NUCLEAR FORCES
& ab initio calculations of atomic nuclei

Ulf-G. Meißner, Univ. Bonn & FZ Jülich

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

CONTENTS

- Intro: Gerry and the nuclear force problem
- Nuclear forces from chiral EFT
- Quark mass dependence of the nuclear force
- Ab initio calculation of atomic nuclei
- Nuclear lattice simulations: results
- The fate of carbon-based life as a function of fundamental parameters
- Towards medium-mass nuclei
- Back to square one

Gerry and the nuclear force problem

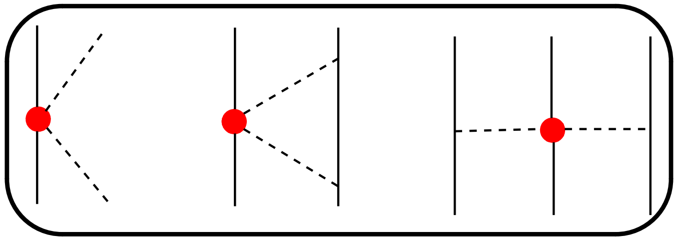
HOW TO BUILD A SERIOUS NUCLEAR FORCE MODEL

- Gerry knew about all the key ingredients!! [a condensation of decades of hard work]

- Ingredient 1: **Chiral symmetry**

  fixes pion interactions to pions and matter fields

  relates seemingly unrelated processes



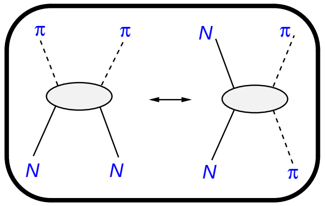
- Ingredient 2: **Three- and four-body forces**

  a precise description of few-nucleon systems requires 3NFs

  4NFs become relevant in heavy nuclei/nuclear matter

- Ingredient 3: **TPE from pion-nucleon scattering**

  model-independent determination using
  dispersion relations: $\pi N \to \pi N \leftrightarrow \bar{N} N \to \pi\pi$



$\Rightarrow$ almost all the ingredients for an EFT approach except power counting

A FEW PERTINENT PAPERS

Brown, Green, Gerace, Nyman, “Four-body forces in nuclear matter,” Nucl. Phys. **A118** (1968) 1

Brown, Green, Gerace, “PCAC and three-body forces in nuclei,” Nucl. Phys. **A118** (1968) 435

Riska, Brown, “Two-pion exchange contribution to the nucleon-nucleon interaction and an effective σ-meson,” Nucl. Phys. **A153** (1970) 8

Brown, “Isn’t it time to calculate the nucleon-nucleon force?,” Comments Nucl. Part. Phys. **4** (1970) 140

Brown and Durso, “Soft pioneering determination of the intermediate range nucleon nucleon interaction,” Phys. Lett. B **35** (1971) 120.

Barshay, Brown, “Chiral field theories and and three-body forces in nuclei,” Phys. Rev. Lett. **34** (1975) 1106

Durso, Saarela, Brown, Jackson, “Isobars, transition potentials and short-range repulsion in the nucleon-nucleon interaction,” Nucl. Phys. **A278** (1977) 445

Brown, “Chiral Symmetry And The Nucleon Nucleon Interaction,” in Rho M, Wilkinson D: Mesons In Nuclei, Vol.I*, Amsterdam 1979, 329-356

Durso, Brown, Saarela, “Chiral symmetry and the A_1 contribution to the nucleon-nucleon interaction,” Nucl. Phys. **A430** (1984) 653

Brown, Machleidt, “Strength of the ρ meson coupling to nucleons,” Phys. Rev. **C 50** (1994) 1731

and of course NN force aspects from bags, Skyrmions and $V_{\rm low-k}, \ldots$

THE MASTERPIECE

THE NUCLEON-NUCLEON INTERACTION

G. E. BROWN
Nordita, Copenhagen
and
State University of New York
Stony Brook N.Y.

and

A. D. JACKSON
State University of New York
Stony Brook N.Y.

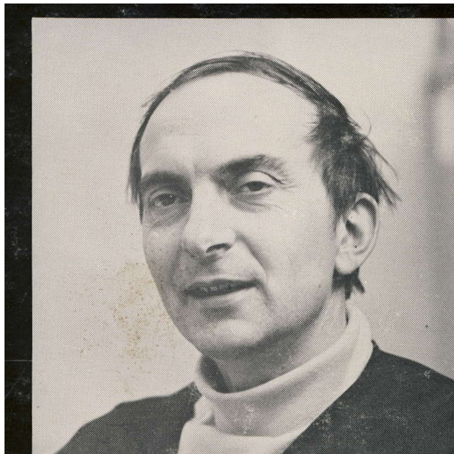
N·H P·C

1976

NORTH-HOLLAND PUBLISHING COMPANY – AMSTERDAM • OXFORD
AMERICAN ELSEVIER PUBLISHING COMPANY, INC. – NEW YORK

⋆ a phlethora of concepts and methods

⋆ many insights into the nuclear force problem



GERALD E. BROWN received his Ph. D. at Yale University in 1950 and his D. Sc. at the University of Birmingham, England where he was Professor until 1960. From 1964–68 he was Professor at Princeton University and since then has headed the Institute for Theoretical Physics at the State University of New York at Stony Brook. Since 1960 he has also been Professor at the Nordic Institute for Theoretical Atomic Physics, Copenhagen, Denmark. Fellow of the Royal Danish Academy and the American Physical Society, he is presently on the NSF Advisory Panel for Physics. Professor Brown has been a constant and distinguished contributor to the literature in the field of Nuclear Physics and is the author of two recent books: *Unified Theory of Nuclear Models and Forces* (3rd. Edition 1971) and *Main-Body Problems* (1972).

