NUCLEAR LATTICE SIMULATIONS

– Status and Perspectives –

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Nuclear forces from chiral EFT

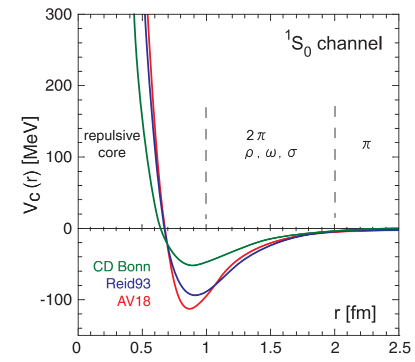
CHIRAL EFT for FEW-NUCLEON SYSTEMS

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



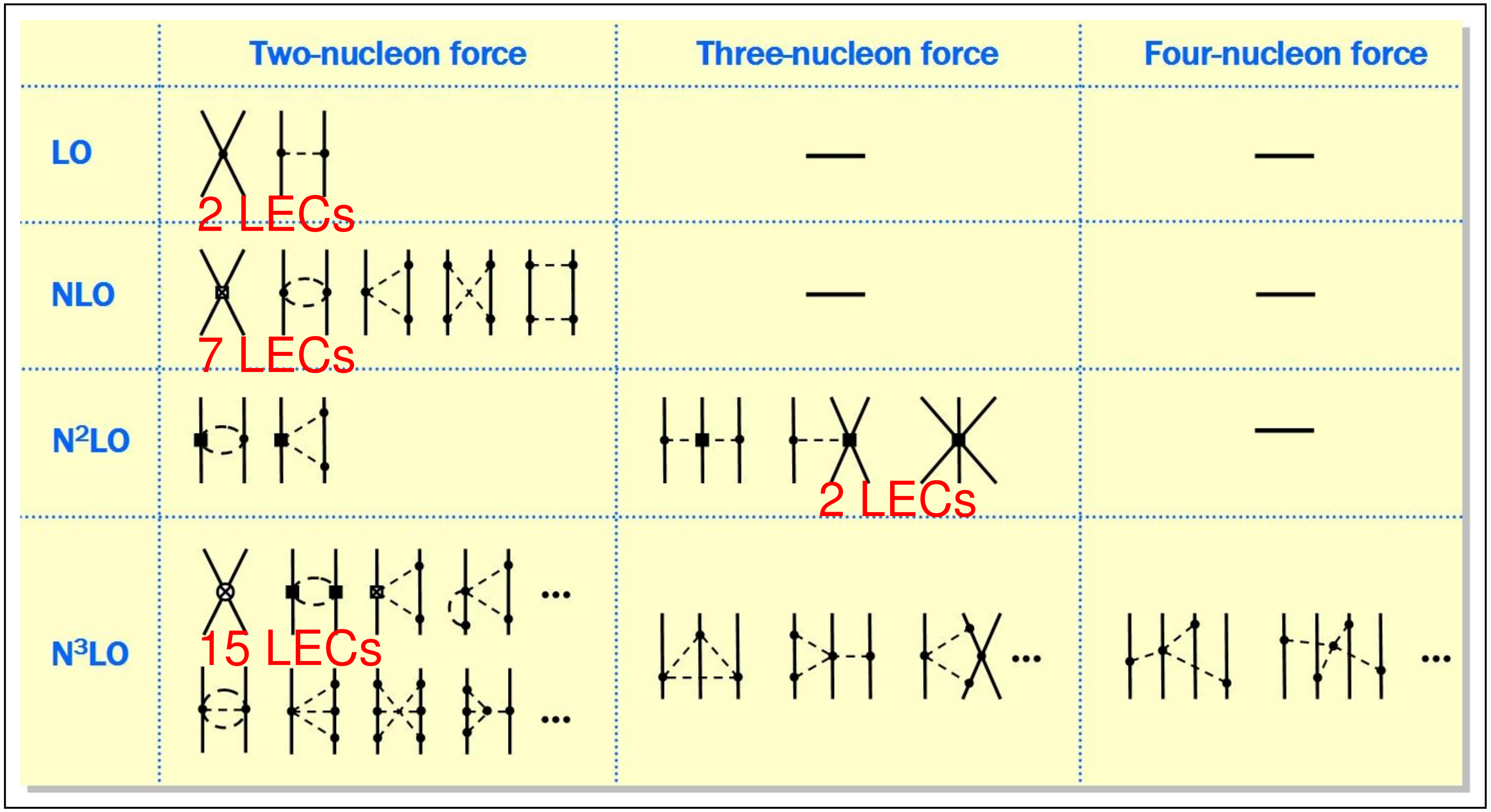
- this can be analyzed in a suitable EFT based on

$$\mathcal{L}_{\rm QCD} \to \mathcal{L}_{\rm EFF} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \ldots$$

