STRUCTURE of NUCLEI from LATTICE SIMULATIONS

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Supported by DFG, SFB/TR-16 and by DFG, SFB/TR-110 and by EU, I3HP EPOS and by BMBF 05P12PDFTE and by HGF VIQCD VH-VI-417

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- Light nuclei and the spectrum of ^{12}C
- Structure and spectrum of ^{16}O
- Towards medium-mass nuclei
- Taming the sign problem: Simulations of ^{10}Be and ^{10}C
- The fate of carbon-based life as a function of fundamental parameters
- Outlook

Ab initio calculations of atomic nuclei

INGREDIENTS

- Nuclear binding is shallow: $E/A \leq 8$ MeV

$\Rightarrow$ Nuclei can be calculated from the A-body Schrödinger equation: $\boxed{H\Psi_A = E\Psi_A}$

- Forces are of (dominant) two- and (subdominant) three-body nature:

$$\boxed{V = V_{\rm NN} + V_{\rm NNN}}$$

$\Rightarrow$ can be calculated **systematically** and to **high-precision** $\rightarrow$slide

Weinberg, van Kolck, Epelbaum, UGM, Entem, Machleidt, . . .

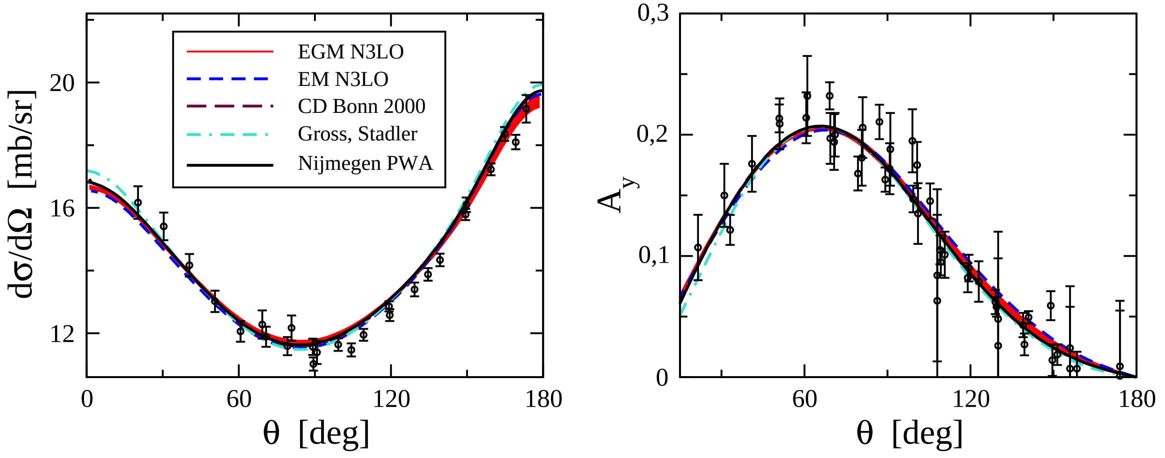
$\Rightarrow$ fit all parameters in $V_{\rm NN} + V_{\rm NNN}$ from 2- and 3-body data

$\Rightarrow$ exact calc's of systems with $A \leq 4$ using Faddeev-Yakubowsky machinery

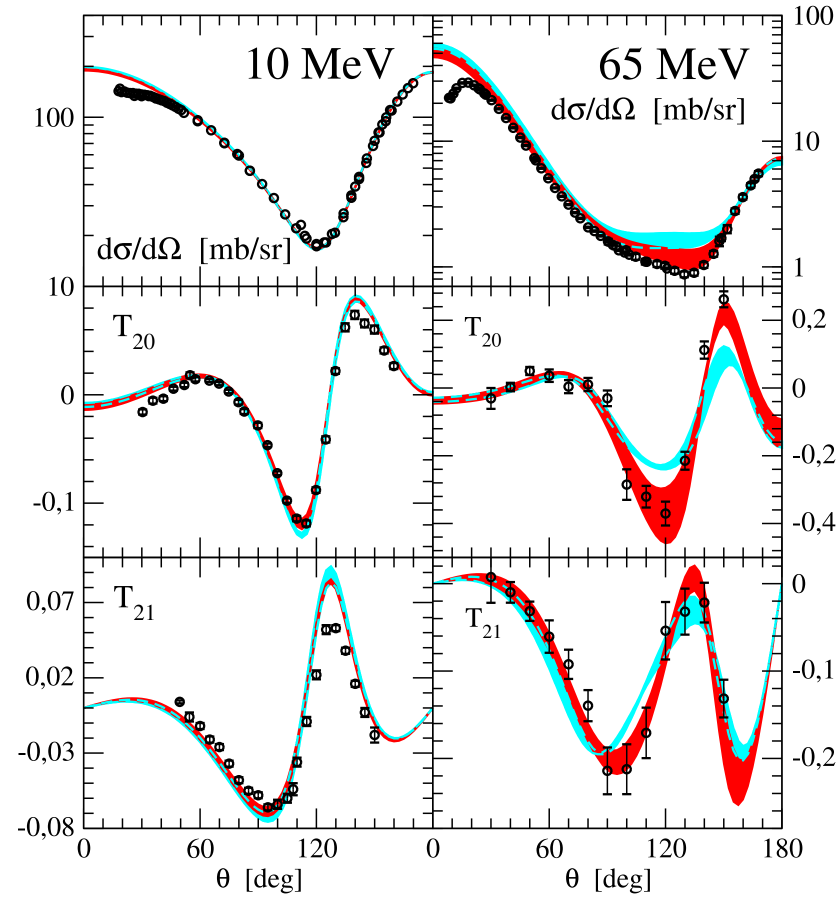
But how about *ab initio* calculations for systems with $A \geq 5$?

FEW-NUCLEON SYSTEMS from CHIRAL EFT

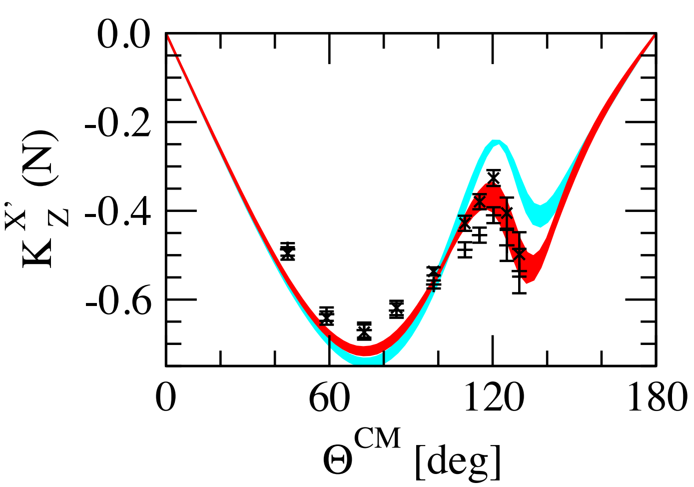
- np scattering



- nd scattering



- pol. transfer in pd scattering



Epelbaum, Hammer, UGM,
Rev. Mod. Phys. **81** (2009) 1773

NUCLEAR LATTICE SIMULATIONS

Frank, Brockmann (1992), Koonin, Müller, Seki, van Kolck (2000) , Lee, Borasoy, Schäfer, Phys.Rev. **C70** (2004) 014007, . . .
Borasoy, Krebs, Lee, UGM, Nucl. Phys. **A768** (2006) 179; Borasoy, Epelbaum, Krebs, Lee, UGM, Eur. Phys. J. **A31** (2007) 105

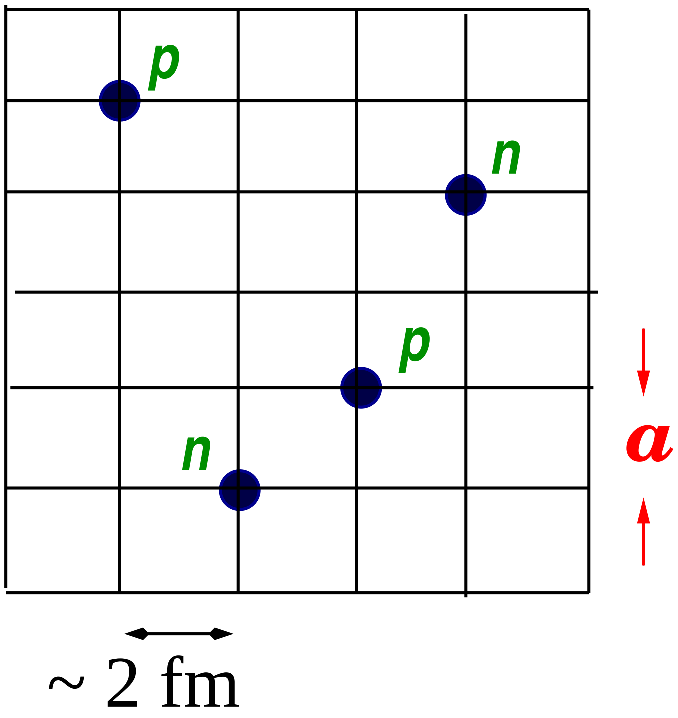
- *new method* to tackle the nuclear many-body problem