Nuclear forces from chiral EFT

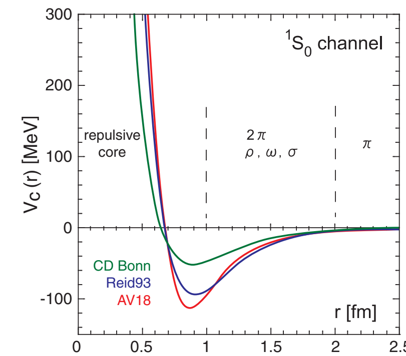
CHIRAL EFT for FEW-NUCLEON SYSTEMS

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



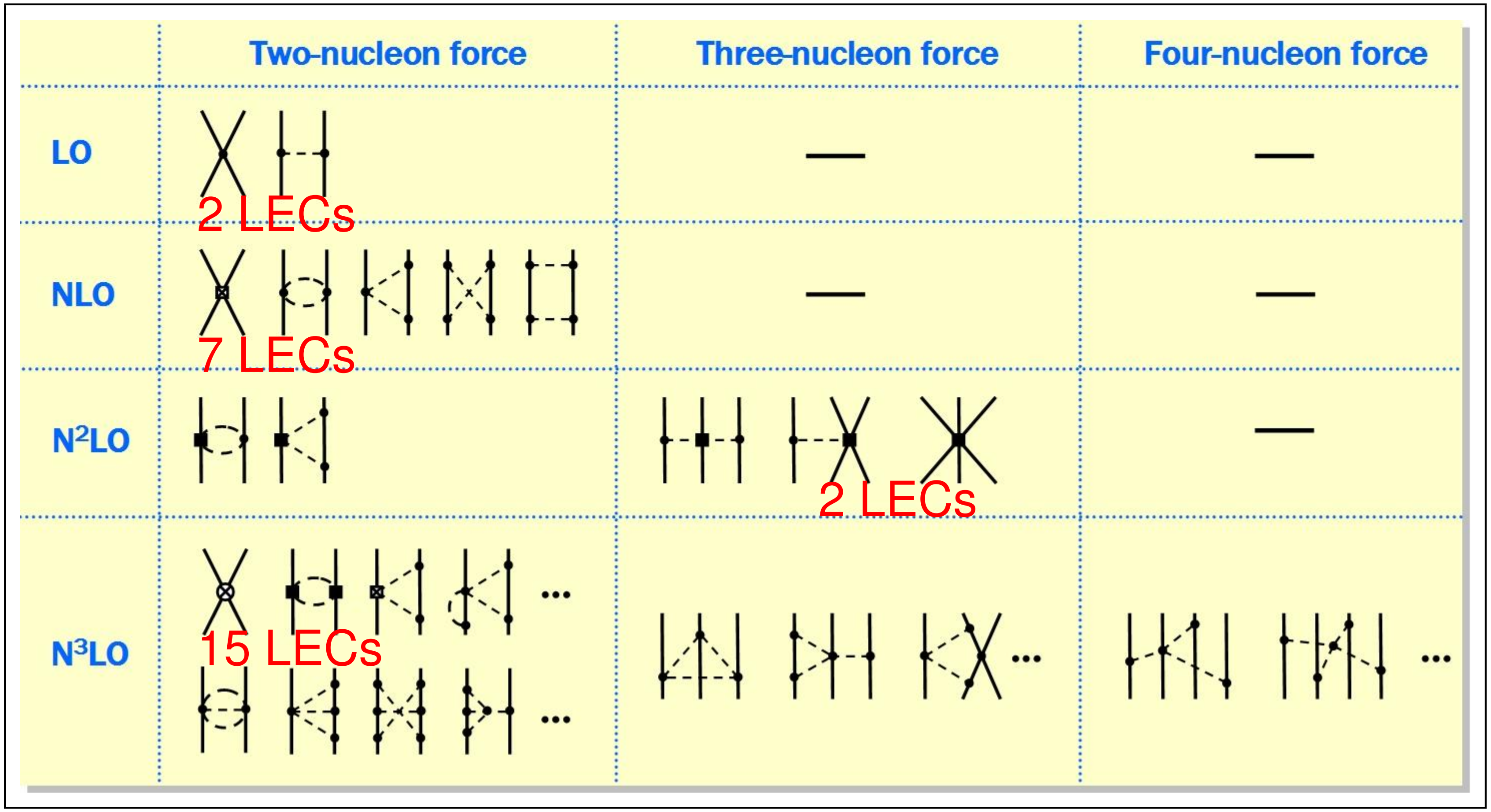
- this can be analyzed in a suitable EFT based on

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

- 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 $V_{\rm NN(N)}$, use in regularized Schrödinger equation