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

→ chirally expand $\mathrm{V_{NN(N)}}$, use in regularized Schrödinger equation

CHIRAL POTENTIAL and NUCLEAR FORCES



$\mathcal{O}((Q/\Lambda_\chi)^{0})$

$\mathcal{O}((Q/\Lambda_\chi)^{2})$

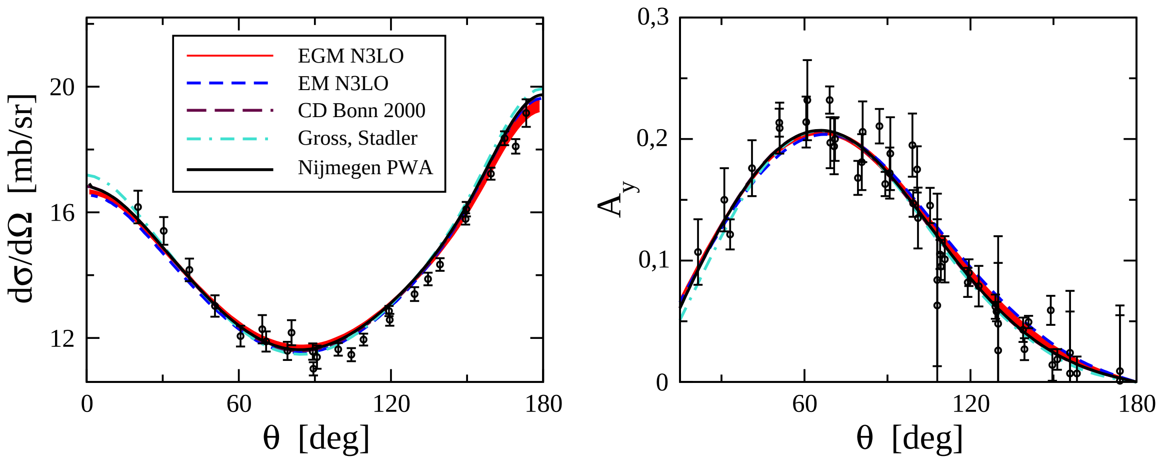
$\mathcal{O}((Q/\Lambda_\chi)^{3})$

$\mathcal{O}((Q/\Lambda_\chi)^{4})$

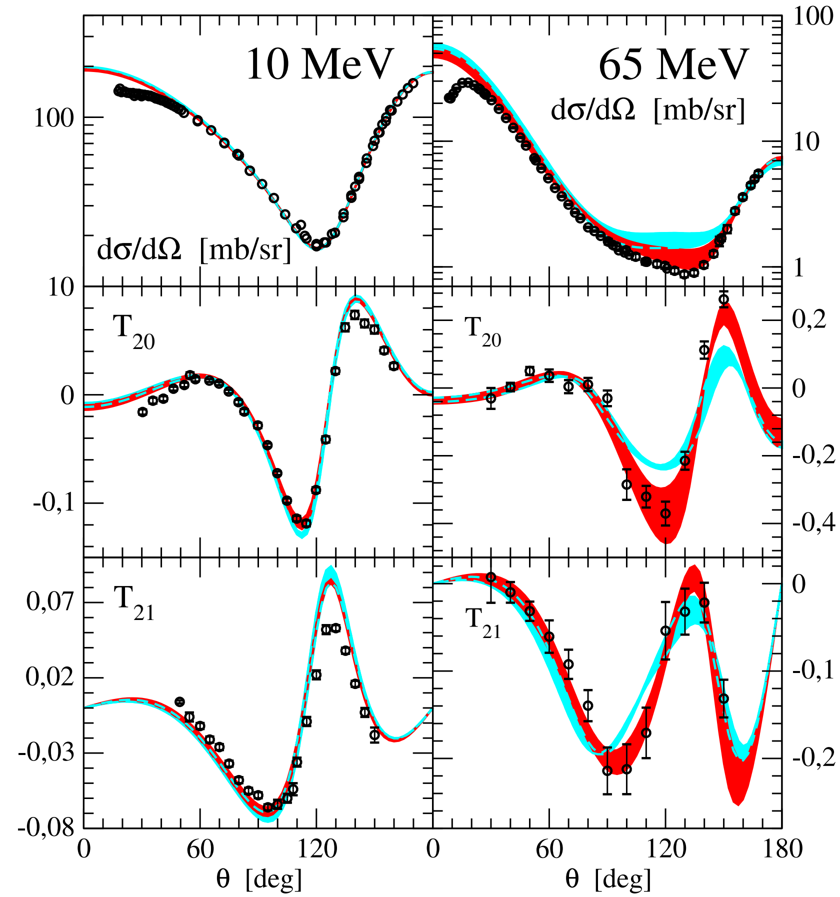
- explains naturally the observed hierarchy of nuclear forces
- MANY successful tests in few-nucleon systems (continuum calc's)

RESULTS

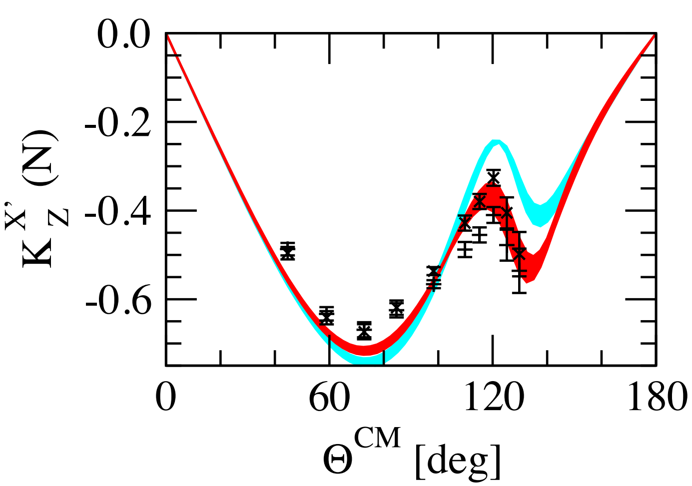
- np scattering



- nd scattering



- pol. transfer in pd scattering



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

Quark mass dependence of the nuclear forces

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

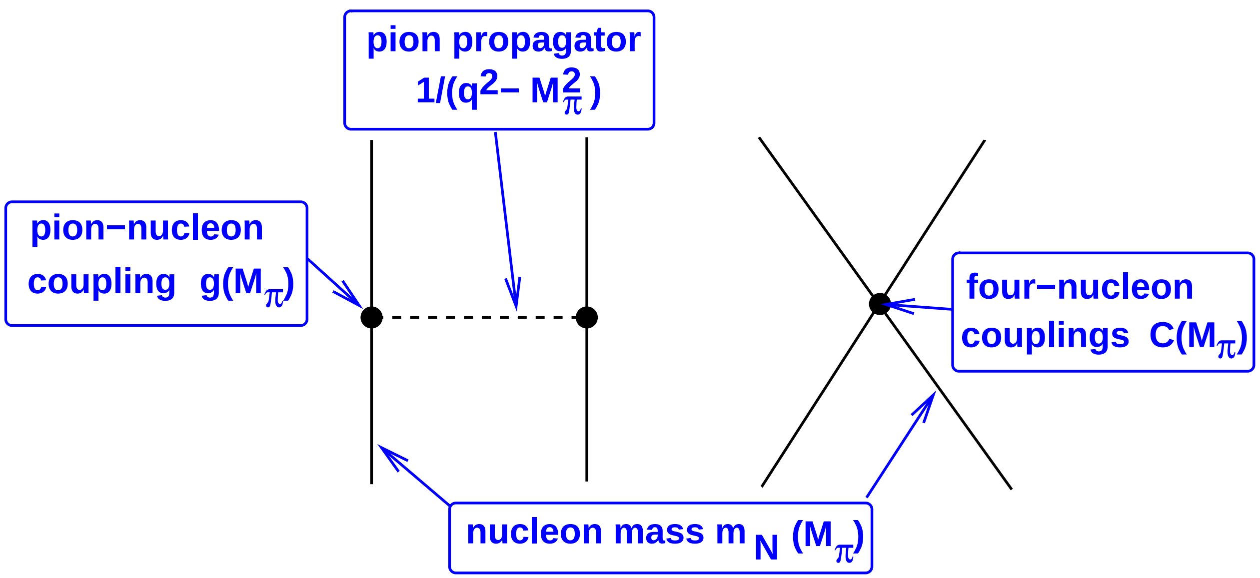
QUARK MASS DEPENDENCE in CHIRAL EFT

- Nuclear forces are given by chiral EFT based on Weinberg's power counting

  Weinberg 1991

⇒ Pion-exchange contributions and short-distance multi-N operators

- graphical representation of the quark mass dependence of the LO potential



- always use the Gell-Mann–Oakes–Renner relation: $M_{\pi^\pm}^2 \sim (m_u + m_d)$

QUARK MASS DEPENDENCE of HADRON MASSES etc[9]

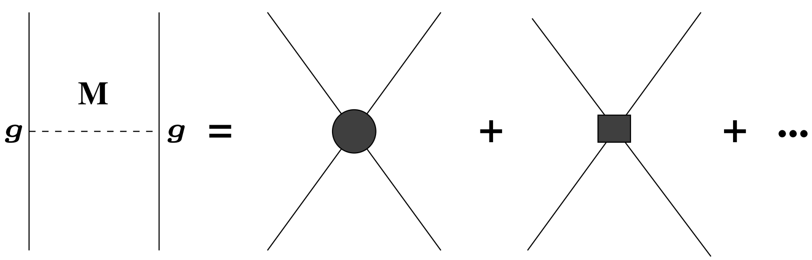
- Quark mass dependence of hadron properties:

$$\frac{\delta O_H}{\delta m_f} \equiv K_H^f \frac{O_H}{m_f}\ , \quad f = u, d, s$$

- Pion and nucleon properties from lattice QCD combined with CHPT

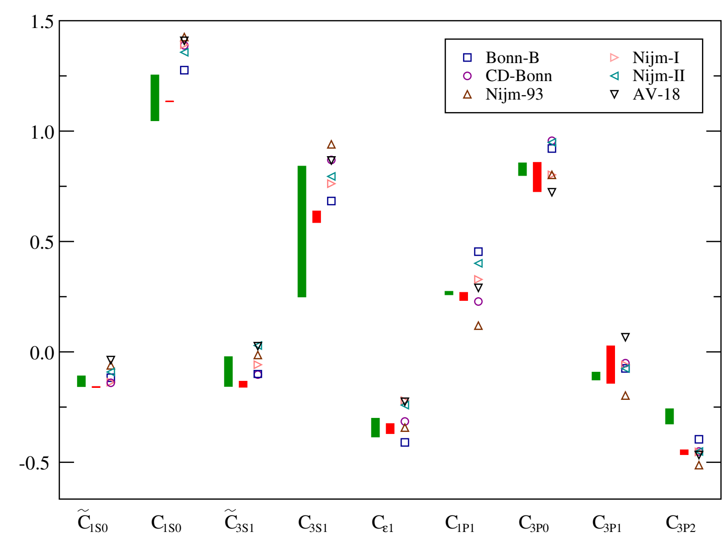
- Contact interactions modeled by heavy meson exchanges