- 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 + Coulomb + I-violation

- typical lattice parameters

$$\Lambda = \frac{\pi}{a} \simeq 300 \text{ MeV [UV cutoff]}$$

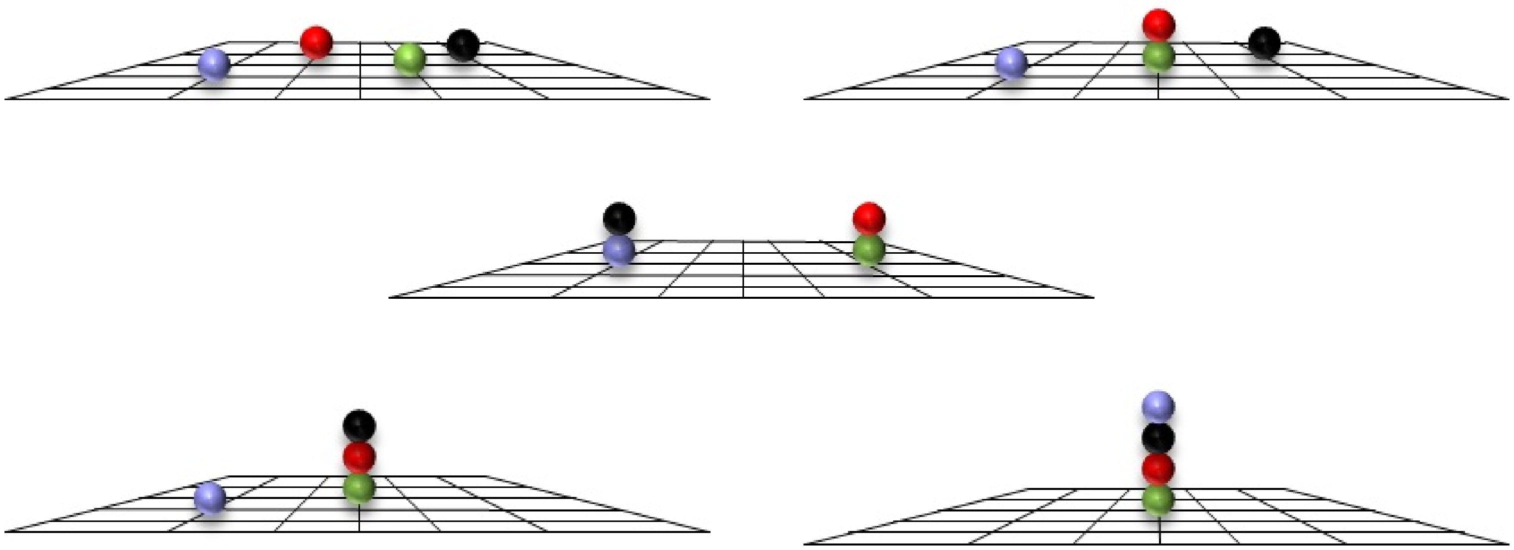


- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

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

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

CONFIGURATIONS



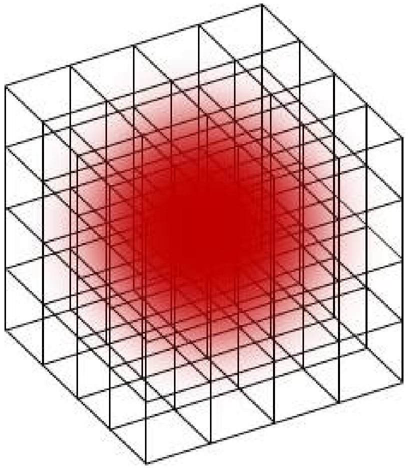
⇒ all *possible* configurations are sampled

⇒ *clustering* emerges *naturally*

⇒ perform *ab initio* calculations using only V_{NN} and V_{NNN} as input

⇒ grand challenge: the spectrum of ^{12}**C** → projection MC

PROJECTION MONTE CARLO TECHNIQUE



- General wave function:

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

- States with well-defined momentum:

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

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

shell-model type

$$\psi_j(\vec{n}) = \exp[-c\vec{n}^2]$$
$$\psi'_j(\vec{n}) = n_x\exp[-c\vec{n}^2]$$
$$\psi''_j(\vec{n}) = n_y\exp[-c\vec{n}^2]$$
$$\psi'''_j(\vec{n}) = n_z\exp[-c\vec{n}^2]$$

cluster type

$$\psi_j(\vec{n}) = \exp[-c(\vec{n}-\vec{m})^2]$$
$$\psi'_j(\vec{n}) = \exp[-c(\vec{n}-\vec{m}')^2]$$
$$\psi''_j(\vec{n}) = \exp[-c(\vec{n}-\vec{m}'')^2]$$
$$\psi'''_j(\vec{n}) = \exp[-c(\vec{n}-\vec{m}''')^2]$$

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

COMPUTATIONAL EQUIPMENT

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

6 Pflops

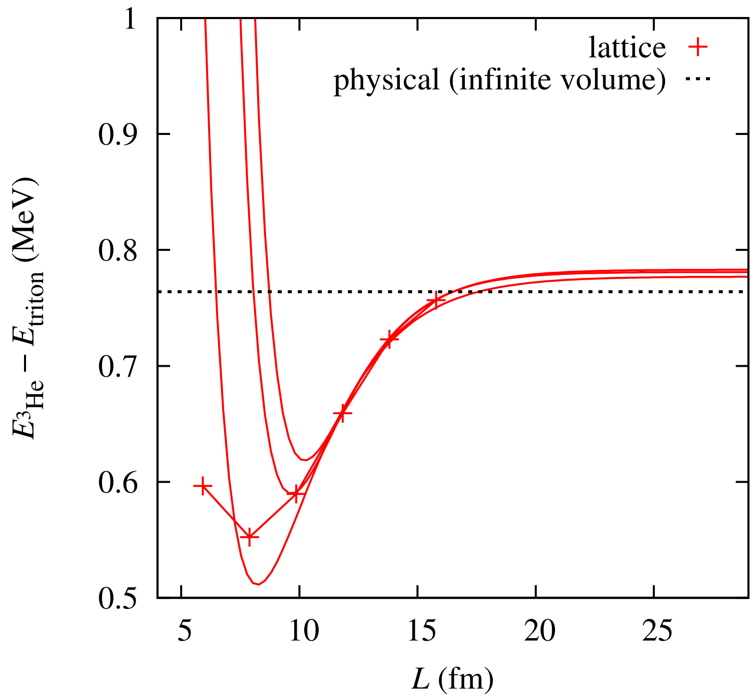
Light nuclei and the spectrum of ^{12}C

RESULTS

- fix parameters from 2N scattering and two 3N observables [NNLO: 9+2]

- some ground state energies and differences

E [MeV]	NLEFT	Exp.
^{3}He -^{3}H	0.78(5)	0.76
^{4}He	$-28.3(6)$	-28.3
^{8}Be	$-55(2)$	-56.5
^{12}C	$-92(3)$	-92.2



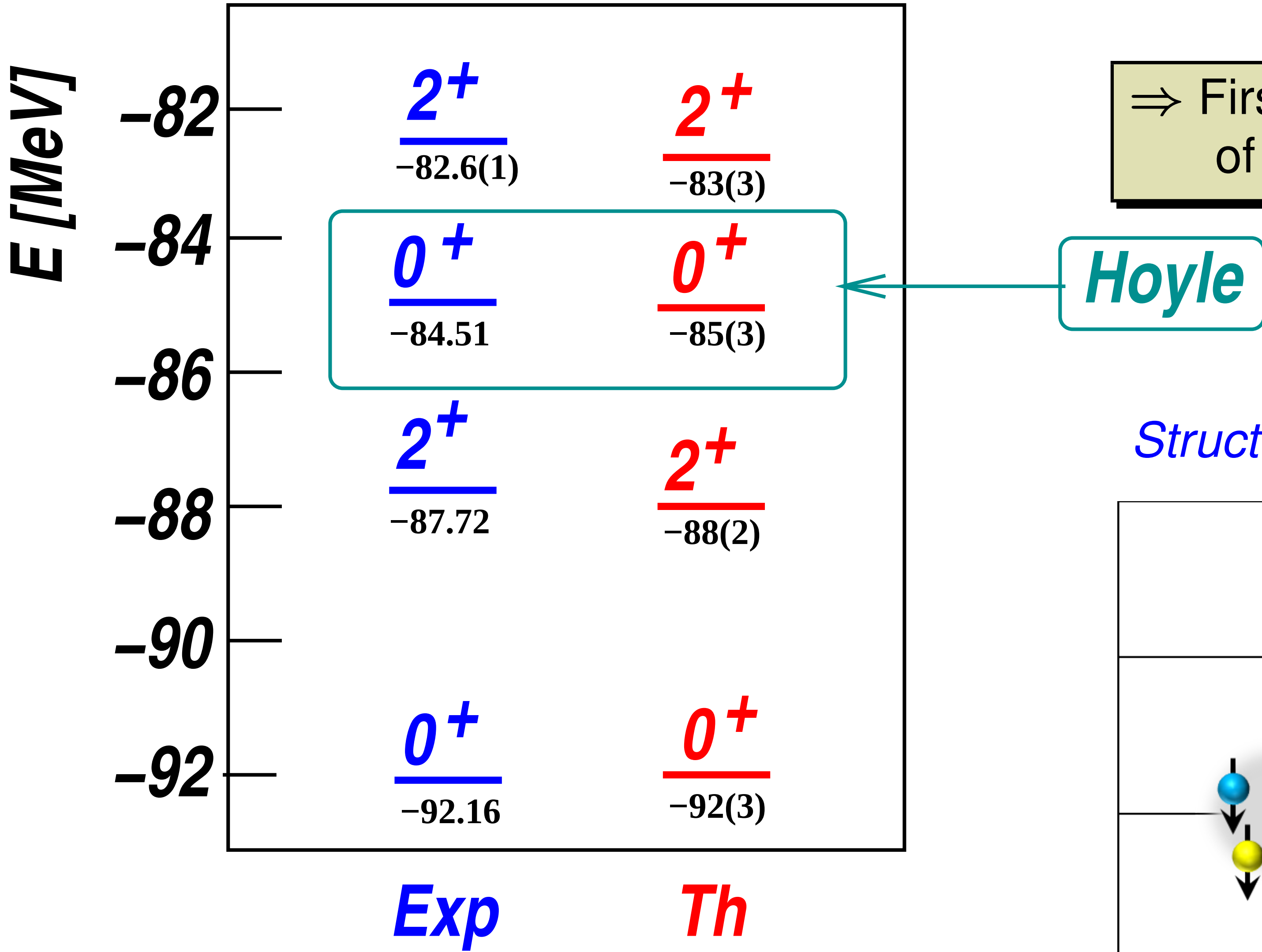
- promising results [3NFs very important]