CHIRAL POTENTIAL and NUCLEAR FORCES



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

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

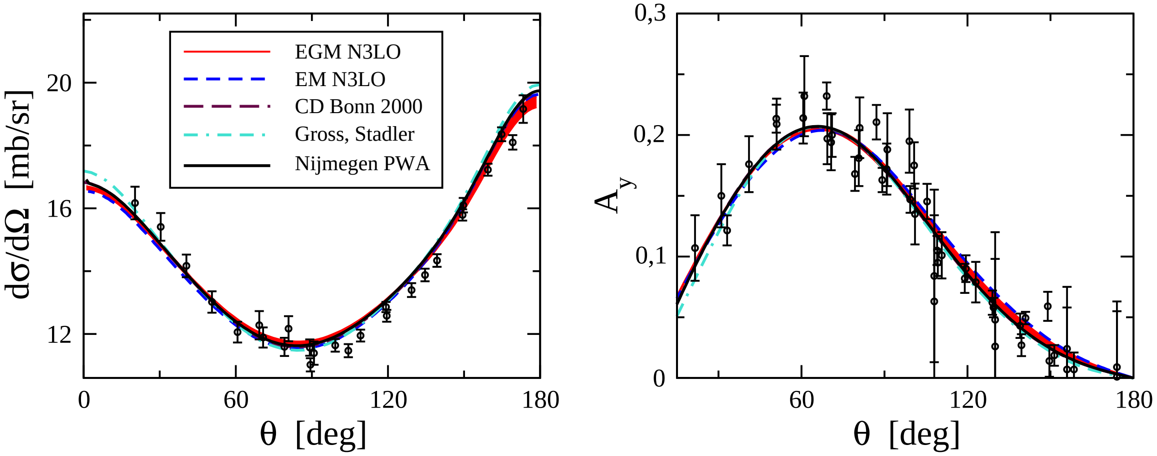
$\mathcal{O}((Q/\Lambda_\chi)^3)$

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

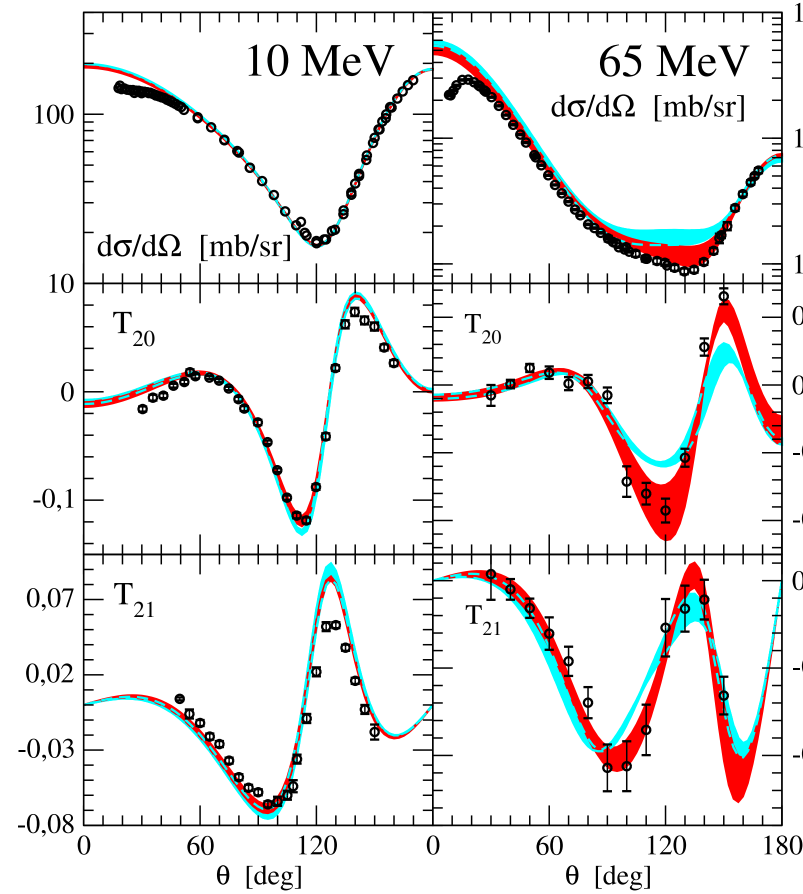
- explains naturally the observed hierarchy of nuclear forces
- MANY successfull tests in few-nucleon systems (continuum calc's)

RESULTS

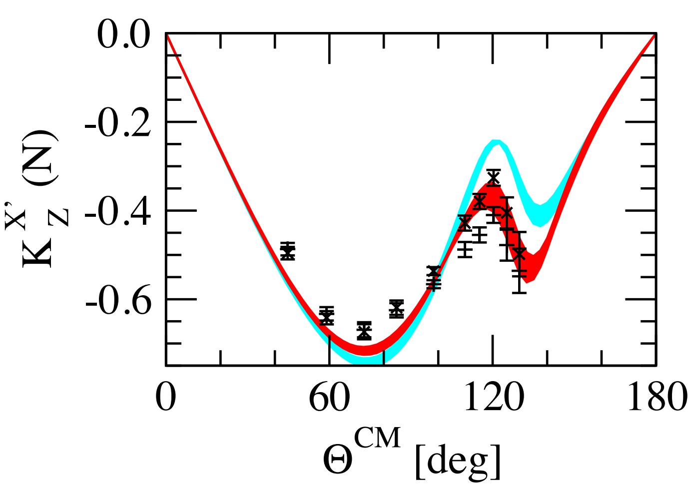
- np scattering



- 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

GERRY'S COLOURFUL WORLDS

- how does nuclear binding change when N_c and/or $m_{\rm quark}$ varies?
- study OBE for different N_c and $m_{\rm quark}$
- construction of the 2π spectral function $\rightarrow$ effective σ-exchange w/ $M_\sigma, g_{\sigma NN}(N_c, m_{\rm quark})$

$\Rightarrow$ "our world is wedged into a small corner of the two-dimensional manifold of $m_{\rm quark}$ versus N_c"

$\Rightarrow$ reanalyze this in chiral EFT

Nuclear Physics **A462** (1987) 701–726
North-Holland, Amsterdam

NUCLEAR PHYSICS IN COLOURFUL WORLDS*
Quantumchromodynamics and nuclear binding

H. MÜTHER[1], C.A. ENGELBRECHT[2] and G.E. BROWN

Department of Physics, State University of New York at Stony Brook, Stony Brook, NY 11794, USA

Received 14 January 1985
(Revised 20 June 1986)

Abstract: When quantumchromodynamics (QCD) is generalized from SU(3) to an SU(N_c) gauge theory, where N_c is the number of colours, it depends on only two parameters: N_c and the bare quark mass m_q. A more general understanding of nuclear physics can be achieved by considering what it would be like in worlds with the number of colours different from 3, and bare quark masses different from the "empirical" ones. Such an investigation can be carried out within a framework of meson-exchange interactions. The empirical binding energy of nuclear matter results from a very near cancellation between attractive and repulsive terms which are two orders of magnitude larger and may be expected to depend sensitively on the parameters of QCD. It is indeed found that our world is wedged into a small corner of the two-dimensional manifold of m_q versus N_c. If the number of colours were decreased by one, or the bare quark masses raised by more than 20%, nuclear matter would become unbound. By tracing the origin of this state of affairs, one obtains a clearer picture of the relative importance of various effects on the behaviour of the bulk nuclear matter. In particular, correlations like those embodied in the Coester band of saturation points appear to have a broader degree of validity than is implied by fits to the actual physical world only.