Epelbaum, UGM, Glöckle, Elster (2002)



$$\frac{g^2}{t-M^2} = -\frac{g^2}{M^2} - \frac{g^2\, t}{M^4} + \ldots$$

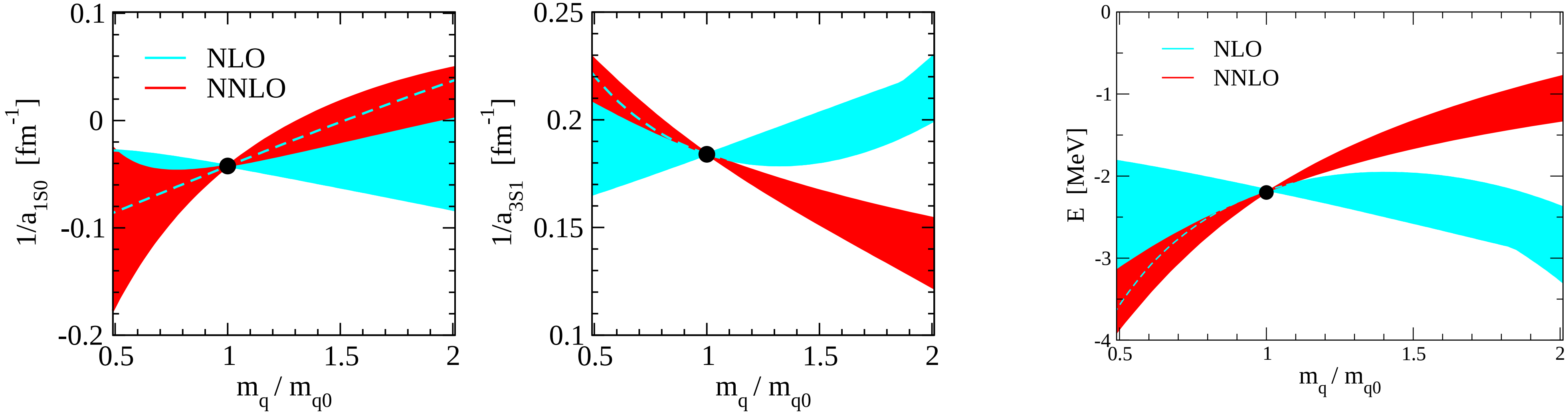
$\hookrightarrow$



RESULTS for the NN SYSTEM

- Putting pieces together for the two-nucleon system:

$$K^q_{a,1S0} = 2.3^{+1.9}_{-1.8},\quad K^q_{a,3S1} = 0.32^{+0.17}_{-0.18},\quad K^q_{\rm B(deut)} = -0.86^{+0.45}_{-0.50}$$



- Nuclear forces are very sensitive to variations in $m_{\rm quark}$
- Extends and improves earlier work based on EFTs and models

  Müther, Engelbrecht, Brown (1986), Beane, Savage (2003), Epelbaum, UGM, Glöckle (2003), Mondejar, Soto (2007), Flambaum, Wiringa (2007), Bedaque, Luu, Platter (2011), ...
- constraints from BBN on quark mass variations → spares

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**

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 $A \geq 5$?

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

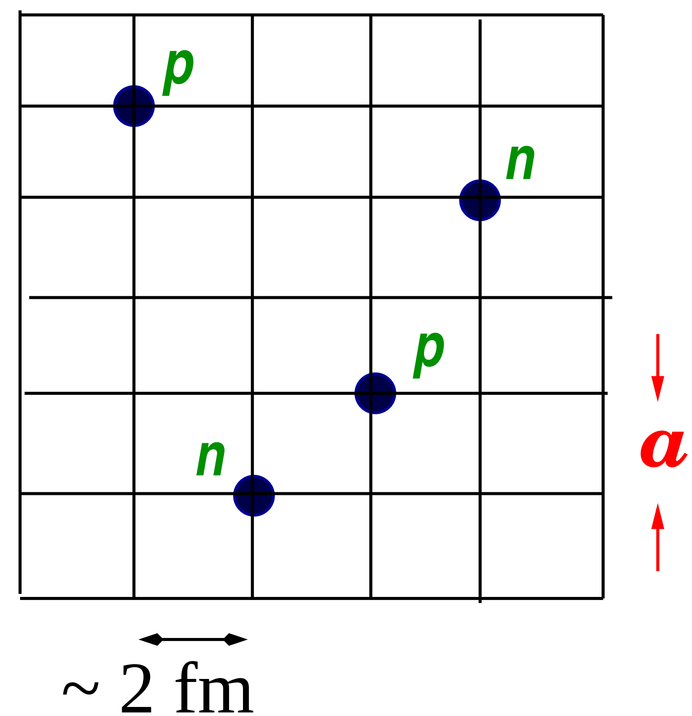
- *new method* to tackle the nuclear many-body problem

