbidden states”.

Energy spectrum of the lowest $^{12}\text{C}(0^+)$ states in dependence on the maximally allowed eigen value of the operator P



Energy spectrum of the lowest $^{12}\text{C}(2^+)$ states in dependence on the maximally allowed eigen values of the operator P



Possible first order quantum phase transition !?

From the weakly bound phase to a deep phase.

For the $0+$ spectrum: *a critical eigen function (critical point)* and corresponding *critical eigen value of the threebody projector*, which is responsible for the quantum phase transition.

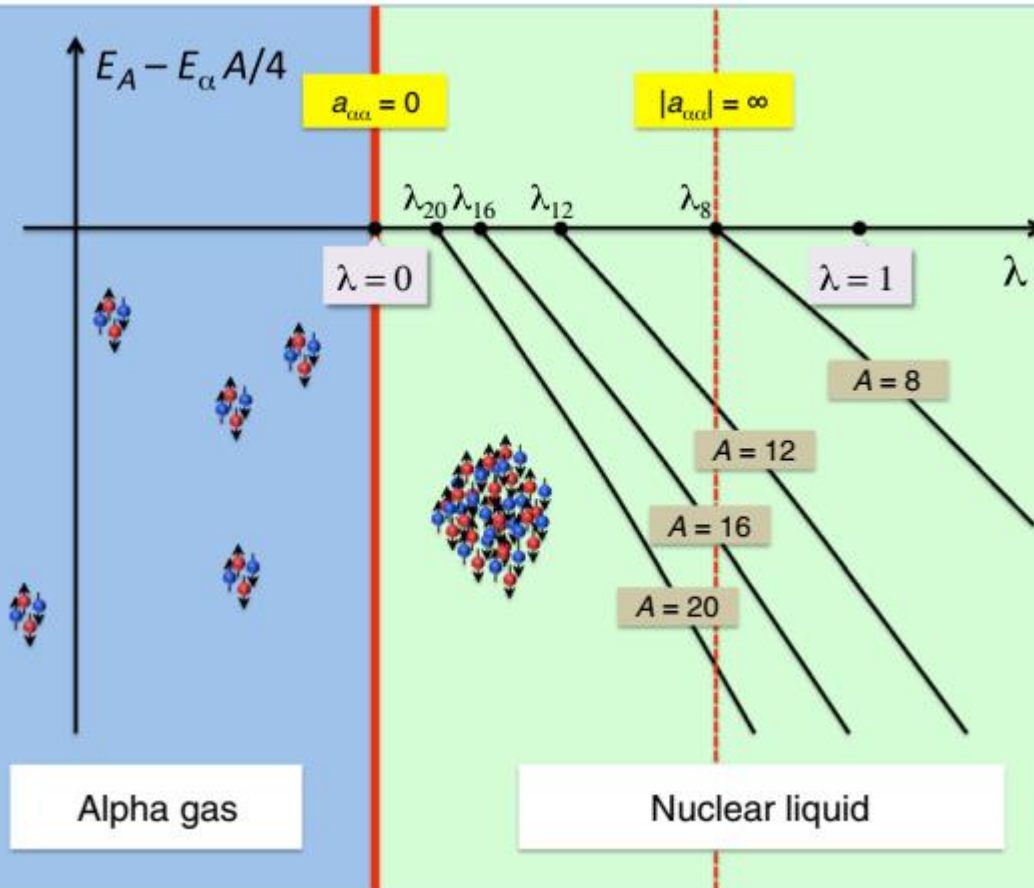
On the left-hand side of the critical point the lowest $0+$ state mostly presents the Hoyle state, while *on the right-hand side* of the critical point the lowest state *becomes the ground state of the ^{12}C nucleus in the deep phase*. An overlap of the critical eigen function of the three-body projector with the ground state is close to unity, while its overlap with the Hoyle state is almost zero. This means that the *ground state of the ^{12}C nucleus in the deep phase is created by the critical eigen function of the Pauli projector*.

A behavior of the $2+$ levels is analogous.

Nuclear Binding Near a Quantum Phase Transition

PRL 117, 132501
(2016)

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$$V_\lambda = (1 - \lambda)V_A + \lambda V_B$$

λ - strength of the locality of the ChEFT NN-interaction pot-al.

While the properties of few nucleon systems vary only slightly with λ , the many-body ground state of V_λ undergoes a **quantum phase transition from a Bose condensed gas to a nuclear liquid**.

Conclusions

- The energy spectrum of the ^{12}C nucleus has been analyzed within the 3α model. The Pauli forbidden states were treated by the OPP and exact orthogonalisation methods.
- An evidence of possible first order quantum phase transition has been examined. It was shown that there are effects of possible **QPT** in the lowest $^{12}\text{C}(0^+_{1})$ and $^{12}\text{C}(2^+_{1})$ states from the weakly bound *gas-like phase* to a *deep liquid-like* phase.
- There is a *critical eigen function and corresponding critical eigen value of the 3-body Pauli projector* which are responsible for the quantum phase transition.
- On the left-hand side of the critical point the lowest 0^+ state mostly presents the *Hoyle state*, while on the *right-hand side* of the critical point the lowest state becomes *the ground state of the ^{12}C nucleus in the deep phase*.
- *The same behavior was found in the 2^+ sector.*

THANKS !!!