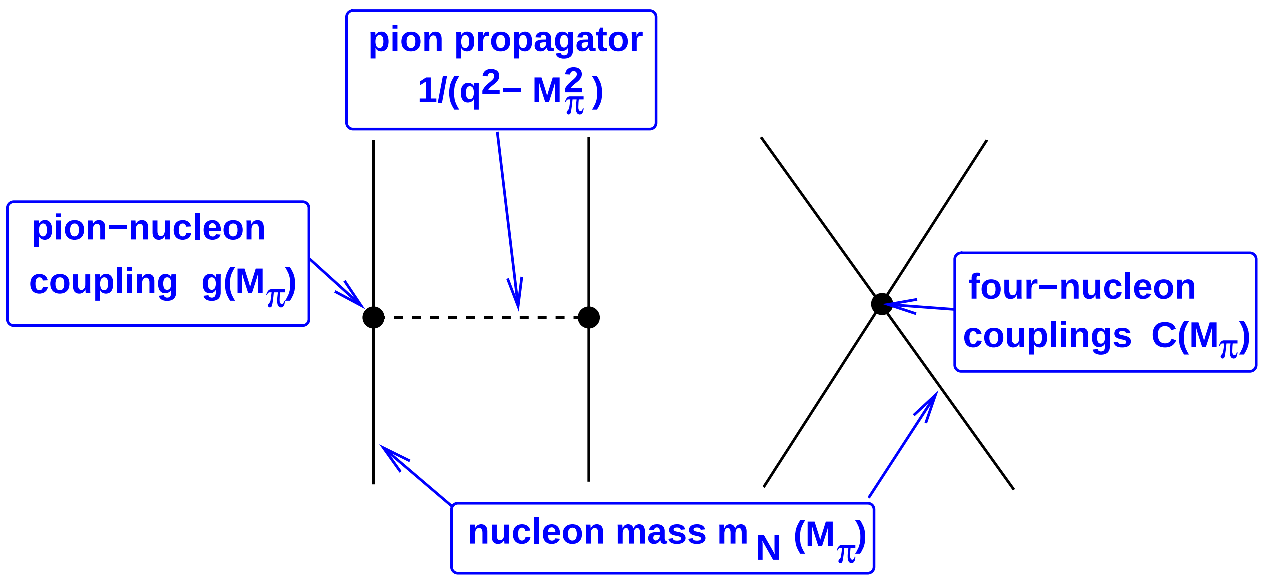
QUARK MASS DEPENDENCE in CHIRAL EFT

- 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: $M^2_{\pi^\pm} \sim (m_u + m_d)$

QUARK MASS DEPENDENCE of HADRON MASSES etc

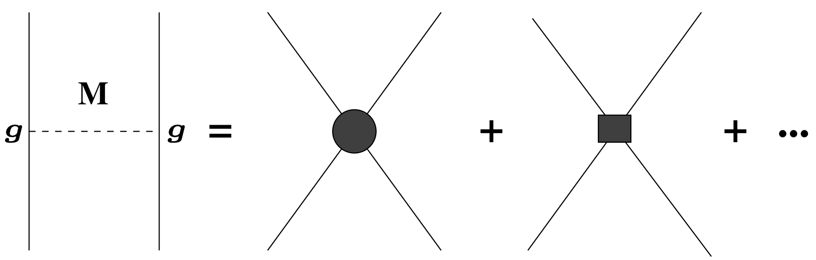
- Quark mass dependence of hadron properties:

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

- Pion and nucleon properties from lattice QCD combined with CHPT

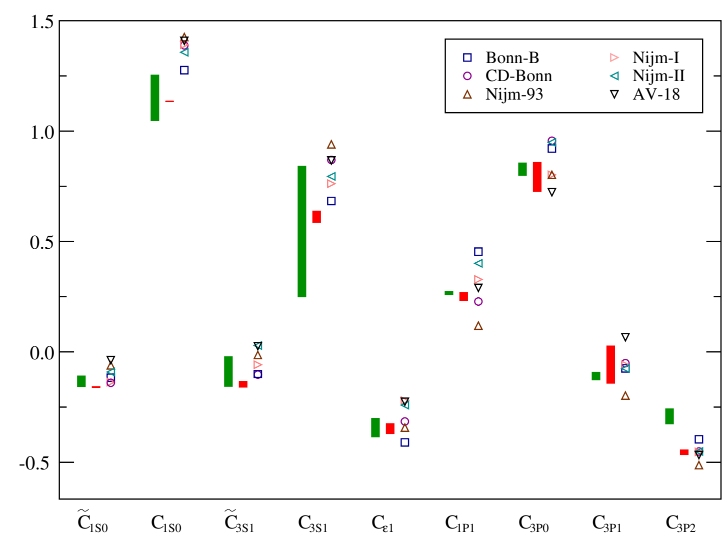
- Contact interactions modeled by heavy meson exchanges

Epelbaum, UGM, Glöckle, Elster (2002)



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

$\hookrightarrow$



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

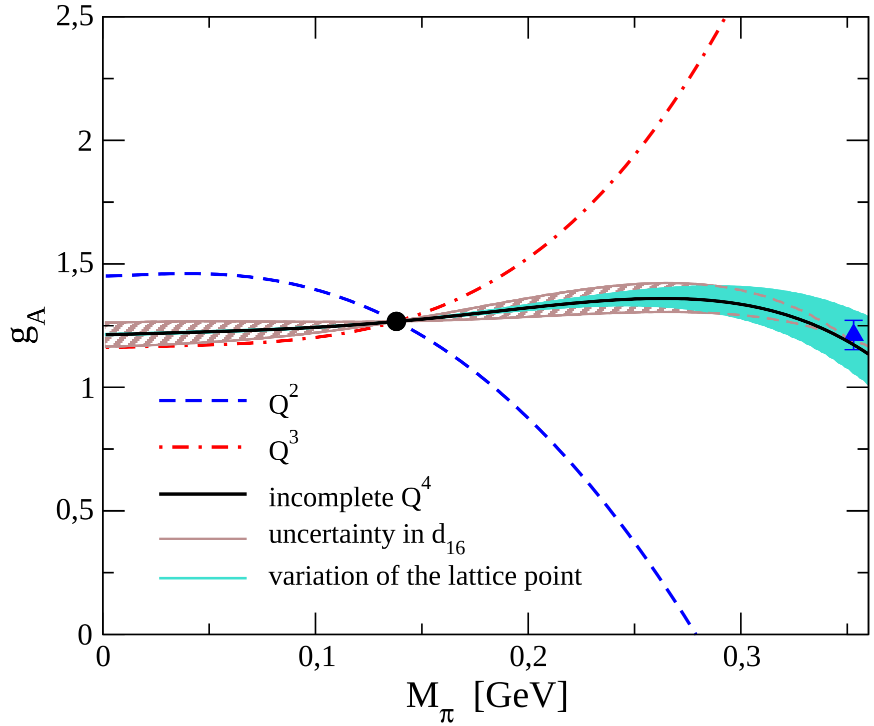
LQCD data show little quark mass dep.