- 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

- typical lattice parameters

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

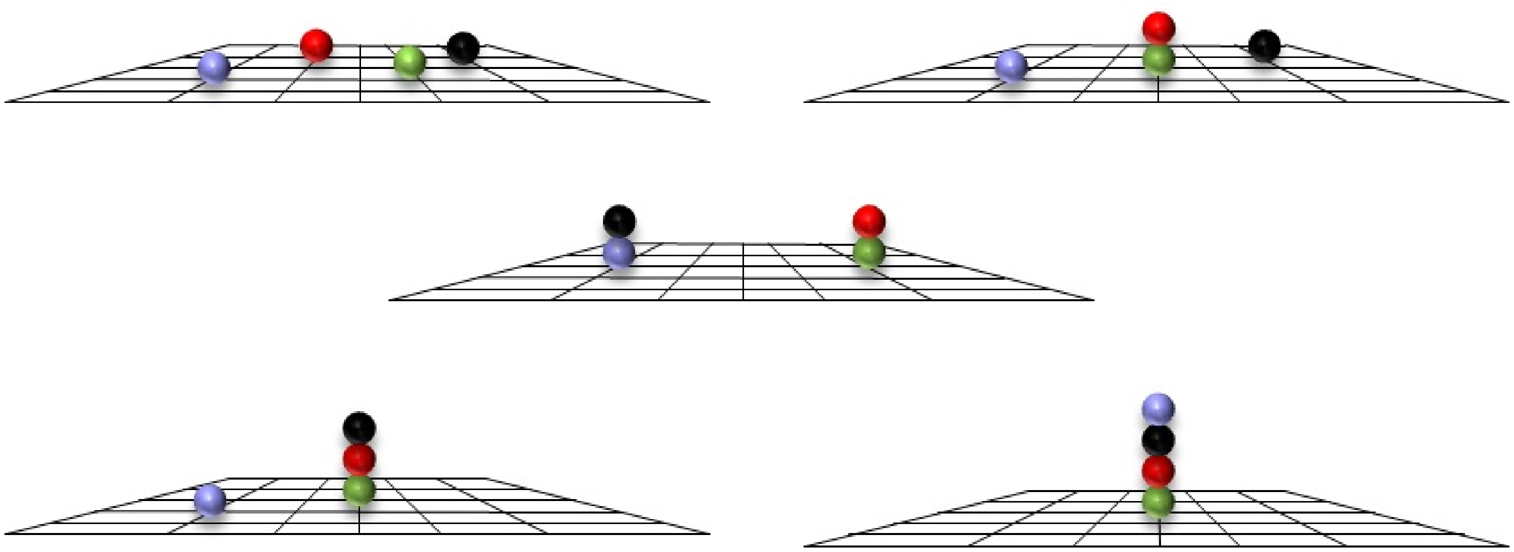


- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

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**

COMPUTATIONAL EQUIPMENT

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

6 Pflops

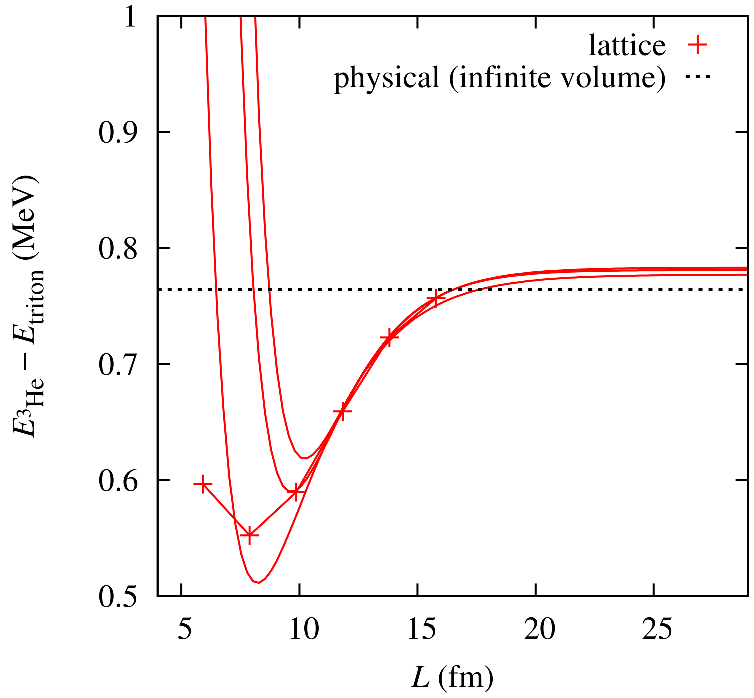
Nuclear lattice simulations
– results –

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



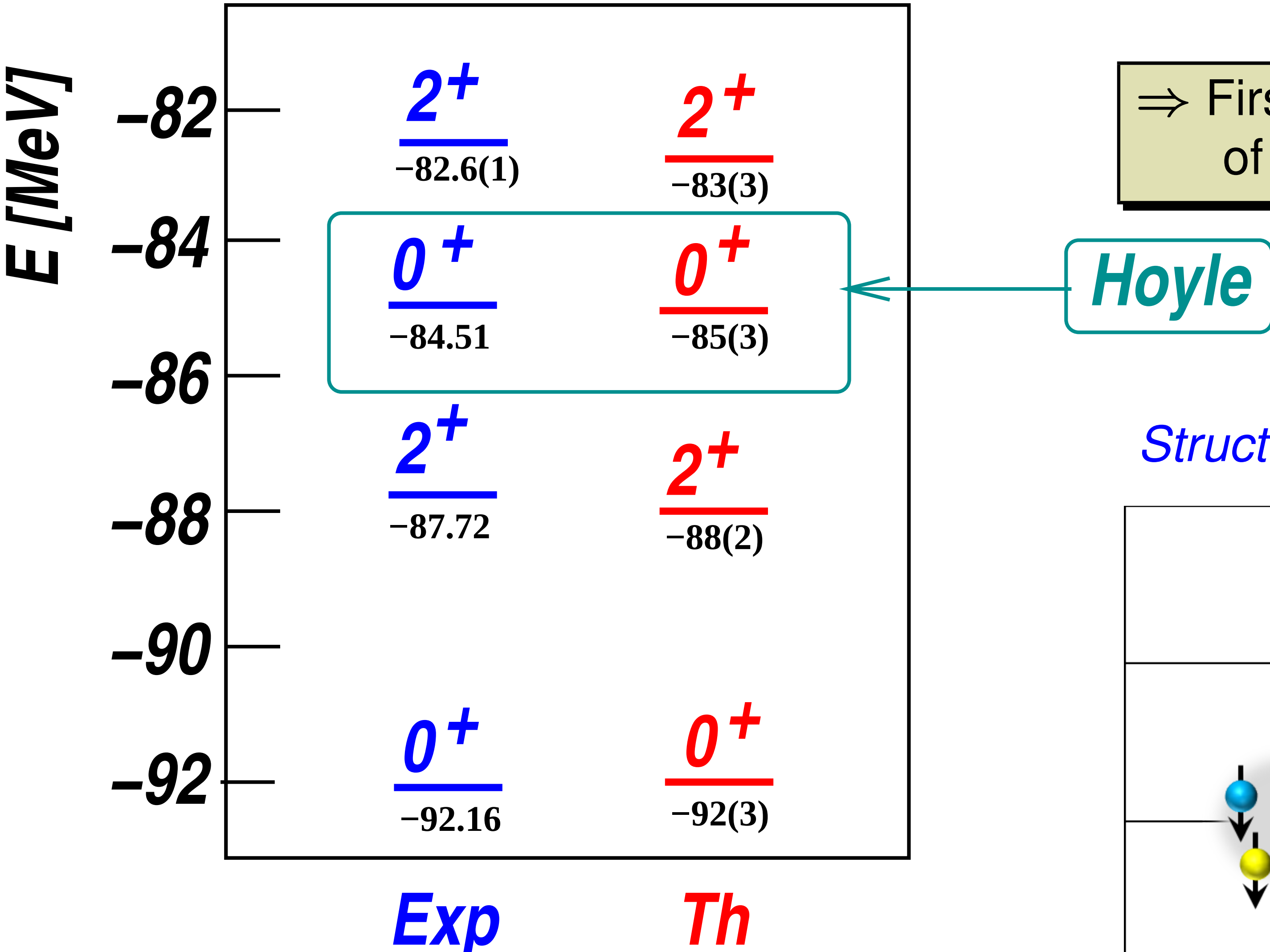
- promising results [3NFs very important]

- excited states more difficult

$\Rightarrow$ new projection MC method [large class of initial wfs] $\rightarrow$ spares

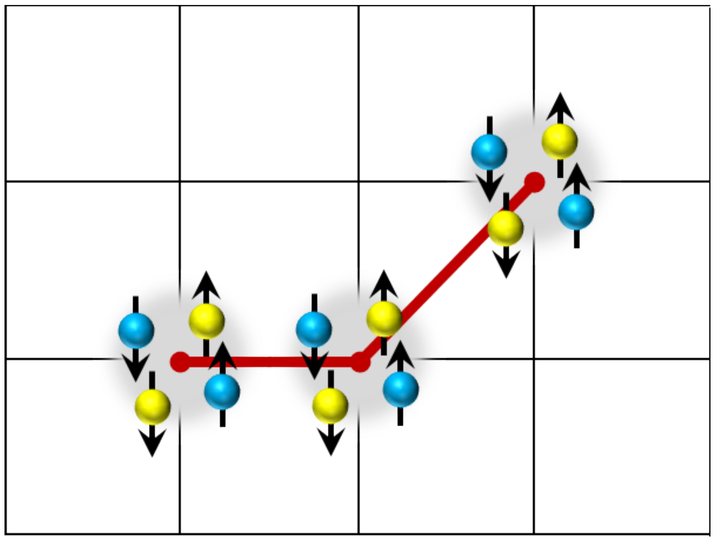
The SPECTRUM of CARBON-12

- 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., arXiv:1303.4326 [nucl-ex]