- new method to decrease the systematic errors (triangulation)

$\Rightarrow$ uncertainties reduced by a factor of 10, e.g. E(^{8}Be) = $\mathbf{-56.3(2)}$ MeV

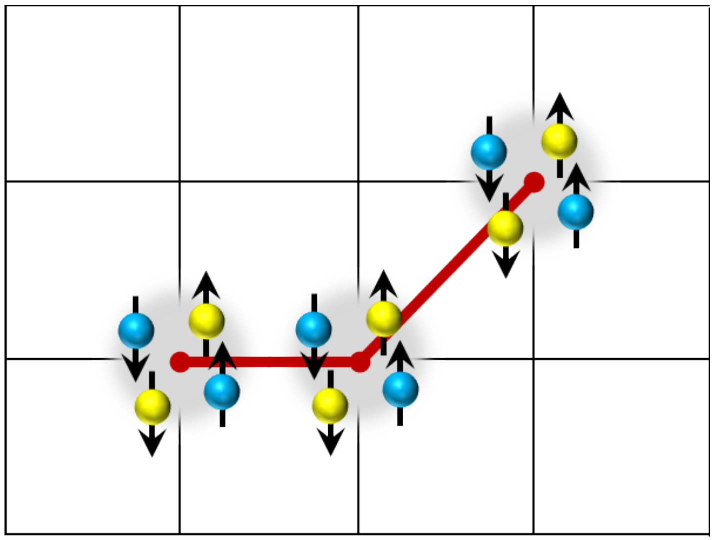
The SPECTRUM of CARBON-12

- After $8 \cdot 10^6$ hrs JUGENE/JUQUEEN (and “some” human work)



⇒ First ab initio calculation of the Hoyle state ✓

Structure of the Hoyle state:



SPECTRUM of ^{12}C

- Summarizing the results for carbon-12 at NNLO:

	0_1^+	2_1^+	0_2^+	2_2^+
2N 3N 2N+3N	-77 MeV -15 MeV $-92(3)$ MeV	-74 MeV -15 MeV $-89(3)$ MeV	-72 MeV -13 MeV $-85(3)$ MeV	-70 MeV -13 MeV $-83(3)$ MeV
Exp.	-92.16 MeV	-87.72 MeV	-84.51 MeV	$-82.6(1)$ MeV [1,2] $-82.32(6)$ MeV [3] $-81.1(3)$ MeV [4] $-82.13(11)$ MeV [5]

[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] Zimmermann et al., Phys. Rev. Lett. 110 (2013) 152502

- importance of **consistent** 2N & 3N forces
- good agreement w/ experiment, can be improved [partly done]

EM TRANSITIONS, RADII etc.

- So far only LO results (need algorithmic improvements)
- RMS charge radii

	LO	Exp.
0_1^+	2.2(2) fm	2.47(2) fm
2_1^+	2.2(2) fm	—
0_2^+	2.5(2) fm	—
2_2^+	2.5(2) fm	—

- Quadrupole moments

	LO	Exp.
2_1^+	8(1) e fm	6(3) e fm
2_2^+	−13(2) e fm	—

- EM transition strength

	LO	Exp.
$B(E2, 2_1^+ \to 0_1^+)$	7(1) e^2 fm^4	7.6(4) e^2 fm^4
$B(E2, 2_1^+ \to 0_2^+)$	1(1) e^2 fm^4	2.6(4) e^2 fm^4

- consistent with overbinding at LO
- results of other approaches: FMD Chernyak et al. (2007)
  NCSM Forssen, Roth, Navratil (2011)

Spectrum & structure of ^{16}O

STRUCTURE of ^{16}O

- Mysterious nucleus, despite modern ab initio calcs

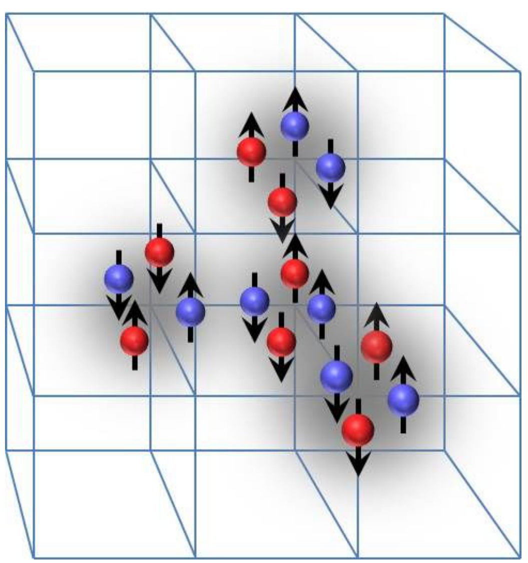
  Hagen et al. (2010), Roth et al. (2011), Hergert et al. (2013)

- Alpha-cluster models since decades, some exp. evidence

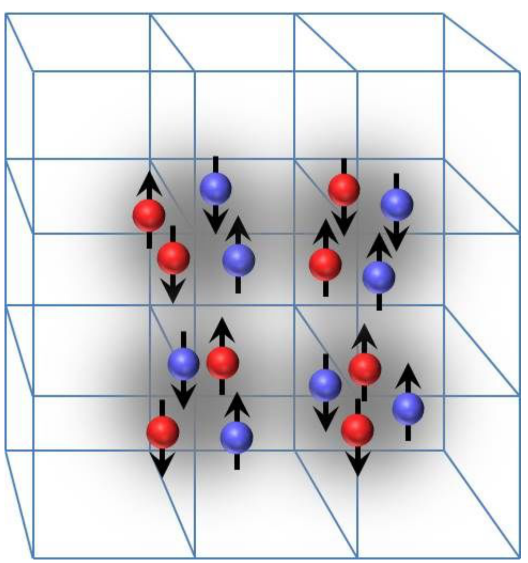
  Wheeler (1937), Dennison (1954), Robson (1979), . . ., Freer et al. (2005)

- Relevant configurations:

Tetrahedron (A)



Square (narrow (B) and wide (C))



DECODING the STRUCTURE of ^{16}O

Epelbaum, Krebs, Lähde, Lee, UGM, Rupak, Phys. Rev. Lett. **112** (2014) 102501

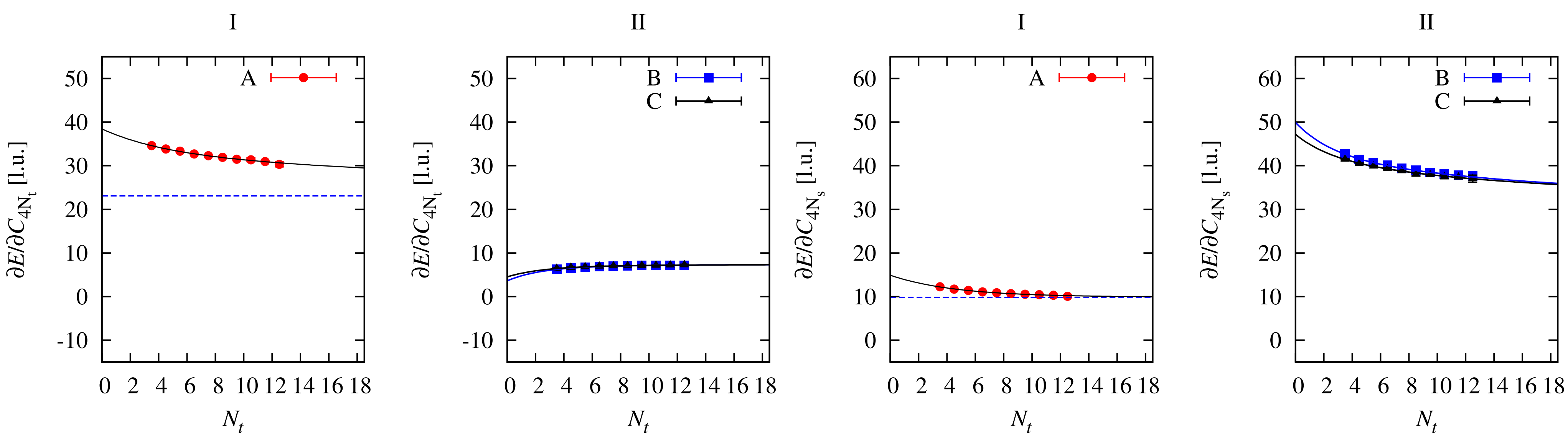
- measure the 4N density, where each of the nucleons is placed at adjacent points

$\Rightarrow$ $\mathbf{0_1^+}$ ground state: mostly tetrahedral config

$\Rightarrow$ $\mathbf{0_2^+}$ excited state: mostly square configs

$\mathbf{2_1^+}$ excited state: rotational excitation of the $\mathbf{0_2^+}$

overlap w/ tetrahedral config. overlap w/ square configs.