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

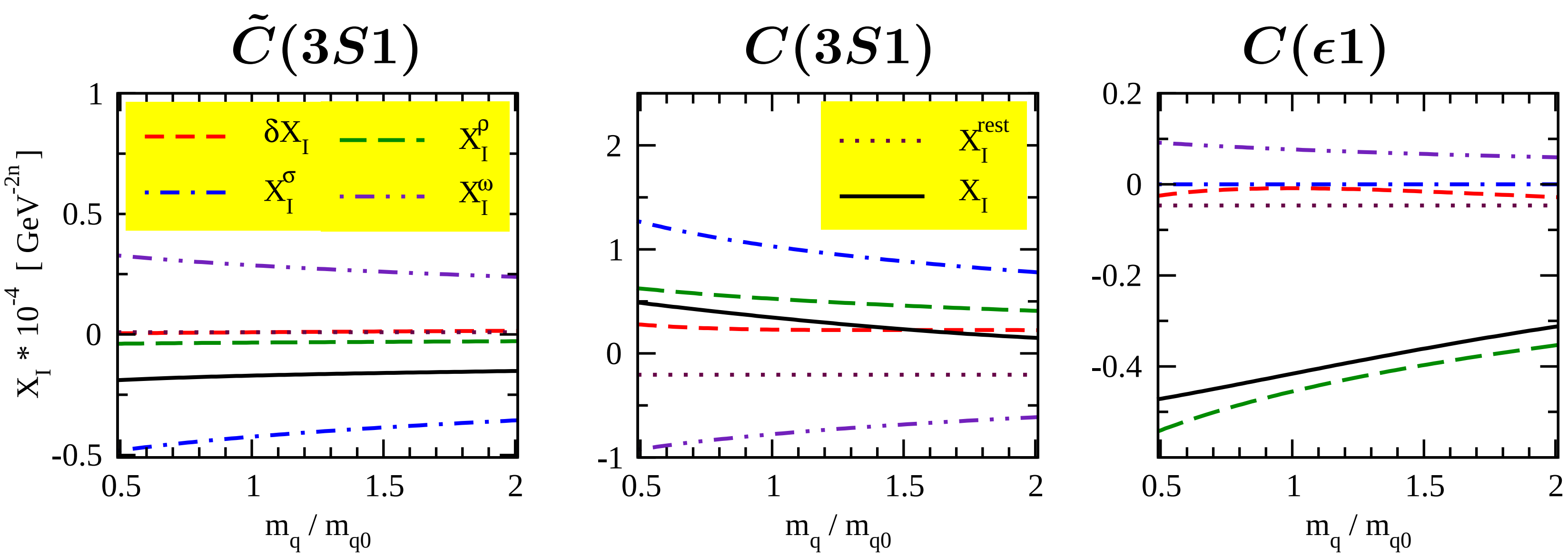
Hanhart, Pelaez, Rios (2008)

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

$\Rightarrow$ 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

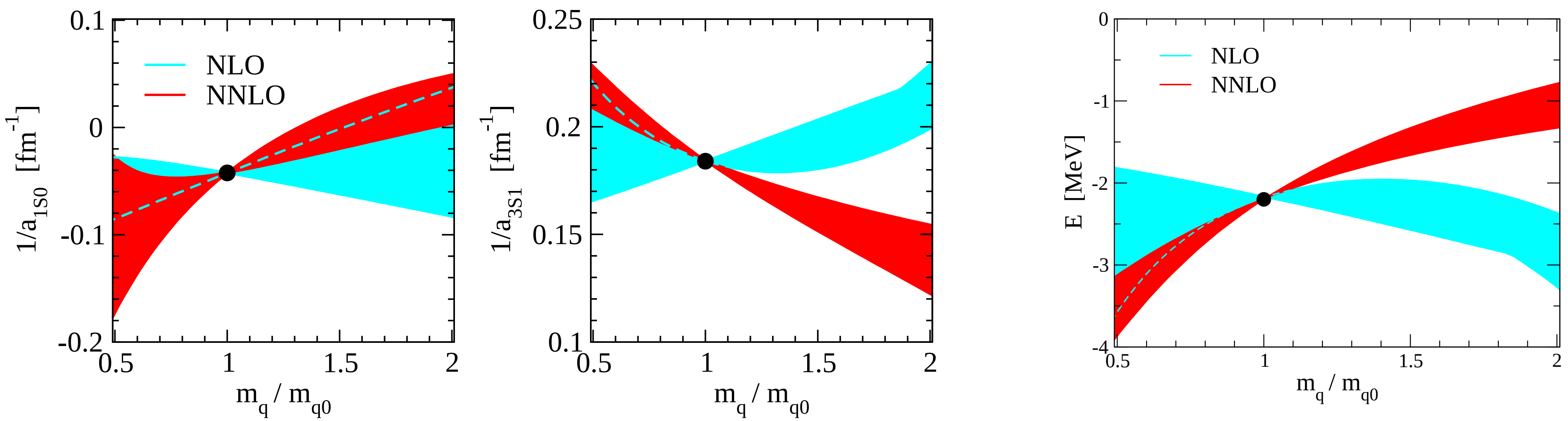
$\Rightarrow$



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 $m_{\rm quark}$ (as Gerry told us)
- 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), . . .