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

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

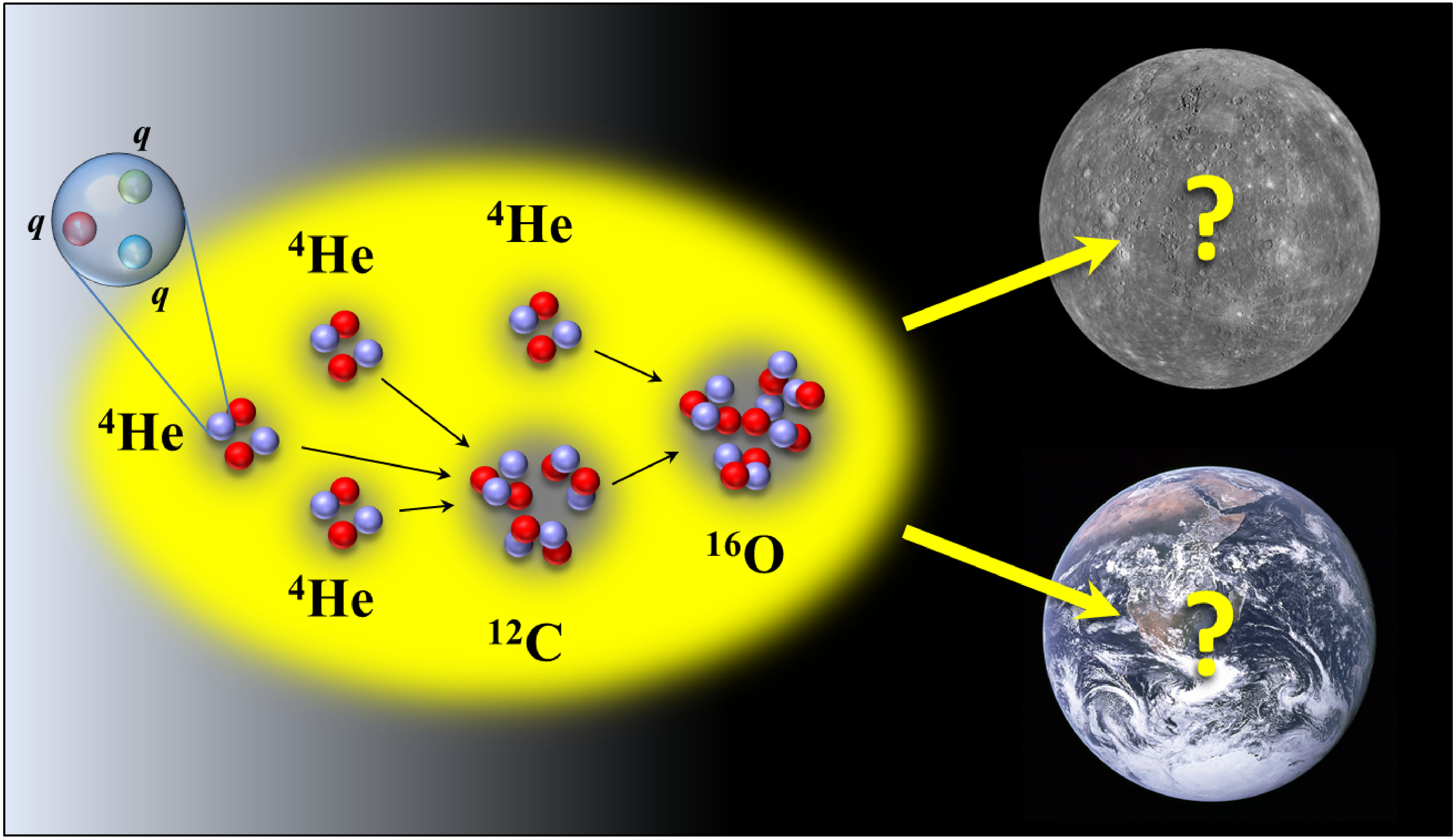
- consistent with overbinding at LO

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

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

FINE-TUNING of FUNDAMENTAL PARAMETERS

Fig. courtesy Dean Lee

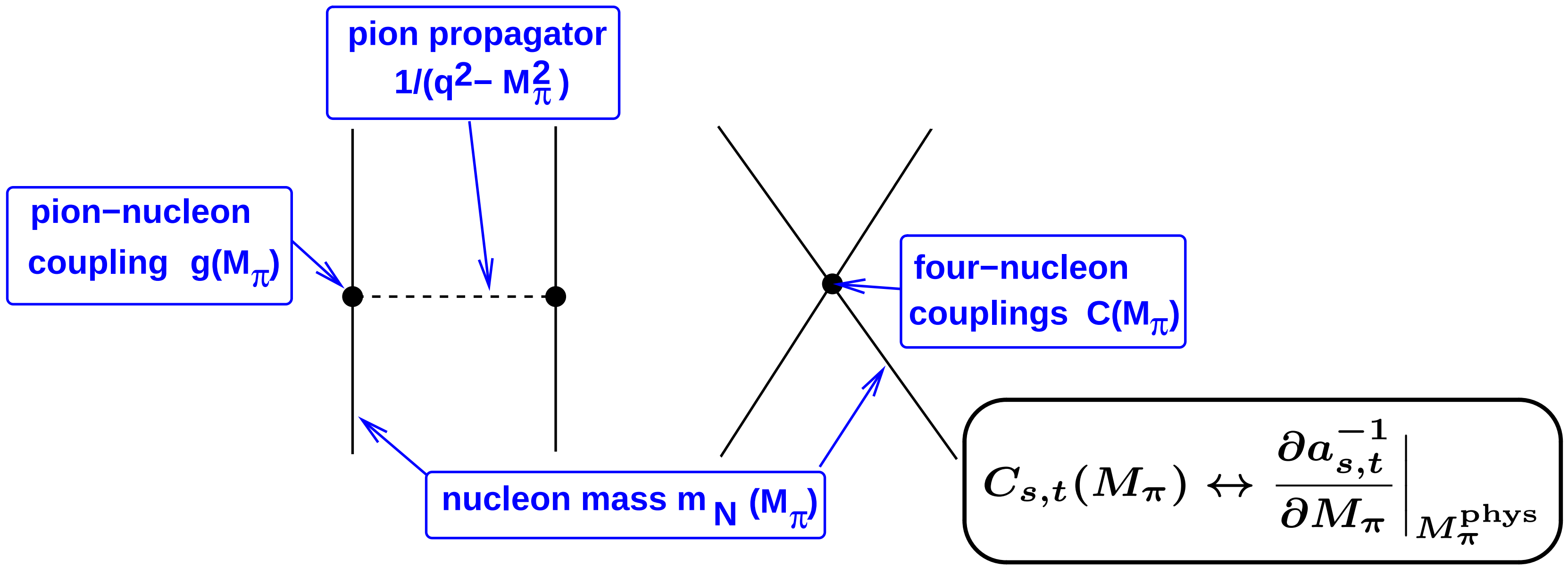


FINE-TUNING: MONTE-CARLO ANALYSIS

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

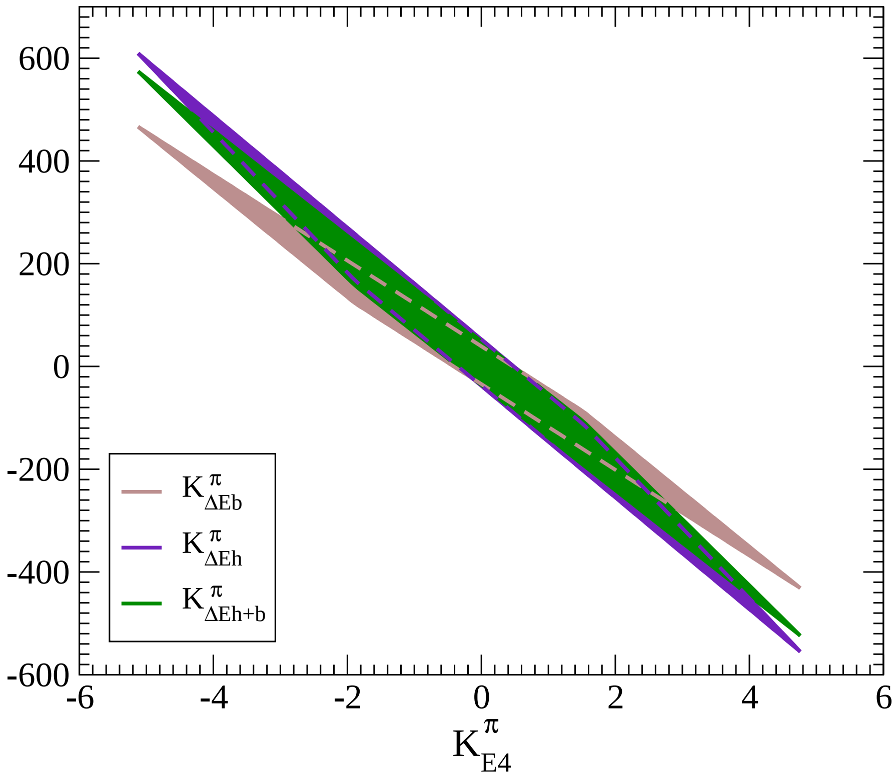
- simulations allow to vary $m_{\rm quark}$ and α_{EM}
- quark mass dependence $\equiv$ pion mass dependence: $\boxed{M^2_{\pi^\pm} \sim (m_u + m_d)}$

