





Status of Nuclear Lattice Simulations

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Nuclear Lattice Effective Field Theory collaboration

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CONTENTS

- Introduction: Effective Field Theory for Nuclear Physics
- Nuclear lattice simulations: methods
- Nuclear lattice simulations: results
- Status summary

Introduction: Effective Field Theory for Nuclear Physics

only a brief reminder \rightarrow details in

E. Epelbaum, H.-W. Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773 [arXiv:0811.1338 [nucl-th]]

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CHIRAL EFT FOR FEW-NUCLEON SYSTEMS

Gasser, Leutwyler, Weinberg, van Kolck, Epelbaum, Bernard, Kaiser, UGM, . . .

• Scales in nuclear physics:

Natural: $\lambda_{\pi} = 1/M_{\pi} \simeq 1.5$ fm (Yukawa 1935)

Unnatural: $|a_{np}({}^1S_0)| = 23.8\,{
m fm}$, $a_{np}({}^3S_1) = 5.4\,{
m fm} \gg 1/M_\pi$

• this can be analyzed in a suitable EFT based on

$$\mathcal{L}_{ ext{QCD}}
ightarrow \mathcal{L}_{ ext{EFF}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \dots$$

- pion and pion-nucleon sectors are perturbative in $Q/\Lambda_{\chi}
 ightarrow$ chiral perturbation th'y
- \mathcal{L}_{NN} collects short-distance contact terms, to be fitted
- NN interaction requires non-perturbative resummation

 \rightarrow chirally expand V_{NN(N)}, use in regularized LS/FY equation

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CHIRAL POTENTIAL and NUCLEAR FORCES



- explains naturally the observed hierarchy of nuclear forces
- MANY successfull tests in few-nucleon systems (continuum calc's)

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Nuclear lattice simulations – Formalism –

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NUCLEAR LATTICE SIMULATIONS

Frank, Brockmann (1992), Koonin, Müller, Seki, van Kolck (2000), Lee, Schäfer (2004), . . . Borasoy, Krebs, Lee, UGM, Nucl. Phys. **A768** (2006) 179; Borasoy, Epelbaum, Krebs, Lee, UGM, Eur. Phys. J. **A31** (2007) 105

- new method to tackle the nuclear many-body problem
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$: nucleons are point-like fields on the sites
- discretized chiral potential w/ pion exchanges and contact interactions
- typical lattice parameters

$$\Lambda = rac{\pi}{a} \simeq 300 \, {
m MeV} \, [{
m UV} \, {
m cutoff}]$$



• strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

J. W. Chen, D. Lee and T. Schäfer, Phys. Rev. Lett. 93 (2004) 242302

• hybrid Monte Carlo & transfer matrix (similar to LQCD)

CONFIGURATIONS







 \Rightarrow all *possible* configurations are sampled \Rightarrow *clustering* emerges *naturally*

TRANSFER MATRIX METHOD

- Correlation–function for A nucleons: $Z_A(t) = \langle \Psi_A | \exp(-tH) | \Psi_A \rangle$ with Ψ_A a Slater determinant for A free nucleons
- Ground state energy from the time derivative of the correlator

$$E_A(t) = -rac{d}{dt}\,\ln Z_A(t)$$

 \rightarrow ground state filtered out at large times: $E_A^0 = \lim_{t \to \infty} E_A(t)$

 \bullet Expectation value of any normal–ordered operator ${\cal O}$

$$Z_A^{\mathcal{O}} = raket{\Psi_A} \exp(-tH/2) \, \mathcal{O} \, \exp(-tH/2) \ket{\Psi_A}$$

$$\lim_{t o\infty}\,rac{Z_A^{\mathcal{O}}(t)}{Z_A(t)}=\langle\Psi_A|\mathcal{O}\,|\Psi_A
angle$$

TRANSFER MATRIX CALCULATION

• Expectation value of any normal–ordered operator $\boldsymbol{\mathcal{O}}$

$$egin{aligned} &\langle \Psi_A | \mathcal{O} \left| \Psi_A
ight
angle &= \lim_{t o \infty} \; rac{\langle \Psi_A | \exp(-tH/2) \, \mathcal{O} \; \exp(-tH/2) \left| \Psi_A
ight
angle \ &\langle \Psi_A | \exp(-tH) | \Psi_A
angle \end{aligned}$$

• Anatomy of the transfer matrix



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PROJECTION MONTE CARLO TECHNIQUE

• General wave function:

 $\psi_j(ec{n}) \ , \ \ j=1,\ldots,A$

• States with well-defined momentum:

$$L^{-3/2} \sum_{\vec{m}} \psi_j(\vec{n} + \vec{m}) \exp(i ec{P} \cdot ec{m}) \;, \;\; j = 1, \dots, A$$