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

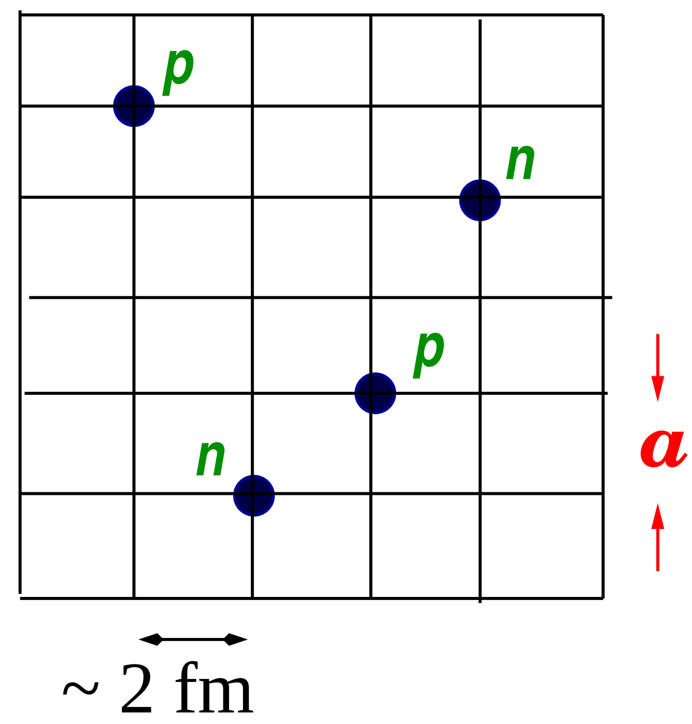
But how about *ab initio* calculations for systems with $A \geq 5$?