RESULTS for ^{16}O

- Spectrum:

	LO	NNLO(2N)	NNLO(3N)	$4N_{\rm eff}$	Exp.
0_1^+	-147.3(5)	-121.4(5)	-138.8(5)	-131.3(5)	-127.62
0_2^+	-145(2)	-116(2)	-136(2)	-123(2)	-121.57
2_1^+	-145(2)	-116(2)	-136(2)	-123(2)	-120.70

- LO charge radius: $r(0_1^+) = 2.3(1)$ fm Exp. $r(0_1^+) = 2.710(15)$ fm

$\Rightarrow$ compensate for this by recscaling with appropriate units of $r/r_{\rm LO}$

- LO EM properties:

	LO	LO(r-scaled)	Exp.
$Q(2_1^+)$ [e fm^2]	10(2)	15(3)	—
$B(E2, 2_1^+ \to 0_2^+)$ [e^2 fm^4]	22(4)	46(8)	65(7)
$B(E2, 2_1^+ \to 0_1^+)$ [e^2 fm^4]	3.0(7)	6.2(1.6)	7.4(2)
$M(E0, 0_2^+ \to 0_2^+)$ [e fm^2]	2.1(7)	3.0(1.4)	3.6(2)

$\Rightarrow$ gives credit to the interpretation of the 2_1^+ as rotational excitation

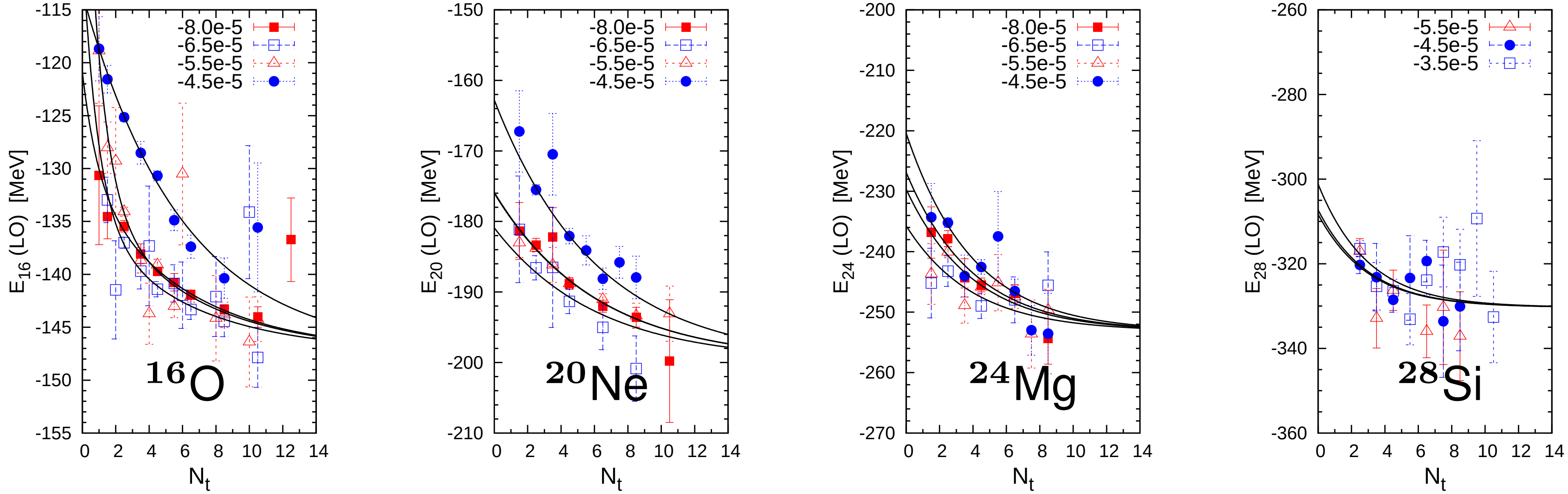
Towards medium-mass nuclei

GOING up the ALPHA CHAIN

- Consider the α ladder ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si as $t_{\rm CPU} \sim A^2$
- Improved "multi-state" technique to extract ground state energies

  $\Rightarrow$ higher A, better accuracy

  $\Rightarrow$ overbinding at LO beyond $A = 12$ persists up to NNLO



$$E = -131.3(5) \quad [-127.62]$$
$$E = -165.9(9) \quad [-160.64]$$
$$E = -232(2) \quad [-198.26]$$
$$E = -308(3) \quad [-236.54]$$

REMOVING the OVERBINDING

Lähde et al., Phys. Lett. B732 (2014) 110 [arXiv:1311.0477 [nucl-th]]

- Overbinding is due to four α clusters in close proximity

$\Rightarrow$ remove this by an effective 4N operator [long term: N3LO]

$$V^{(4\mathrm{N}_{\mathrm{eff}})} = D^{(4\mathrm{N}_{\mathrm{eff}})} \sum_{1 \le (\vec{n}_i - \vec{n}_j)^2 \le 2} \rho(\vec{n}_1)\rho(\vec{n}_2)\rho(\vec{n}_3)\rho(\vec{n}_4)$$

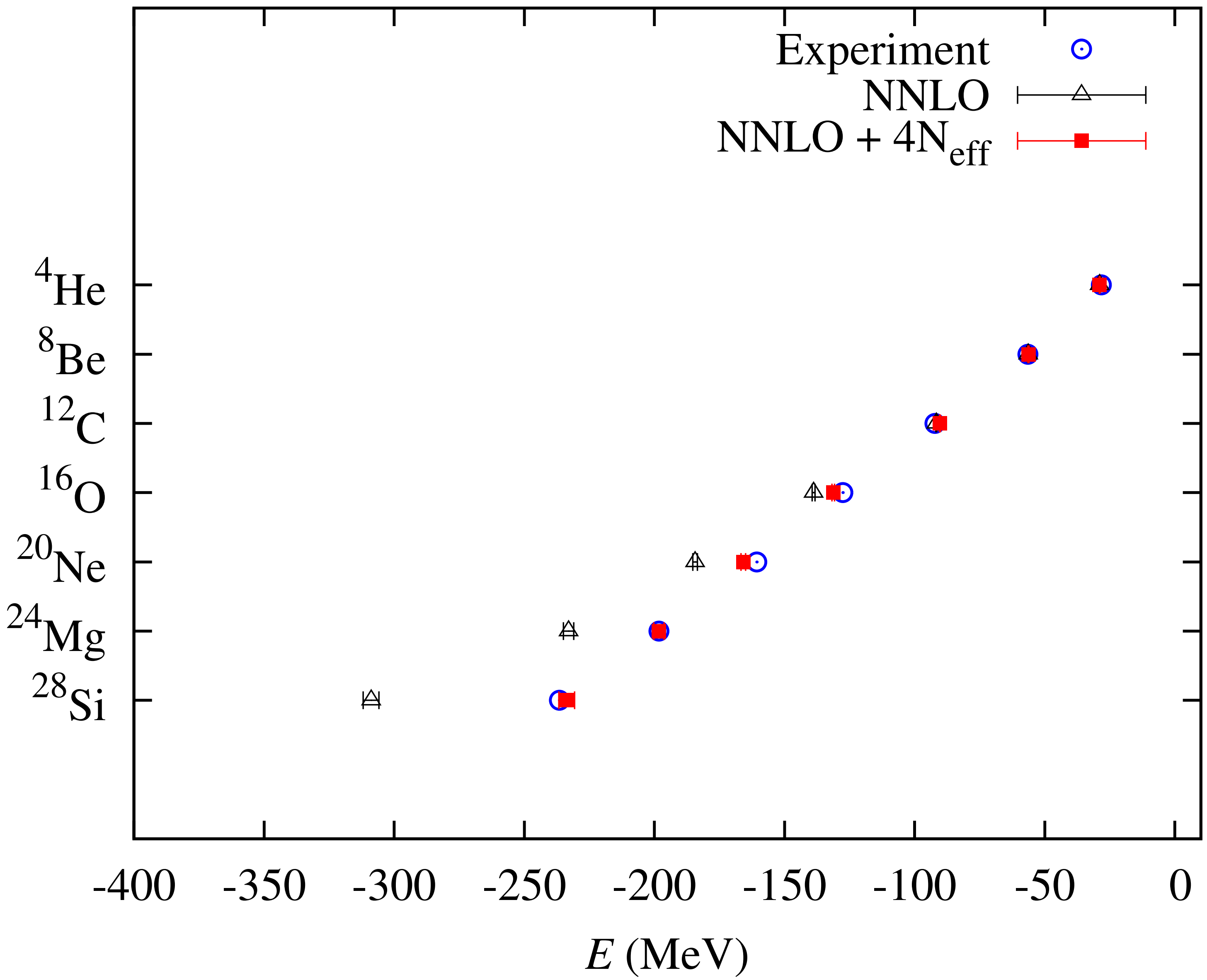
- fix the coefficient $D^{(4\mathrm{N}_{\mathrm{eff}})}$ from the BE of ^{24}Mg