- Insert clusters of nucleons at initial/final states (spread over some time interval)
 → allows for all type of wave functions (shell model, clusters, ...)
 - \rightarrow removes directional bias

shell-model type

$$egin{aligned} \psi_j(ec{n}) &= \exp[-cec{n}^2] \ \psi_j'(ec{n}) &= n_x \exp[-cec{n}^2] \ \psi_j''(ec{n}) &= n_y \exp[-cec{n}^2] \ \psi_j'''(ec{n}) &= n_z \exp[-cec{n}^2] \end{aligned}$$

cluster type

$$egin{aligned} \psi_j(ec{n}) &= \exp[-c(ec{n}-ec{m})^2] \ \psi_j'(ec{n}) &= \exp[-c(ec{n}-ec{m}')^2] \ \psi_j''(ec{n}) &= \exp[-c(ec{n}-ec{m}'')^2] \ \psi_j'''(ec{n}) &= \exp[-c(ec{n}-ec{m}''')^2] \end{aligned}$$

ullet shell-model w.f.s do not have enough 4N correlations $\sim \langle (N^\dagger N)^2
angle$

PROJECTION MONTE CARLO TECHNIQUE II

- Example: two basic configurations in the spectrum of ¹²C (a = 1.97 fm)
 - compact triangle config.12 rotational orientations

bent arm configuration24 rotational orientations





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MONTE CARLO with AUXILIARY FILEDS

• Contact interactions represented by auxiliary fields s, s_I



• Correlation function = path-integral over pions & auxiliary fields



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COMPUTATIONAL EQUIPMENT

- Past = JUGENE (BlueGene/P)
- Present = JUQUEEN (BlueGene/Q)



Nuclear lattice simulations – Results –







neutron matter

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FIXING PARAMETERS & FIRST PREDICTIONS

- work at NNLO including strong and em isospin breaking
- 9 NN LECs from np scattering and Q_d
- 2 LECs for isospin-breaking (np, pp, nn)
- 2 LECs D, E related to the leading 3NF
- \Rightarrow make predictions
- pp vs np scattering
- nd spin-3/2 quartet channel

40 0 20 40 60 80 100 120 140 0 20 40 60 80 100 120 140 $p_{\rm CM}\,({\rm MeV})$ $p_{\rm CM}$ (MeV) ${}^{1}S_{0}$ ĹΟ 140 NLO + IB + EM 0.15 PWA93 (pp) 120 × 0.10 $\delta(^{1}S_{0})$ (degrees) 08 08 08 09 o cot & (fm⁻¹) 0.05 0 -0.05 or p-d (exp.) n-d (exp.) 40 -0.10 × LO NLO 20 -0.15 A NNLO 60 80 100 120 140 160 20 40 0 0 0.10 0.20 0.30 0.40 $p_{\rm CM}$ (MeV) p^2 (fm⁻²)

LÒ.

NLO₃

PWA93 (np)

140

120

40

20

 ${}^{3}S_{1}$

LÓ₂

NLO₃

PWA93 (np)

180

160

 $(32)^{(32)}$ (degrees) (140 (120)

80

60

Ground states

Epelbaum, Krebs, Lähde, Lee, UGM, arxiv:1208.1328

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PREDICTIONS: TRITON & HELIUM-3

Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. 104 (2010) 142501; Eur. Phys. J. A 45 (2010) 335

• binding energies of 3N systems: $E(L) = B.E. - \frac{a}{L} \exp(-bL)$

see also Hammer, Kreuzer (2011)

 $< \land \nabla$

 \Rightarrow predict the energy difference $E(^{3}He) - E(^{3}H)$



Ground state of ⁴He

L = 11.8 fm



Ground state of ⁸Be

L = 11.8 fm



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Ground state of ¹²C

L = 11.8 fm



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Ground state of ¹⁶O

L = 11.8 fm



SPECTRUM OF ¹²C & the HOYLE STATE

Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. **106** (2011) 192501 Viewpoint: Hjorth-Jensen, Physics **4** (2011) 38 Epelbaum, Krebs, Lähde, Lee, UGM, arxiv:1208.1328 (numbers from this ref.)