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

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

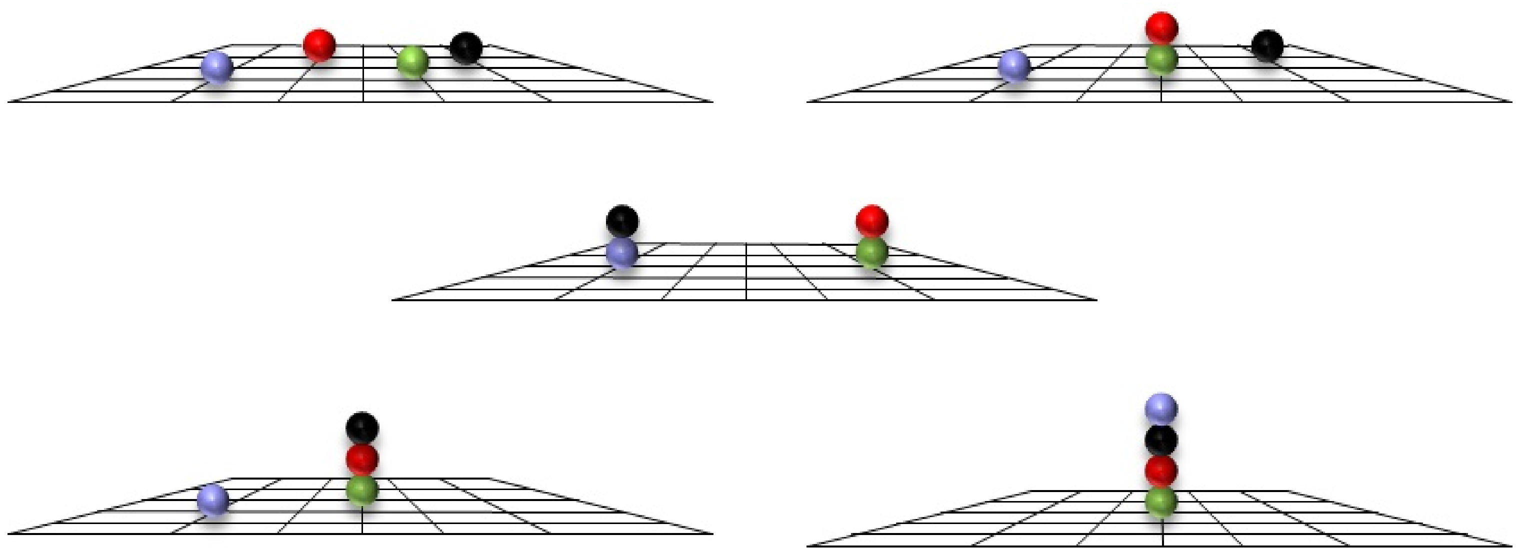


- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

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

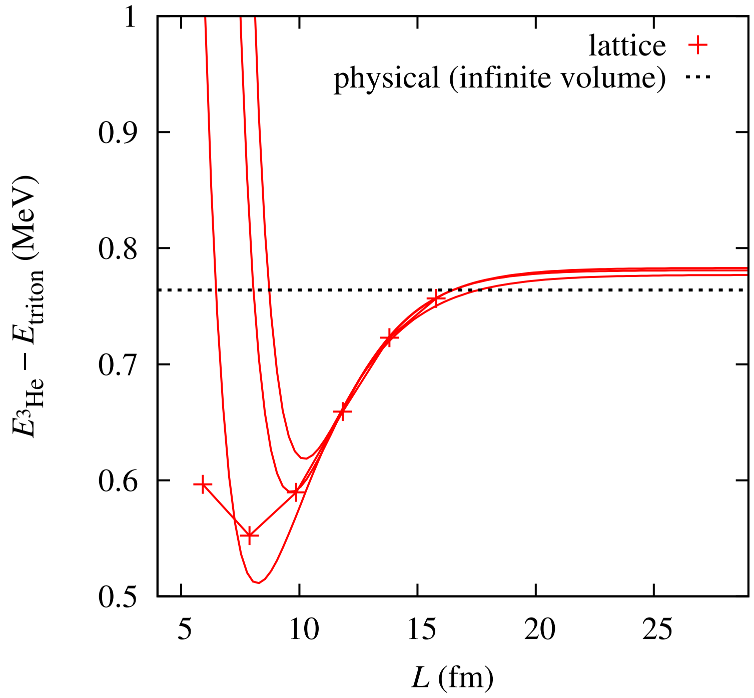
Nuclear lattice simulations – results –

RESULTS

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

- some groundstate 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



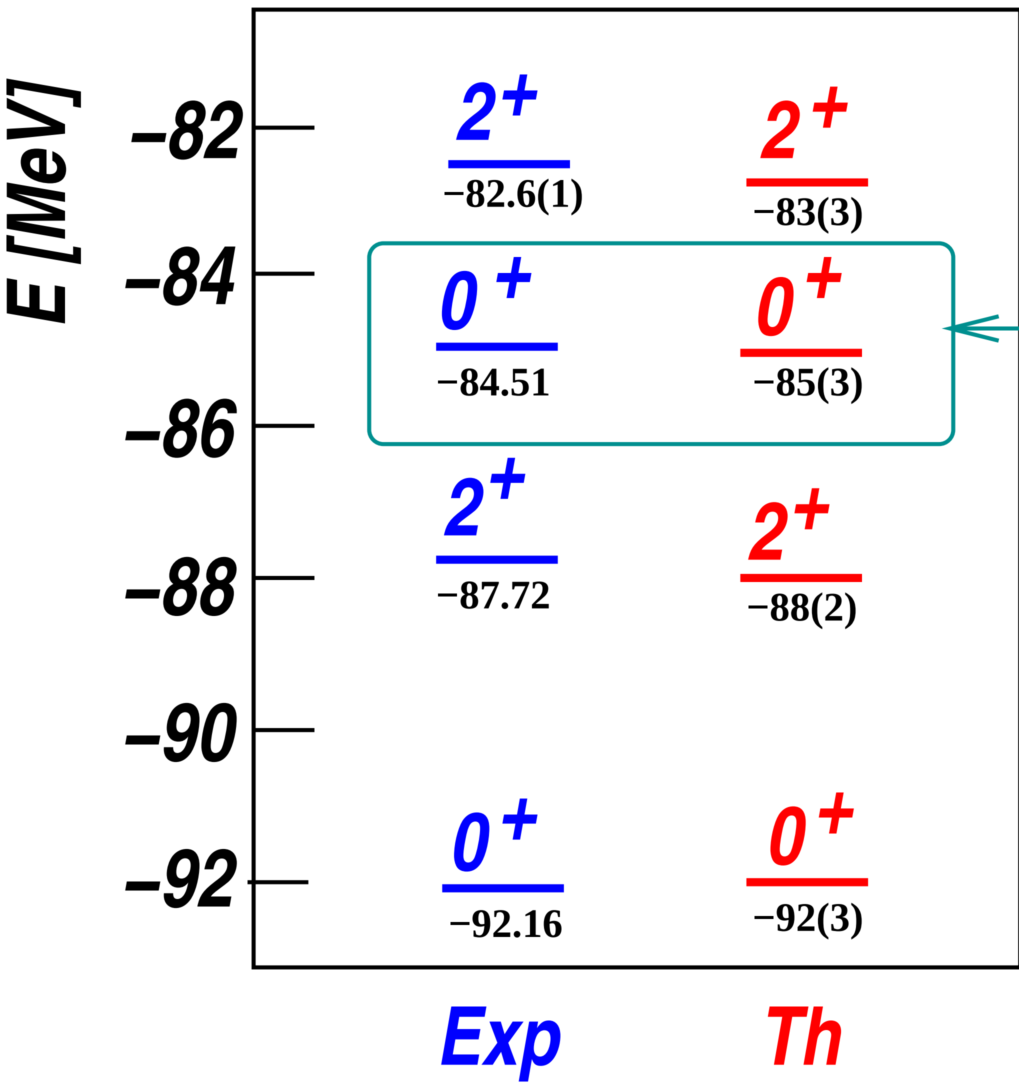
- promising results [3NFs very important]

- excited states more difficult

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

The SPECTRUM of CARBON-12

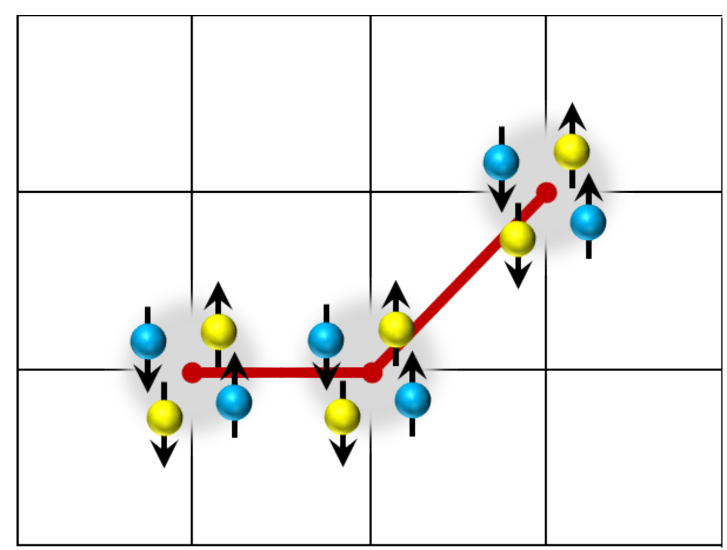
- After $8 \cdot 10^6$ hrs JUGENE/JUQUEEN (and “some” human work)



Hoyle

⇒ 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]