$\Rightarrow$ excellent description of the ground state energies

A	12	16	20	24	28
Th	$-90.3(2)$	$-131.3(5)$	$-165.9(9)$	$-198(2)$	$-233(3)$
Exp	-92.16	-127.62	-160.64	-198.26	-236.54

$\rightarrow$ ultimately, reduce lattice spacing [interaction more repulsive] & N^{3}LO

GROUND STATE ENERGIES



Taming the sign problem: Simulations of ^{10}Be & ^{10}C

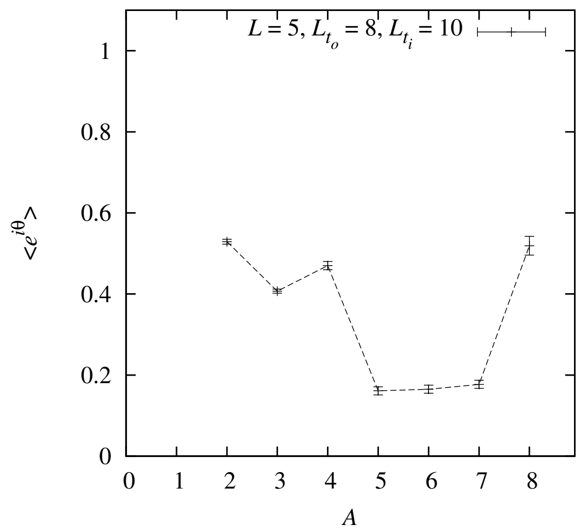
SYMMETRY-SIGN INTERPOLATION METHOD

Epelbaum, Krebs, Lähde, Lee, UGM, Rupak, in preparation

- so far: nuclei with $N = Z$, and $A = 4 \times \text{int}$ as these have the least sign problem due to the approximate SU(4) symmetry

$$\langle \text{sign} \rangle = \langle \exp(i\theta) \rangle = \langle \frac{\det M(t_o, t_i, \ldots)}{|\det M(t_o, t_i, \ldots)|} \rangle$$

$M(t_o, t_i, \ldots)$ is the transition matrix



Borasoy et al. (2007)

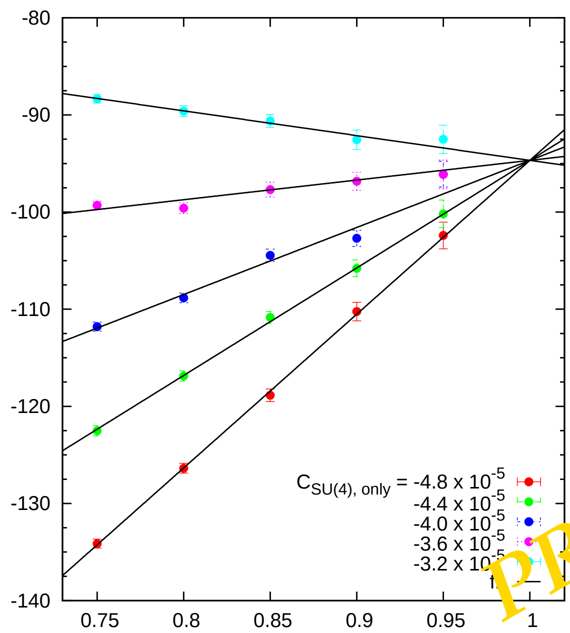
- Symmetry-sign interpolation method: control the sign oscillations

$$\boxed{H_d = d \cdot H_{\text{phys}} + (1 - d) \cdot H_{\text{SU}(4)}} \qquad H_{\text{SU}(4)} = \tfrac{1}{2} C_{\text{SU}(4)} (N^\dagger N)^2$$

$\hookrightarrow$ for a given d, dial the SU(4) coupling $C_{\text{SU}(4)}$ so that the LO value of the g.s. energy for $d = 1$ is reproduced

SYMMETRY-SIGN INTERPOLATION: RESULTS

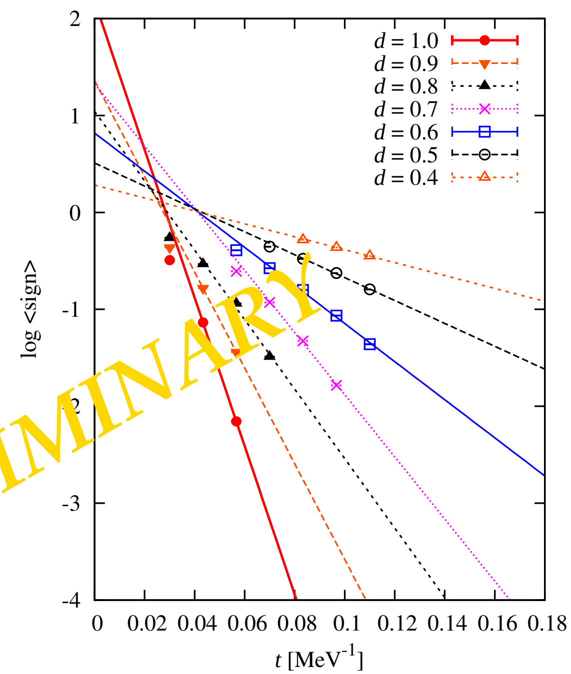
- A first test: ^{12}C



$E(^{12}\mathrm{C}) = -94.68(34)$ MeV

at $t = 0.07\,\mathrm{MeV}^{-1}$

- First results: $A = 10$



$\langle(H_{\mathrm{phys}})\rangle \sim 0.01$
$\Rightarrow \langle(H_{0.7})\rangle \sim 0.1$

$\langle(H_{\mathrm{phys}})\rangle \sim 0.001$
$\Rightarrow \langle(H_{0.5})\rangle \sim 0.1$

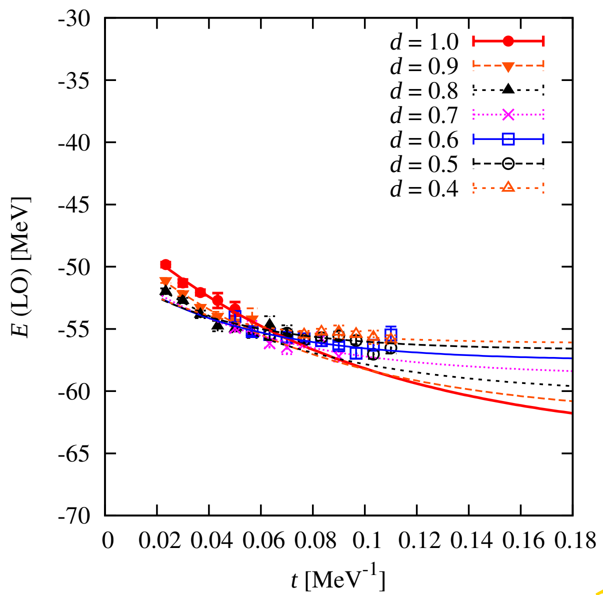
$\langle(H_{\mathrm{phys}})\rangle \sim 0.00000001$
$\Rightarrow \langle(H_{0.35})\rangle \sim 0.1$

$\rightarrow \log\langle\mathrm{sign}\rangle \sim -d^2\, t$

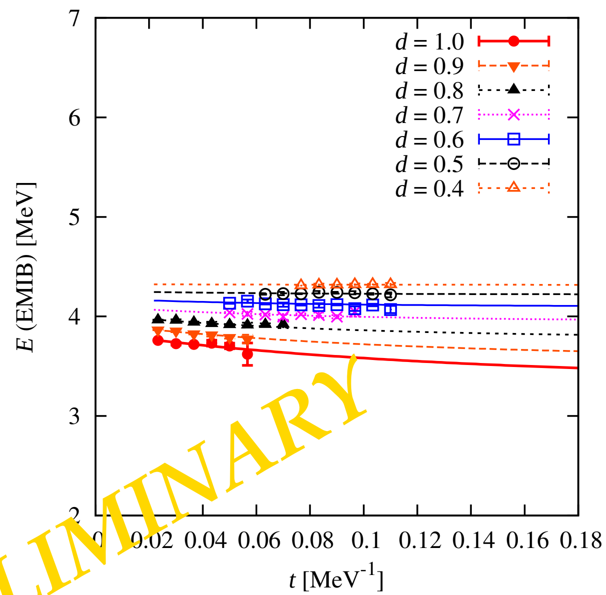
- tremendous suppression of the sign oscillations