  Gell-Mann, Oakes, Renner (1968)
- explicit and implicit pion mass dependences



CORRELATIONS

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



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

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

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

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

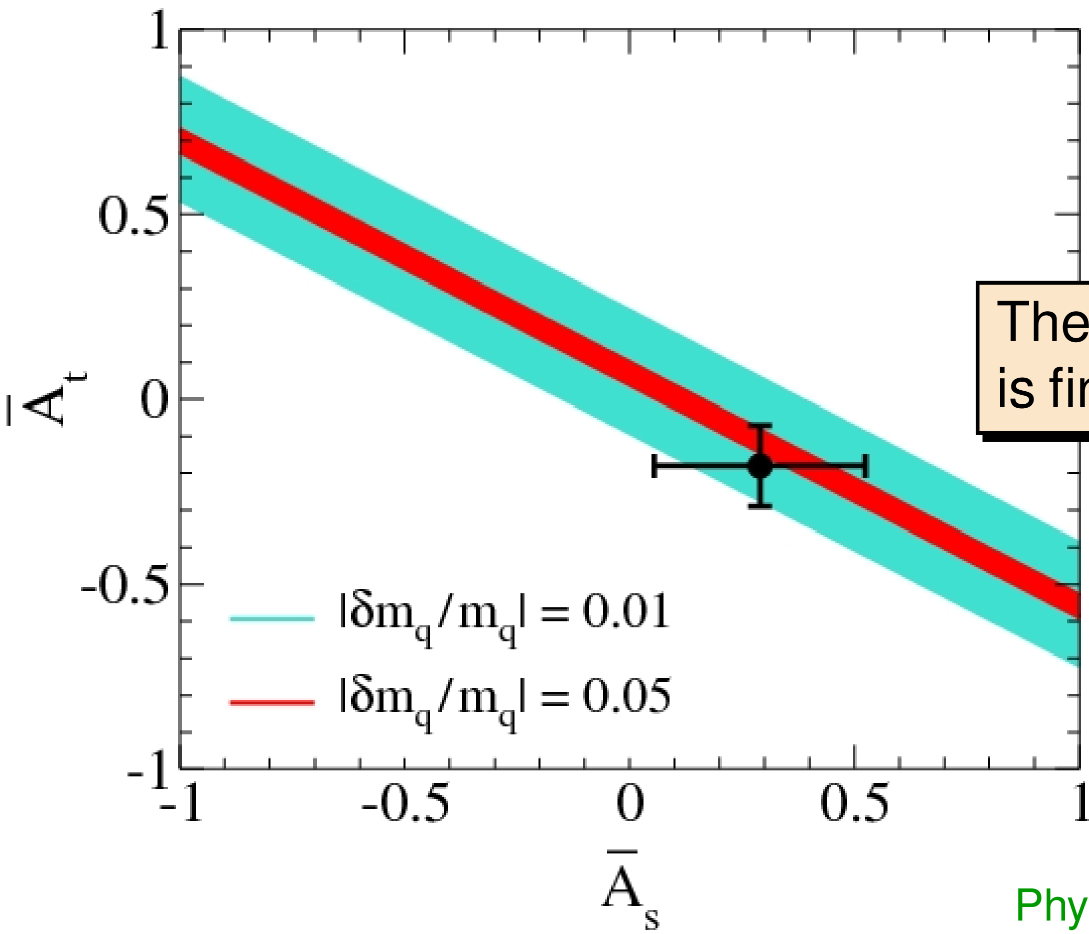
- clear correlations: α-particle BE and the energies/energy differences

$\Rightarrow$ 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)

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



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

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

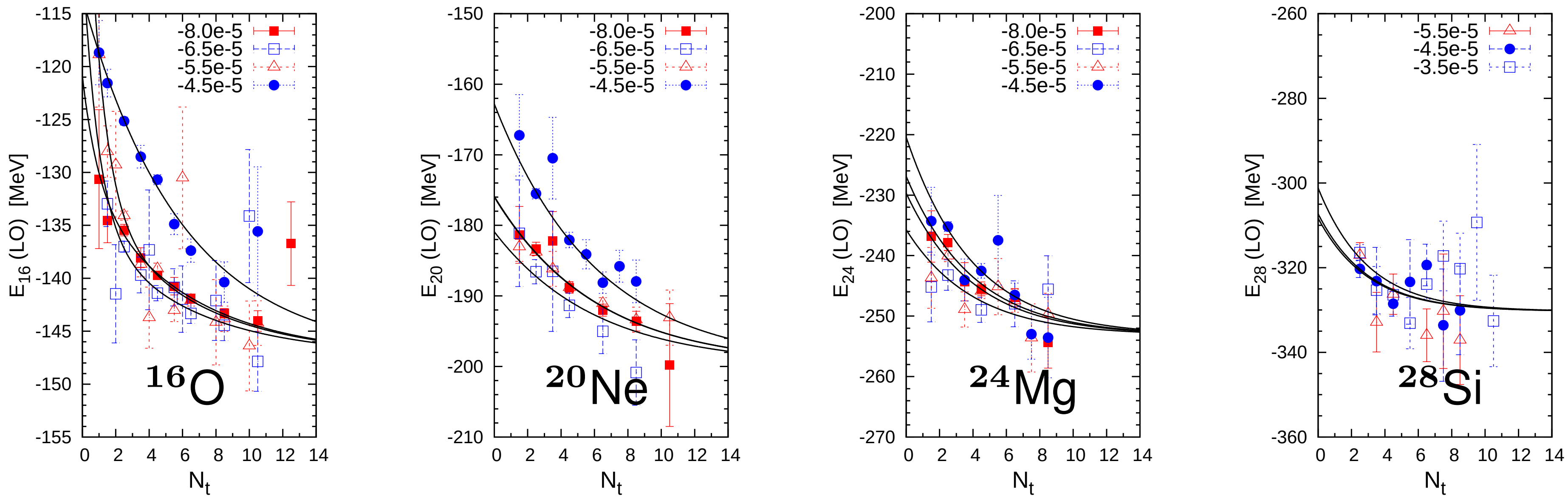
Towards medium-mass nuclei

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



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

REMOVING the OVERBINDING

Lähde et al., 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]