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EXCITED STATES of ¹²C



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THE HOYLE STATE (0_2^+)

- energy: $E(0_2^+) = -85(3) \, \text{MeV}$
- close to $E(^{4}\text{He}) + E(^{8}\text{Be}) = -83.3(2.0) \text{ MeV}$
- structure: "bent" alpha-chain like (not "BEC")



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A HOYLE STATE EXCITATION (2_2^+)

- a 2^+ state 2 MeV above the Hoyle state
- interpretation:

a rotational band of the Hoyle state generated from excitations of the alpha-chain

• what's in the data ?

a 2^+ state 3.51 MeV above the Hoyle state seen in ${}^{11}B(d,n){}^{12}C$ not included in the level scheme! Ajzenberg-Selove, Nucl. Phys. A506 (1990) 1

a 2⁺ state 3.8(4) MeV above the Hoyle state seen in ${}^{12}C(\alpha, \alpha){}^{12}C$ Bency John et al., Phys. Rev. C 68 (2003) 014305

• and much more, see next slide

 \Rightarrow ab initio prediction requires experimental confirmation



SPECTRUM OF ¹²C

• Summarizing the results for carbon-12:

| | 0_1^+ | 2^+_1 | 0^+_2 | 2^+_2 |
|------|------------------------|------------|------------|--------------------|
| LO | -96(2) MeV | -94(2) MeV | -89(2) MeV | -88(2) MeV |
| NLO | -77(3) MeV | -74(3) MeV | -72(3) MeV | -70(3) MeV |
| NNLO | -92(3) MeV | -89(3) MeV | -85(3) MeV | -83(3) MeV |
| | | | | -82.6(1) MeV [1,2] |
| Exp. | $-92.16~{	extsf{MeV}}$ | -87.72 MeV | -84.51 MeV | -82.32(6) MeV [3] |
| | | | | -81.1(3) MeV [4] |
| | | | | -82.13(11) MeV [5] |

• importance of consistent 2N & 3N forces

[1] Freer et al., Phys. Rev. C 80 (2009) 041303
[2] Zimmermann et al., Phys. Rev. C 84 (2011) 027304
[3] Hyldegaard et al., Phys. Rev. C 81 (2010) 024303
[4] Itoh et al., Phys. Rev. C 84 (2011) 054308
[5] Weller et al., in preparation

- good agreement w/ experiment, can be improved
- test of the Anthropic Principle possible, intriguing results

A FIRST LOOK at EM PROPERTIES

• LO em results obtained (NLO/NNLO requires longer time simulations)

| Observable | LO theory | Experiment |
|---|-----------|------------|
| $r(0_1^+)$ [fm] | 2.2(2) | 2.47(2) |
| $Q(2_1^+) [e^2 fm]$ | 6(2) | 6(3) |
| $B(E2;\!2^+_1 	o 0^+_1) [\mathrm{e}^2 \mathrm{fm}^4]$ | 5(2) | 7.6(4) |
| $B(E2;\!2^+_1 	o 0^+_2) \ [\mathrm{e}^2 \ \mathrm{fm}^4]$ | 1.5(7) | 2.6(4) |
| m(E0; $0^+_2 ightarrow 0^+_1)$ [e fm ²] | 3(1) | 5.5(1) |

- satisfying agreement for LO calculation
- other radii, quadrupole moments and transition strengths also computed
- FMD and cluster models predict e.g. $r(0_2^+) = (3.5 3.9)$ fm
- higher order corrections are in the works

STATUS SUMMARY

2012/2

- detailed investigation of the ¹²C nucleus, in part. the structure of the Hoyle state
- \rightarrow achieved, publication submitted, more details to come

2013

- detailed investigation (spectrum and wave function) of ¹⁴N
- \rightarrow postponed, do the more interesting nucleus ¹⁶O first (same CPU time)

2014

- detailed investigation of spectrum and wave function of ¹⁶O
- \rightarrow ground state done, spectrum runs start 09/2012 (JUQUEEN and RWTH Bull CI.)

2015

- formulation of the lattice set-up to perform simulations of light hyper-nuclei based on the leading order hyperon-nucleon interactions
- \rightarrow start to develop a new method w/ hyperons in nuclear background field

2016/1

- lattice simulations of light hyper-nuclei
- ightarrow if method works, will be done \ldots

Testing the Anthropic Principle

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MC ANALYSIS of the AP

- consider QCD only ightarrow calculate $\partial \Delta E / \partial M_{\pi}$
- relevant quantities (energy *differences*)

$$\Delta E_h \equiv E_{12}^* - E_8 - E_4, \quad \Delta E_b \equiv E_8 - 2E_4 \left| -\Delta E_c \equiv E_{12}^* - E_{12} \right|$$