GROUND STATES of ^{10}Be and ^{10}C

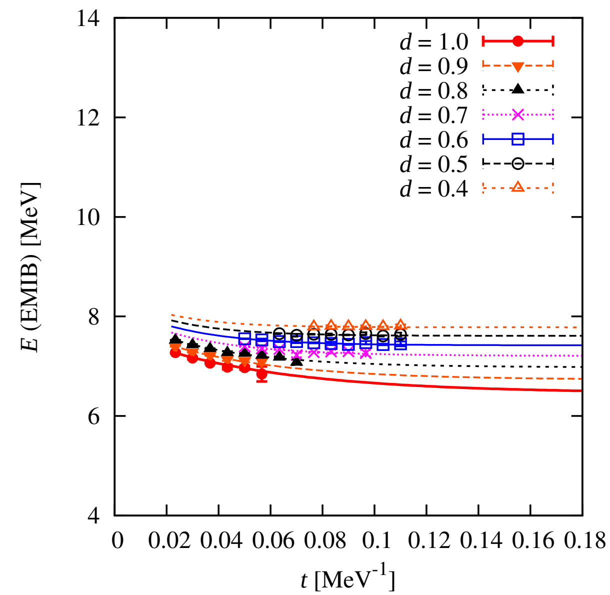
- LO energy



- NLO IV energy ^{10}Be



- NLO IV energy ^{10}C



PRELIMINARY

	LO	NLO	NNLO	Exp.
^{10}Be	$-64(2)$	$-55(2)$	$-63(2)$	-64.98
^{10}C	$-64(2)$	$-52(2)$	$-59(2)$	-60.32

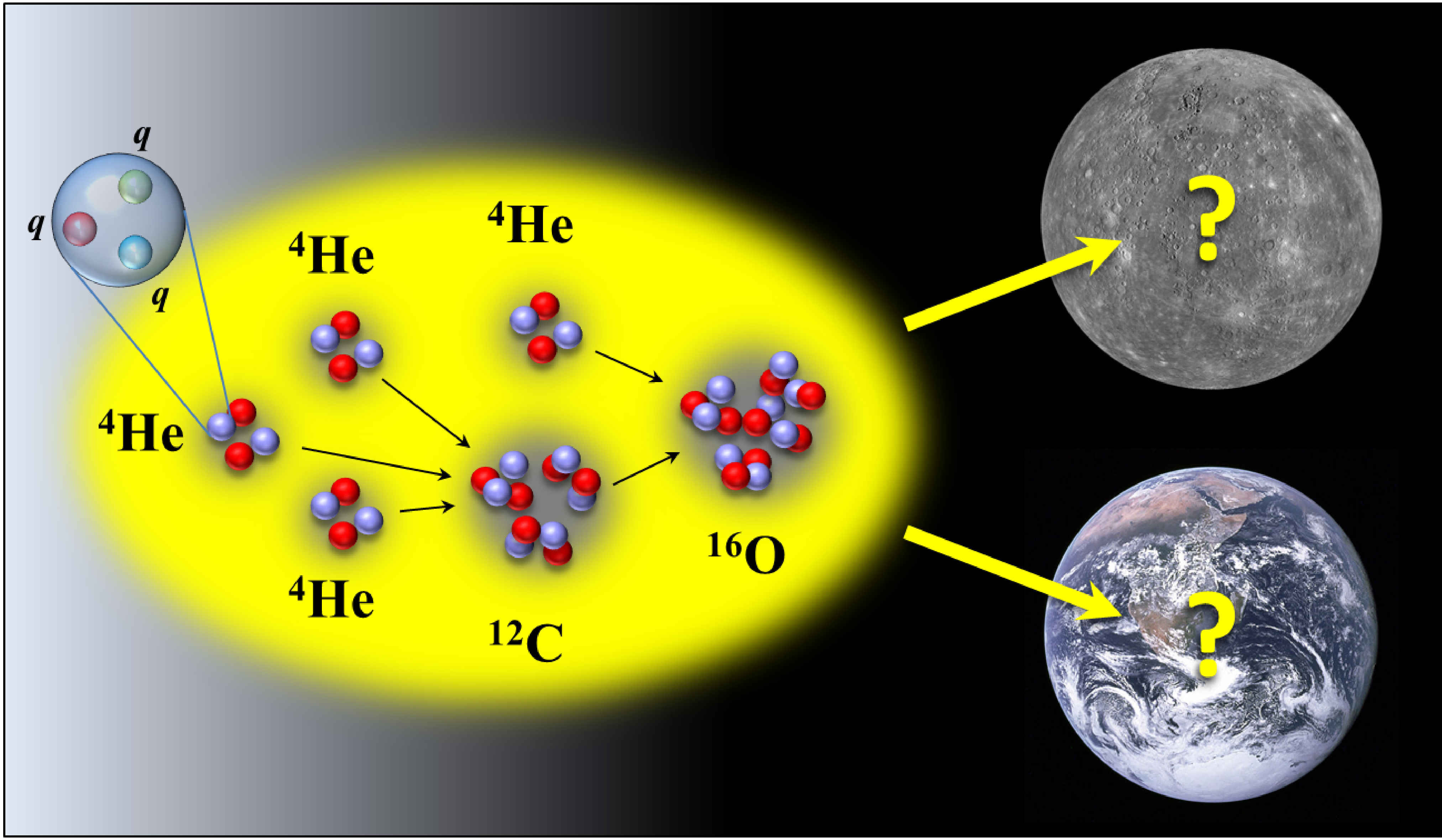
$\rightarrow$ promising results!

$\rightarrow$ major step towards halos, drip lines, . . .

The fate of carbon-based life as a function of the quark mass

FINE-TUNING of FUNDAMENTAL PARAMETERS

Fig. courtesy Dean Lee



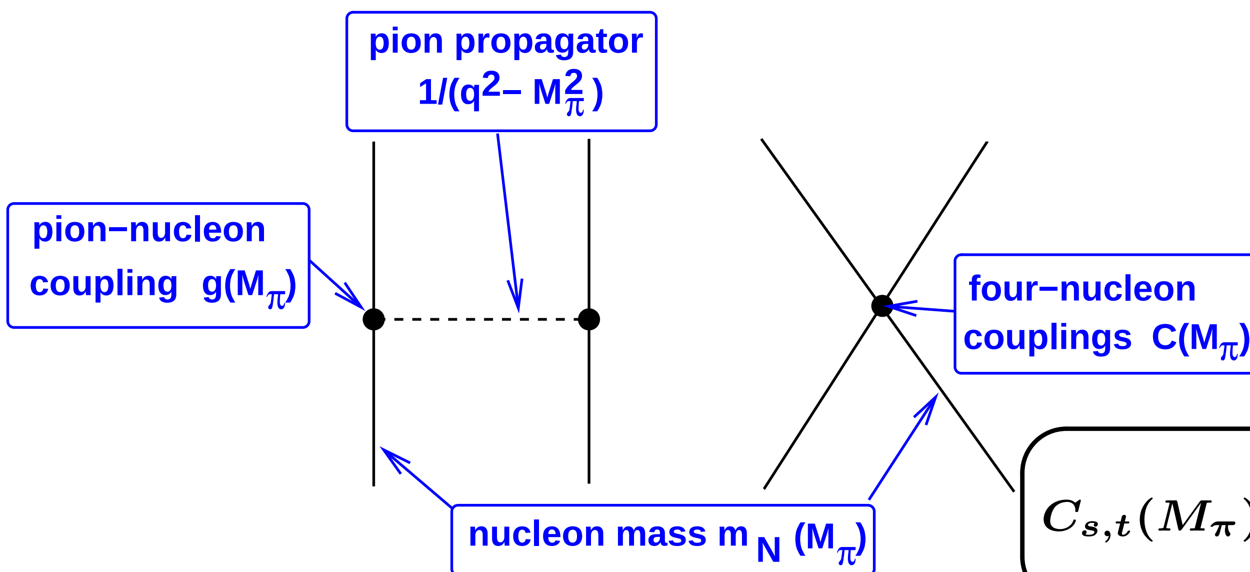
FINE-TUNING: MONTE-CARLO ANALYSIS

Epelbaum, Krebs, Lähde, Lee, UGM, PRL **110** (2013) 112502, Eur. Phys. J. **A49** (2013) 82

- simulations allow to vary $m_{\rm quark}$ and α_{EM}
- quark mass dependence $\equiv$ pion mass dependence: $\boxed{M^2_{\pi^\pm} \sim (m_u + m_d)}$

Gell-Mann, Oakes, Renner (1968)

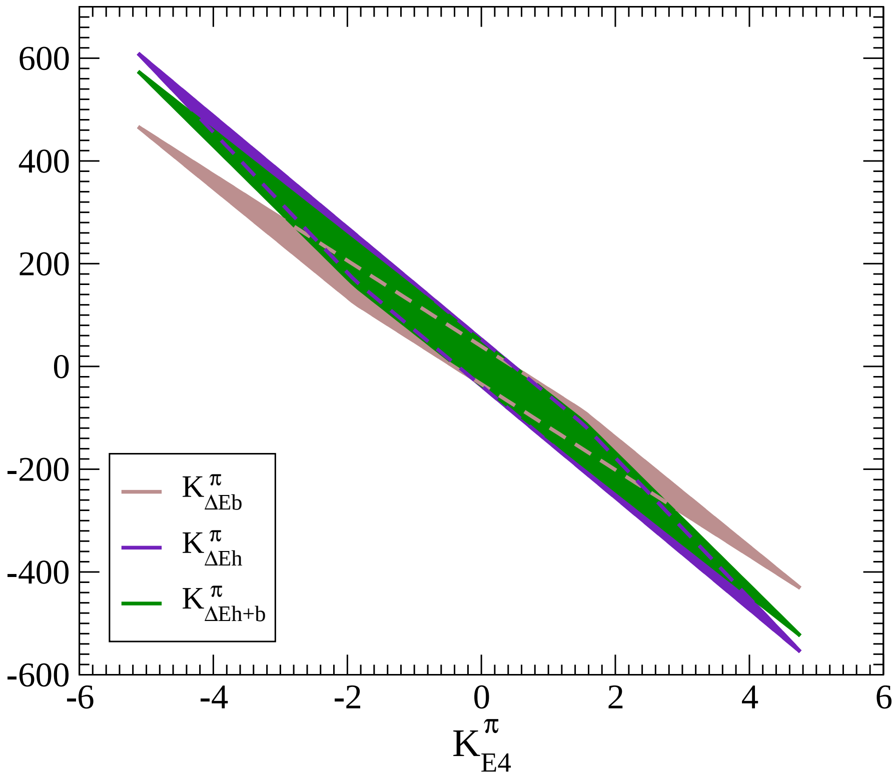
- explicit and implicit pion mass dependences



$$C_{s,t}(M_\pi) \leftrightarrow \frac{\partial a^{-1}_{s,t}}{\partial M_\pi}\bigg|_{M_\pi^{\rm phys}}$$