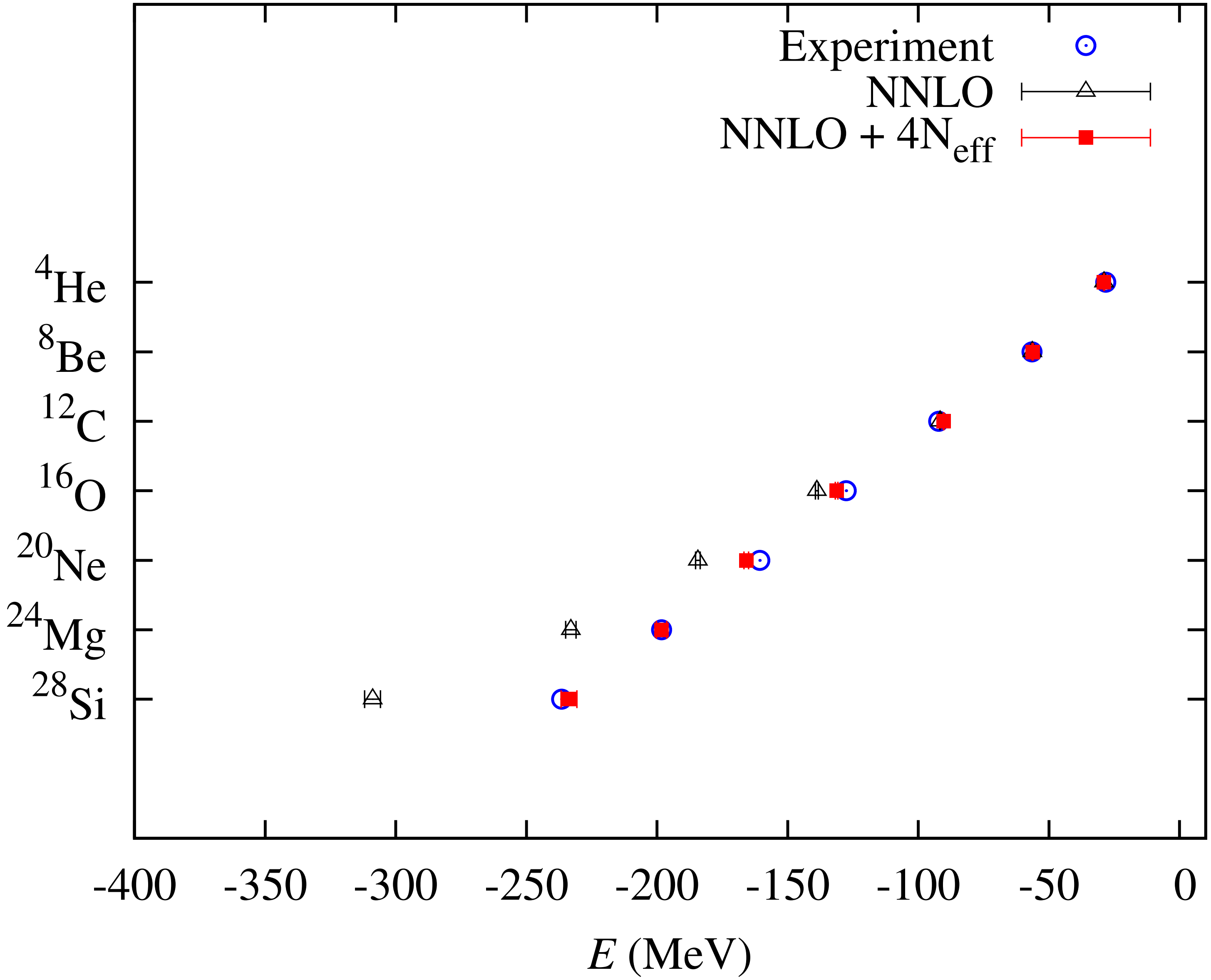
$$V^{(4\text{N}_{\text{eff}})} = D^{(4\text{N}_{\text{eff}})} \sum_{1 \le (\vec{n}_i - \vec{n}_j)^2 \le 2} \rho(\vec{n}_1)\rho(\vec{n}_2)\rho(\vec{n}_3)\rho(\vec{n}_4)$$

- fix the coefficient $D^{(4\text{N}_{\text{eff}})}$ 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

GROUND STATE ENERGIES



Spectrum & structure of ^{16}O

STRUCTURE of ^{16}O

- Mysterious nucleus, despite modern ab initio calcs

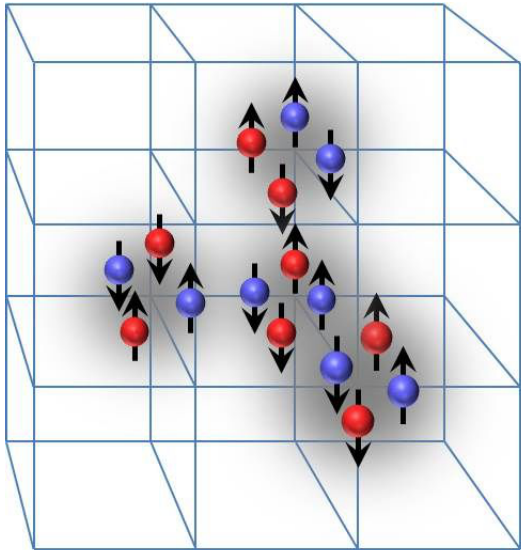
  Hagen et al. (2010), Roth et al. (2011), Hergert et al. (2013)

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

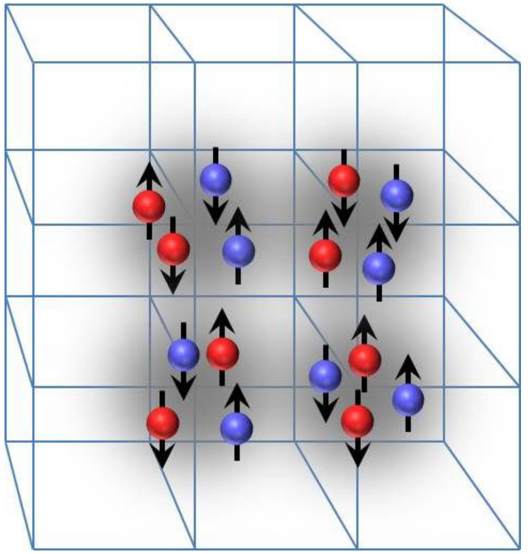
  Wheeler (1937), Dennison (1954), Robson (1979), . . ., Freer et al. (2005)

- Relevant configurations:

Tetrahedron (A)



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



DECODING the STRUCTURE of ^{16}O

Epelbaum, Krebs, Lähde, Lee, UGM, Rupak, *in prep.*

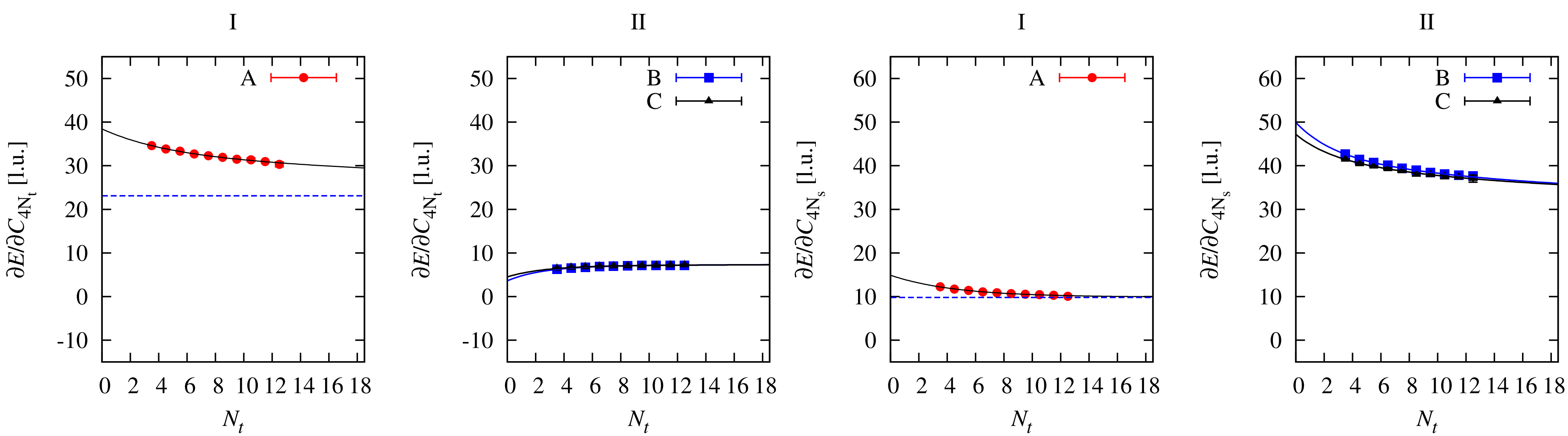
- measure the 4N density, where each of the nucleons is placed at adjacent points

$\Rightarrow$ $\mathbf{0_1^+}$ 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)
$M(E0, 0_2^+ \to 0_1^+)$ [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

OUTLOOK

- **Algorithmic improvements:**
  - tame the sign problem $\Rightarrow N \neq Z$ nuclei
  - 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