• energy differences depend on parameters of QCD (LO analysis)

$$E_i = E_i \bigg(M_\pi^{\text{OPE}}, m_N(M_\pi), \tilde{g}_{\pi N}(M_\pi), C_0(M_\pi), C_I(M_\pi) \bigg)$$

$${ ilde g}_{\pi N} \equiv {g_A \over 2 F_\pi}$$

 $\boldsymbol{\alpha}$

• remember: $M_{\pi^\pm}^2 \sim (m_u + m_d)$

 \Rightarrow quark mass dependence \equiv pion mass dependence

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PION MASS VARIATIONS

• consider pion mass changes as *small perturbations*

$$\begin{split} \frac{\partial E_i}{\partial M_{\pi}} \Big|_{M_{\pi}^{\rm phys}} &= \left. \frac{\partial E_i}{\partial M_{\pi}^{\rm OPE}} \right|_{M_{\pi}^{\rm phys}} + x_1 \left. \frac{\partial E_i}{\partial m_N} \right|_{m_N^{\rm phys}} + x_2 \left. \frac{\partial E_i}{\partial \tilde{g}_{\pi N}} \right|_{\tilde{g}_{\pi N}^{\rm phys}} \\ &+ x_3 \left. \frac{\partial E_i}{\partial C_0} \right|_{C_0^{\rm phys}} \right. \\ \left. + x_4 \left. \frac{\partial E_i}{\partial C_I} \right|_{C_I^{\rm phys}} \end{split}$$

with

$$x_1 \equiv \left. \frac{\partial m_N}{\partial M_\pi} \right|_{M^{\rm phys}_\pi}, \ x_2 \equiv \left. \frac{\partial \tilde{g}_{\pi N}}{\partial M_\pi} \right|_{M^{\rm phys}_\pi}, \ x_3 \equiv \left. \frac{\partial C_0}{\partial M_\pi} \right|_{M^{\rm phys}_\pi}, \ x_4 \equiv \left. \frac{\partial C_I}{\partial M_\pi} \right|_{M^{\rm phys}_\pi}$$

 \Rightarrow problem reduces to the calculation of the various derivatives using AFQMC and the determination of the x_i

- x_1 and x_2 can be obtained from LQCD plus CHPT
- x_3 and x_4 can be obtained from two-body scattering and its M_{π} -dependence

AFQMC RESUTS for the DERIVATIVES

• ⁴He

-25

-25.5

-26

-26.5

-27

-27.5

-28

-28.5

-20

-1.35

-1.4

-1.45

-1.5

-1.55

-1.6

-1.65

-1.7

1.4

1.35

1.3

1.25

1.2

1.15



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DETERMINATION of the x_i

- x_1 from the quark mass expansion of the nucleon mass: $x_1 \simeq 0.8 \pm 0.2$
- x_2 from the quark mass expansion of the pion decay constant and the nucleon axial-vector constant: $x_2 \simeq -0.056 \dots 0.008$
- x₃ and x₄ can be obtained from a two-nucleon scattering analysis & can be deduced from:

$$-rac{\partial a^{-1}}{\partial M_\pi}\equiv rac{A}{aM_\pi}=rac{1}{\pi L}S'(\eta)rac{\partial \eta}{\partial M_\pi}\,,\;\;\eta\equiv m_N E\left(rac{L}{2\pi}
ight)^2$$

 \Rightarrow while this can straightforwardly be computed, we prefer to use a representation that substitutes x_3 and x_4 by:

$$\left. rac{\partial a_s^{-1}}{\partial M_\pi} \right|_{M^{\mathrm{phys}}_\pi}, \quad \left. rac{\partial a_t^{-1}}{\partial M_\pi} \right|_{M^{\mathrm{phys}}_\pi}$$

 \Rightarrow we are ready to study the pertinent energy differences

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• putting pieces together:

$$\begin{split} \frac{\partial \Delta E_{h}}{\partial M_{\pi}}\Big|_{M_{\pi}^{\rm phys}} &= -0.455(35) \left. \frac{\partial a_{s}^{-1}}{\partial M_{\pi}} \right|_{M_{\pi}^{\rm phys}} - 0.744(24) \left. \frac{\partial a_{t}^{-1}}{\partial M_{\pi}} \right|_{M_{\pi}^{\rm phys}} + 0.056(10) \\ \frac{\partial \Delta E_{b}}{\partial M_{\pi}} \Big|_{M_{\pi}^{\rm phys}} &= -0.117(34) \left. \frac{\partial a_{s}^{-1}}{\partial M_{\pi}} \right|_{M_{\pi}^{\rm phys}} - 0.189(24) \left. \frac{\partial a_{t}^{-1}}{\partial M_{\pi}} \right|_{M_{\pi}^{\rm phys}} + 0.012(9) \\ \frac{\partial \Delta E_{c}}{\partial M_{\pi}} \Big|_{M_{\pi}^{\rm phys}} &= -0.07(3) \left. \frac{\partial a_{s}^{-1}}{\partial M_{\pi}} \right|_{M_{\pi}^{\rm phys}} - 0.14(2) \left. \frac{\partial a_{t}^{-1}}{\partial M_{\pi}} \right|_{M_{\pi}^{\rm phys}} + 0.017(9) \end{split}$$