CORRELATIONS

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



$$\Delta E_b = E(^8\mathrm{Be}) - 2E(^4\mathrm{He})$$

$$\Delta E_h = E(^{12}\mathrm{C}^*) - E(^8\mathrm{Be}) - E(^4\mathrm{He})$$

$$\Delta E_{h+b} = E(^{12}\mathrm{C}^*) - 3E(^4\mathrm{He})$$

$$\boxed{\frac{\partial O_H}{\partial M_\pi} = K_H^\pi \frac{O_H}{M_\pi}}$$

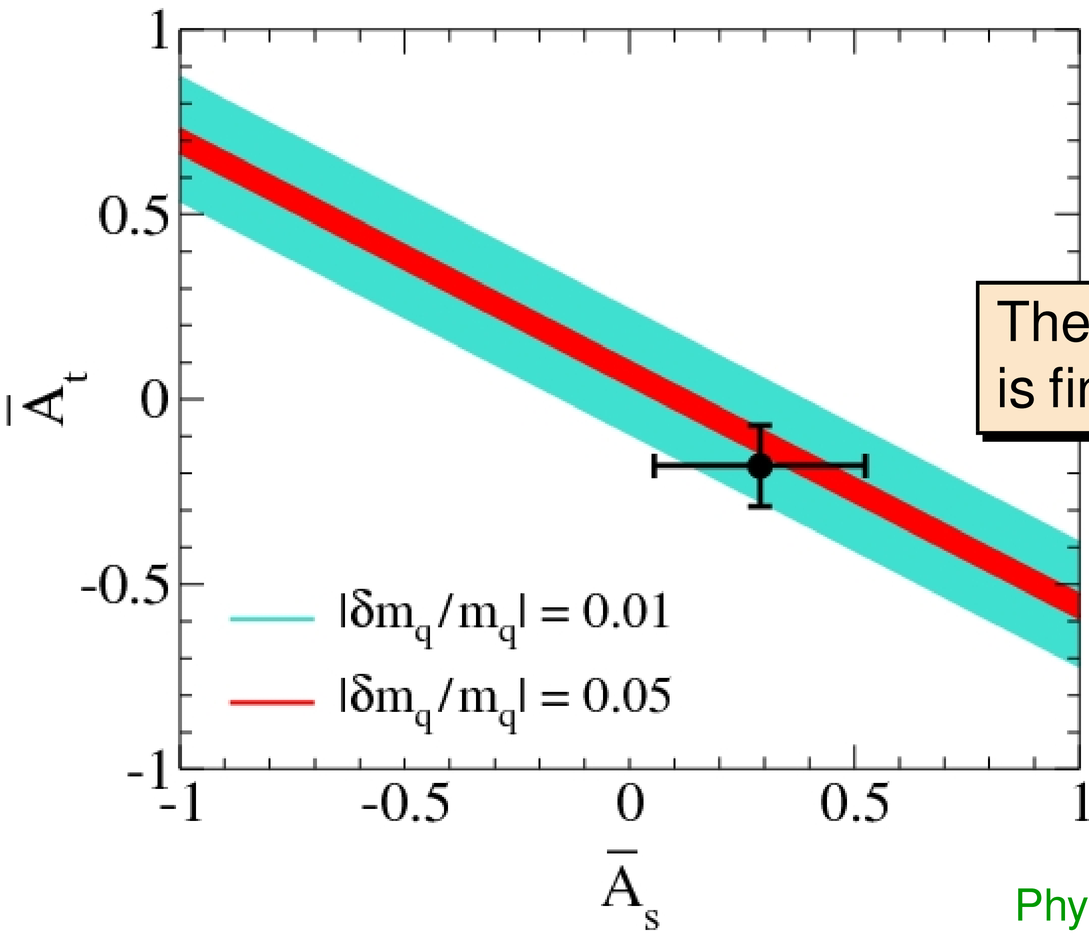
- clear correlations: α-particle BE and the energies/energy differences

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

THE END-OF-THE-WORLD PLOT

- $|\delta(\Delta E_{h+b})| < 100$ keV   Schlattl et al. (2004) [phys. value = 379.47(18) keV]

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



$$\bar{A}_{s,t} \equiv \left.\frac{\partial a_{s,t}^{-1}}{\partial M_\pi}\right|_{M_\pi^{\rm phys}}$$

The light quark mass is fine-tuned to $\simeq 2-3\,\%$

Similarly: $\alpha_{\rm EM}$ is fine-tuned to $\simeq 2.5\%$

Berengut et al., Phys. Rev. **D 87** (2013) 085018

OUTLOOK

- **Algorithmic improvements:**
  - tame the sign problem $\Rightarrow N \neq Z$ nuclei $\boxed{\to \text{first steps!}}$
  - improve extraction of em operator insertions
  - improve action to minimize rotational symmetry breaking

- **Methodological improvements:**
  - study the finite volume dependence of LO and higher order signals
  - study the finite a dependence of energies etc.
  - work out the forces to NNNLO and implement in MC codes
  - improve EoS for neutron matter and pairing gaps
  - reaction theory, first steps — Lee, Pine, Rupak, ...

$\Rightarrow$ exciting times ahead of us

SPARES

PION EXCHANGE CONTRIBUTIONS

- Work to NNLO, need quark mass dependence of M_π, F_π, m_N, g_A

$\Rightarrow$ using lattice + CHPT gives: $K^q_{M_\pi} = 0.494^{+0.009}_{-0.013}$, $K^q_{F_\pi} = 0.048 \pm 0.012$

$$K^q_{m_N} = 0.048^{+0.002}_{-0.006}$$

- situation for g_A not quite clear

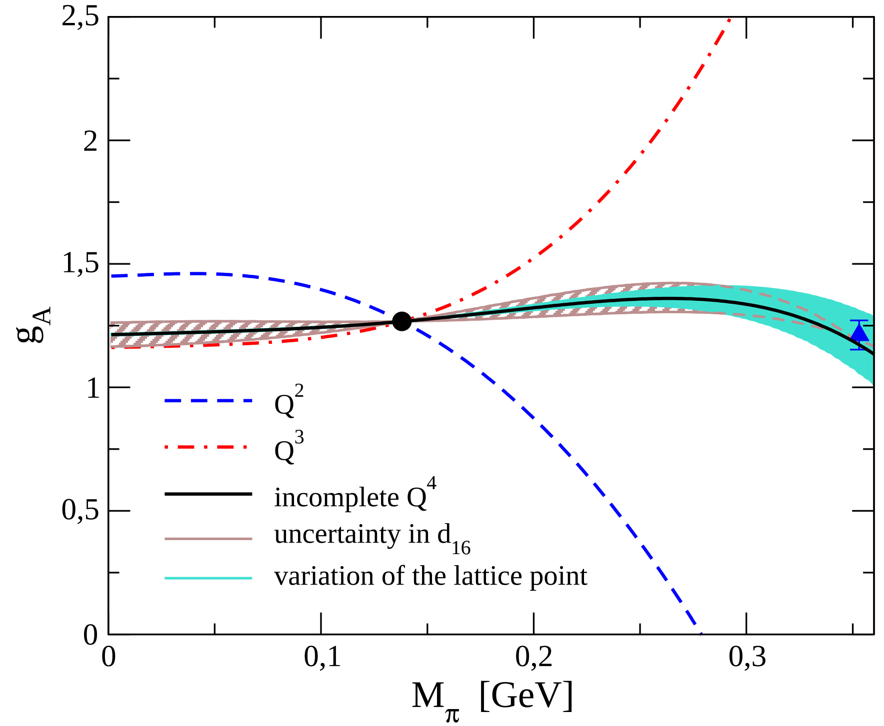
  LQCD data show little quark mass dep.

  chiral expansion converges slowly

  two-loop representation might suffice
  to make contact with flat LQCD data
  Bernard, UGM (2006)

  $\rightarrow$ use a simplified two-loop representation

  $\rightarrow$ fixes quark mass dep. of $V_{1\pi} + V_{2\pi}$



QUARK MASS DEP. of the SHORT-DISTANCE TERMS

- Consider a typical OBEP with $M = \sigma, \rho, \omega, \delta, \eta$
- Quark mass dependence of the sigma and rho from unitarized CHPT