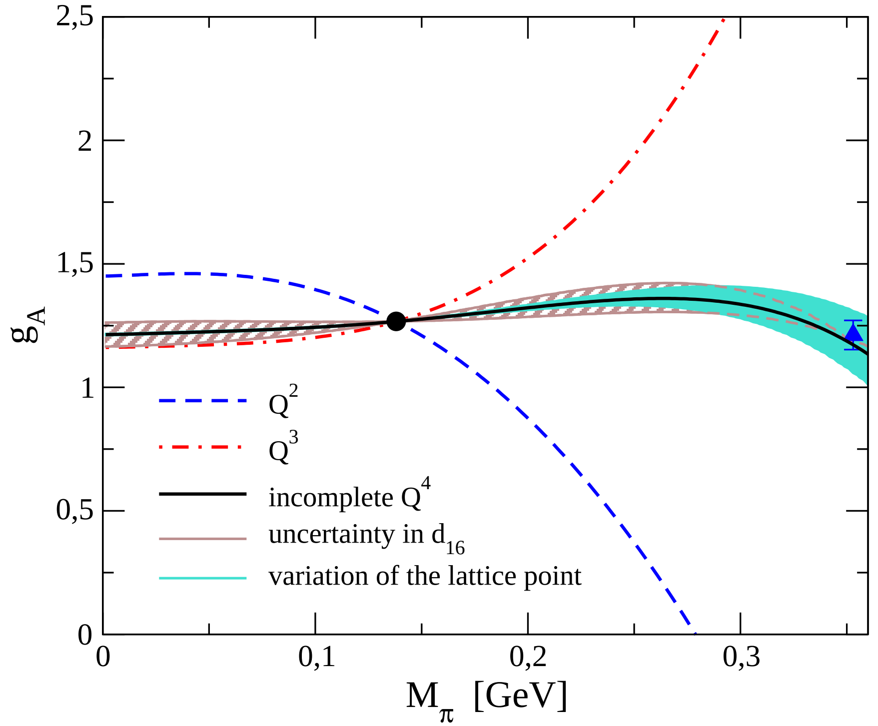
  LQCD data show little quark mass dep.

  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

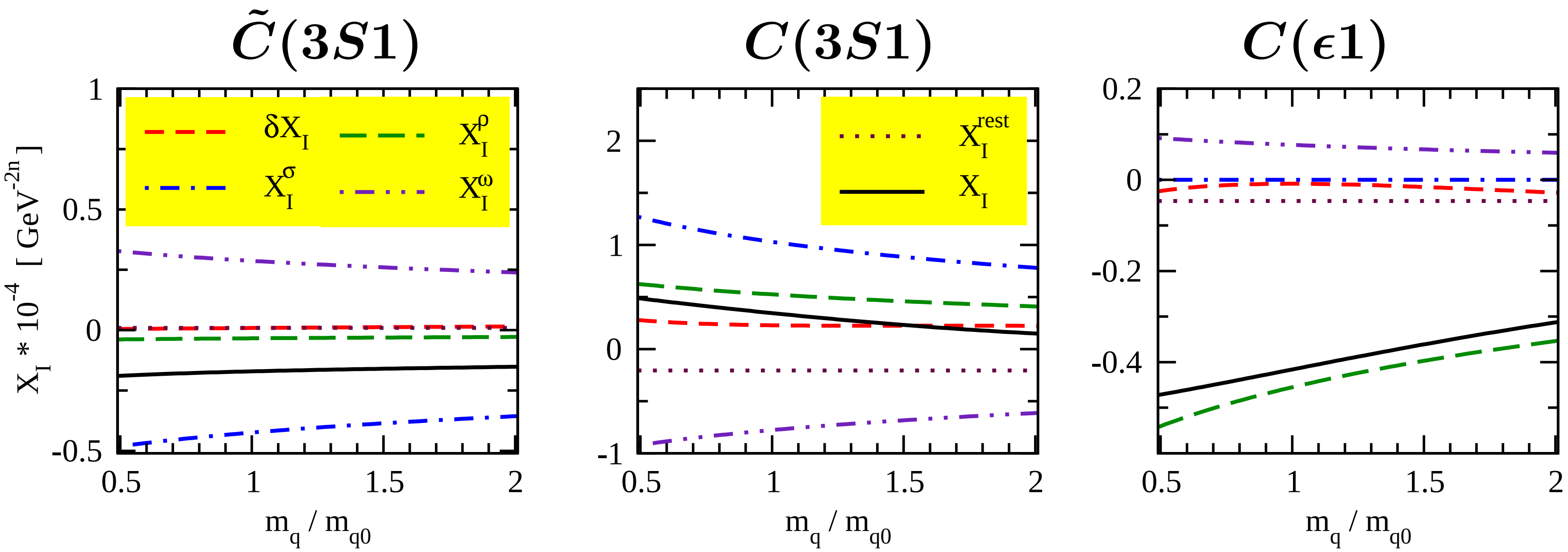
Hanhart, Pelaez, Rios (2008)

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

$\Rightarrow$ 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

$\Rightarrow$



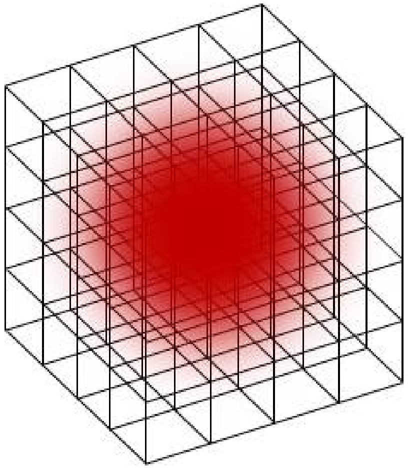
PROJECTION MONTE CARLO TECHNIQUE

- 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)
  - $\rightarrow$ allows for all type of wave functions (shell model, clusters, ...)
  - $\rightarrow$ 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 $\sim \langle (N^\dagger N)^2\rangle$

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:

$$\frac{\delta \ln Y_a}{\delta \ln m_q} = \sum_{X_i} \frac{\partial \ln Y_a}{\partial \ln X_i} K^q_{X_i}$$

- 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

⇒ results are dominated by the ^{4}He abundance:

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

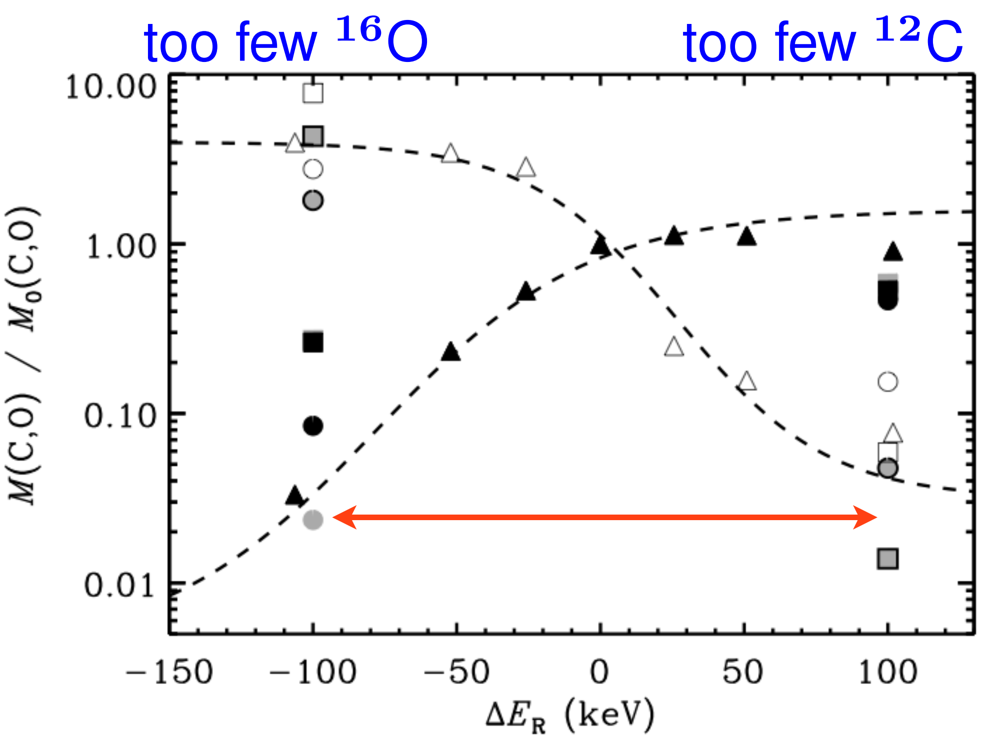
EARLIER STUDIES of the ANTHROPIC PRINCIPLE

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

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

- 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



Oberhummer et al., Science **289** (2000) 88

Csoto et al., Nucl. Phys. A **688** (2001) 560

Schlattl et al., Astrophys. Space Sci. **291** (2004) 27

[Livio et al., Nature **340** (1989) 281]