- x_1 and x_2 only affect the small constant terms
- also calculated the shifts of the individual energies (not shown here)

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INTERPRETATION

- $(\partial \Delta E_h / \partial M_\pi) / (\partial \Delta E_b / \partial M_\pi) \simeq 4$ $\Rightarrow \Delta E_h$ and ΔE_b cannot be independently fine-tuned
- Within error bars, $\partial \Delta E_h / \partial M_\pi \& \partial \Delta E_b / \partial M_\pi$ appear unaffected by the choice of x_1 and $x_2 \rightarrow$ indication for α -clustering
- For ΔE_h & ΔE_b , the dependence on M_π is small when

$$\partial a_s^{-1}/\partial M_\pi \simeq -1.6 \times \partial a_t^{-1}/\partial M_\pi$$

• the triple alpha process is controlled by :

$$\Delta E_{h+b} \equiv \Delta E_h + \Delta E_b = E^{\star}_{12} - 3E_4$$

$$\frac{\partial \Delta E_{h+b}}{\partial M_{\pi}} \Big|_{M_{\pi}^{\rm phys}} = -0.571(14) \left. \frac{\partial a_s^{-1}}{\partial M_{\pi}} \right|_{M_{\pi}^{\rm phys}} - 0.934(11) \left. \frac{\partial a_t^{-1}}{\partial M_{\pi}} \right|_{M_{\pi}^{\rm phys}} + 0.069(6)$$

 \Rightarrow so what can we say about the quark mass dependence of the scattering lengths?

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ONSTRAINTS on the SCATTERING LENGTHS

- Quark mass dependence of hadron properties: ${\delta O_H\over \delta m_f}\equiv K^f_H{O_H\over m_f}\,,\;\;f=u,d,s$
- NN scattering lengths as a function of M_{π} : -

$$-rac{\partial a_{s,t}^{-1}}{\partial M_{\pi}}\equiv rac{A_{s,t}}{a_{s,t}M_{\pi}}, \quad A_{s,t}\equiv rac{K_{a_{s,t}}^q}{K_{\pi}^q}$$

- earlier determinations from chiral EFT at NLO Beane, Savage (2003), Epelbaum, Glöckle, UGM (2003)
- new determination at NNLO:

Epelbaum et al. (2012)

$$K^q_{a_s} = 2.3^{+1.9}_{-1.8} \,, \, K^q_{a_t} = 0.32^{+0.17}_{-0.18}
ightarrow rac{\partial a_t^{-1}}{\partial M_\pi} = -0.18^{+0.10}_{-0.10} \,, \,\, rac{\partial a_s^{-1}}{\partial M_\pi} = 0.29^{+0.25}_{-0.23}$$

• note the *magical* central value:

$$rac{\partial a_s^{-1}/\partial M_\pi}{\partial a_t^{-1}/\partial M_\pi}\simeq -1.6^{+1.0}_{-1.7}$$

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CORRELATIONS

• vary the quark mass derivatives of $a_{s,t}^{-1}$ within $-1, \ldots, +1$:



• clear correlations: α -particle BE and the energies/energy differences

 \Rightarrow anthropic or non-anthropic scenario depends on whether the ⁴He BE moves!

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THE END-OF-THE-WORLD PLOT

$ullet \left| \delta(\Delta E_{h+b}) ight| < 100 \ { m keV}$

$$\rightarrow \left| \left| \left(0.571(14)\bar{A}_s + 0.934(11)\bar{A}_t - 0.069(6) \right) \frac{\delta m_q}{m_q} \right| < 0.0015$$



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SUMMARY & OUTLOOK

- Nuclear lattice simulations as a new quantum many-body approach
- Formulate continuum EFT on space-time lattice $V = L_s imes L_s imes L_s imes L_t$
- New method to extract phase shifts & mixing angles
- Fix parameters in few-nucleon systems \rightarrow predictions
- Promising results for A = 2, 3, 4, 8, 12, 16 at NNLO
- ¹²C spectrum at NNLO \rightarrow Hoyle state & 2⁺ excitation
- First ever ab initio MC calculation of ¹⁶O
- Testing the anthropic principle \rightarrow strong correlations of α -cluster type \Rightarrow the Hoyle state does not appear anthropic (Coulomb to be done)

 \Rightarrow larger A and higher precision