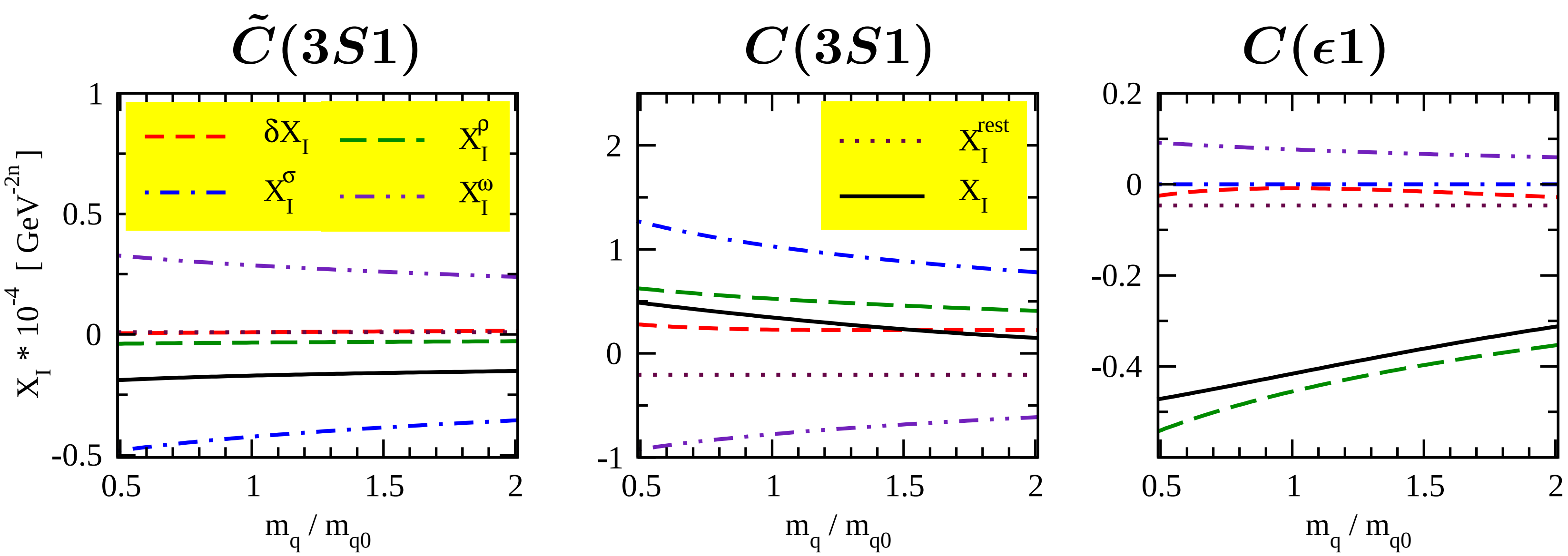
Hanhart, Pelaez, Rios (2008)

$\Rightarrow$ $K^q_{M_\sigma} = 0.081 \pm 0.007, \quad K^q_{M_\rho} = 0.058 \pm 0.002$

$\Rightarrow$ couplings appear quark mass independent (requires refinement in the future)

- assume a) that $K^q_\omega = K^q_\rho$ and b) neglect dep. of δ, η

$\Rightarrow$



Impact on BBN

Berengut, Epelbaum, Flambaum, Hanhart, UGM, Nebreda, Pelaez,
Phys. Rev. D **87** (2013) 085018

QUARK MASS VARIATIONS of HEAVIER NUCLEI

- In BBN, we also need the variation of ^{3}He and ^{4}He. All other BEs are kept fixed.

- use the method of BLP: Bedaque, Luu, Platter, PRC **83** (2011) 045803

$$K^q_{^A\mathrm{He}} = K^q_{a,\,1S0} K^{a,\,1S0}_{^A\mathrm{He}} + K^q_{\mathrm{deut}} K^{\mathrm{deut}}_{^A\mathrm{He}}\ , \quad A = 3, 4$$

with

$$K^{a,\,1S0}_{^3\mathrm{He}} = 0.12 \pm 0.01\ , \quad K^{\mathrm{deut}}_{^3\mathrm{He}} = 1.41 \pm 0.01$$

$$K^{a,\,1S0}_{^4\mathrm{He}} = 0.037 \pm 0.011\ , \quad K^{\mathrm{deut}}_{^4\mathrm{He}} = 0.74 \pm 0.22$$

so that

$$\Rightarrow \boxed{K^q_{^3\mathrm{He}} = -0.94 \pm 0.75, \quad K^q_{^4\mathrm{He}} = -0.55 \pm 0.42}$$

- consistent w/ direct nuclear lattice simulation calc:

$$K^q_{^3\mathrm{He}} = -0.YY \pm 0.XX, \quad K^q_{^4\mathrm{He}} = -0.15 \pm 0.25$$

EKLLM, PRL **110** (2013) 112502

BBN RESPONSE MATRIX

- calculate BBN response matrix of primordial abundances Y_a at fixed baryon-to-photon ratio:

$$\frac{\delta \ln Y_a}{\delta \ln m_q} = \sum_{X_i} \frac{\partial \ln Y_a}{\partial \ln X_i} K_{X_i}^q$$

- use the updated Kawano code

Kawano, FERMILAB-Pub-92/04-A

X	d	^{3}He	^{4}He	^{6}Li	^{7}Li
a_s	−0.39	0.17	0.01	−0.38	2.64
$B_{\rm deut}$	−2.91	−2.08	0.67	−6.57	9.44
$B_{\rm trit}$	−0.27	−2.36	0.01	−0.26	−3.84
$B_{^3{\rm He}}$	−2.38	3.85	0.01	−5.72	−8.27
$B_{^4{\rm He}}$	−0.03	−0.84	0.00	−69.8	−57.4
$B_{^6{\rm Li}}$	0.00	0.00	0.00	78.9	0.00
$B_{^7{\rm Li}}$	0.03	0.01	0.00	0.02	−25.1
$B_{^7{\rm Be}}$	0.00	0.00	0.00	0.00	99.1
τ	0.41	0.14	0.72	1.36	0.43

LIMITS for the QUARK MASS VARIATION

- Average of [deut/H] and ^{4}He(Y_p):

$$\frac{\delta m_q}{m_q} = 0.02 \pm 0.04$$

- in contrast to earlier studies, we provide reliable error estimates (EFT)
- but: BLP find a stronger constraint due to the neutron life time (affects $Y(^4\mathrm{He})$)
- re-evaluate this under the model-independent assumption that *all* quark & lepton masses vary with the Higgs VEV v

$\Rightarrow$ results are dominated by the ^{4}He abundance:

$$\left|\frac{\delta v}{v}\right| = \left|\frac{\delta m_q}{m_q}\right| \le 0.9\%$$

EARLIER STUDIES of the ANTHROPIC PRINCIPLE

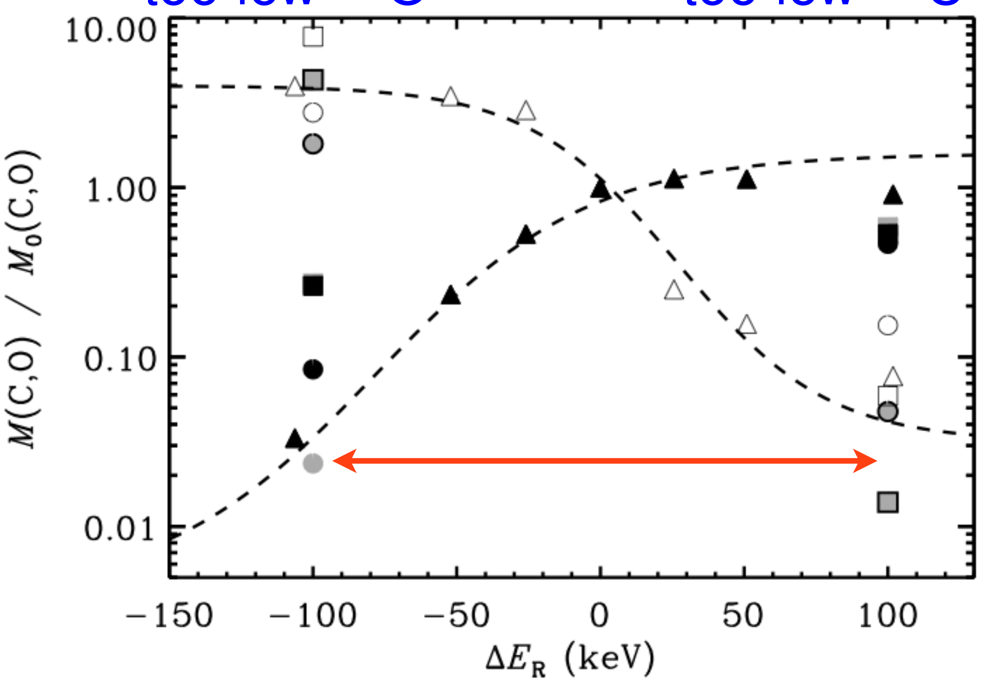
- rate of the 3α-process: $r_{3\alpha} \sim \Gamma_\gamma \, \exp\left(-\frac{\Delta E_{h+b}}{kT}\right)$

$$\Delta E_{h+b} = E_{12}^\star - 3E_\alpha = 379.47(18) \text{ keV}$$

- how much can ΔE_{h+b} be changed so that there is still enough ^{12}C and ^{16}O?

$\Rightarrow$ $|\Delta E_{h+b}| \lesssim 100$ keV

too few ^{16}O too few ^{12}C



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