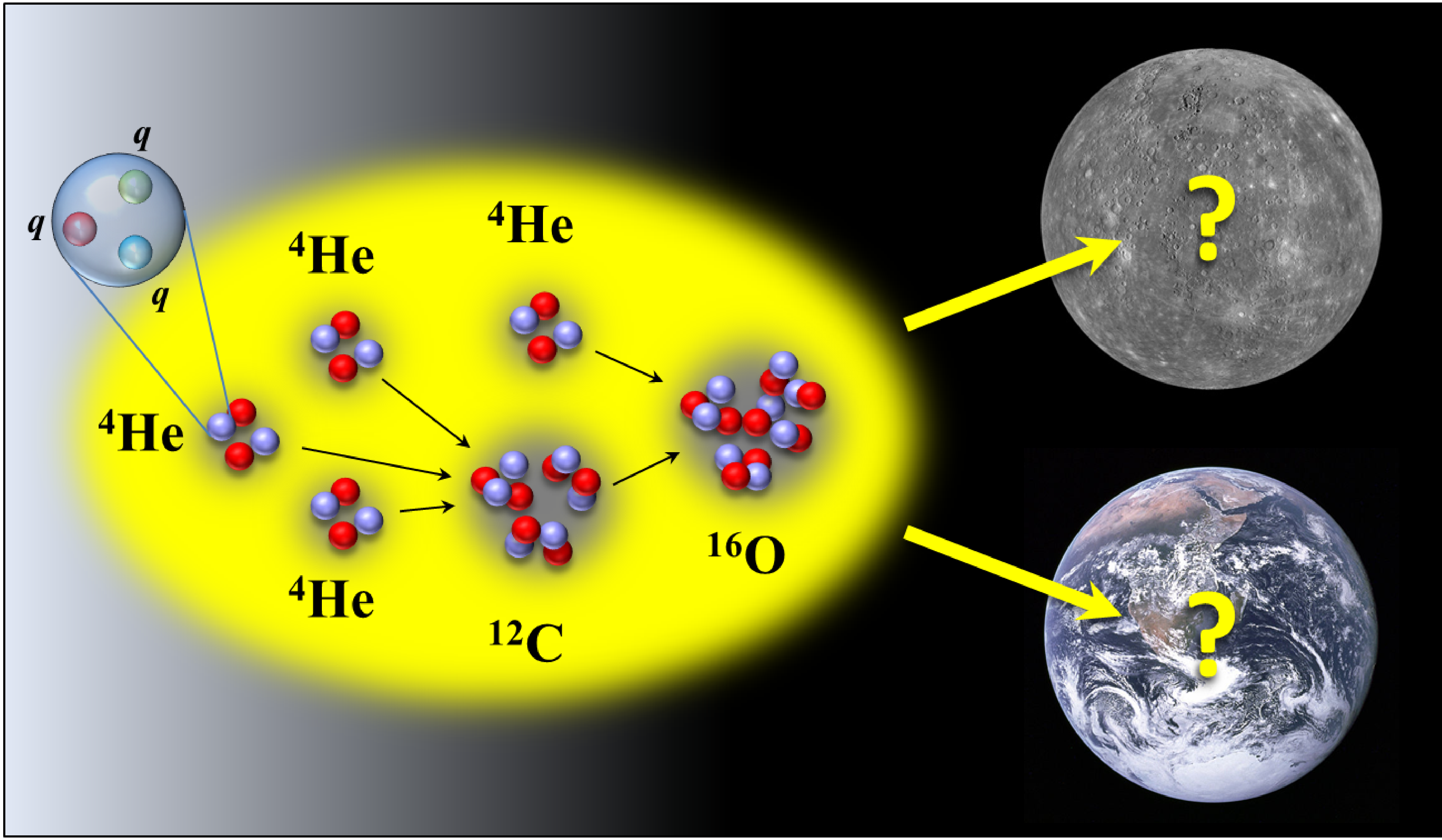
- importance of **consistent** 2N & 3N forces
- good agreement w/ experiment, can be improved

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

The role of carbon abundance is also of relevance to neutron star masses and black hole formation, see Brown, Lee, Rho, Phys.Rev.Lett. **101** (2008) 091101

FINE-TUNING of FUNDAMENTAL PARAMETERS

Fig. courtesy Dean Lee



FINE-TUNING: MONTE-CARLO ANALYSIS

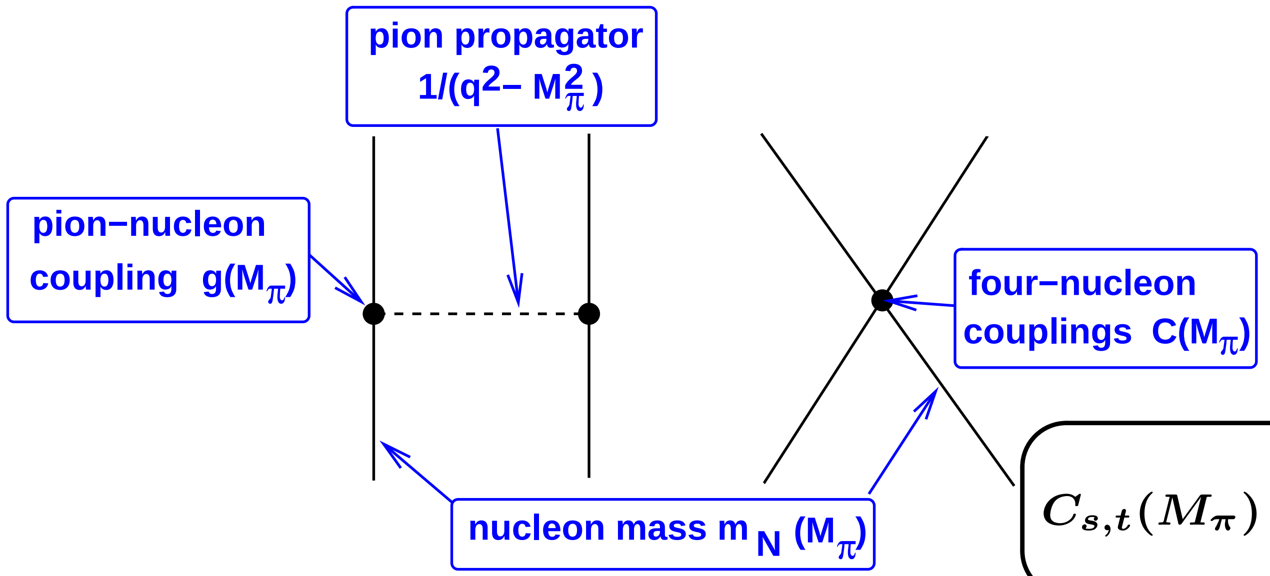
Epelbaum, Krebs, Lähde, Lee, UGM, PRL **110** (2013) 112502, Eur. Phys. J. **A49** (2013) 82

- simulations allow to vary $m_{\rm quark}$ and α_{EM}

- quark mass dependence $\equiv$ pion mass dependence: $M^2_{\pi^\pm} \sim (m_u + m_d)$

Gell-Mann, Oakes, Renner (1968)

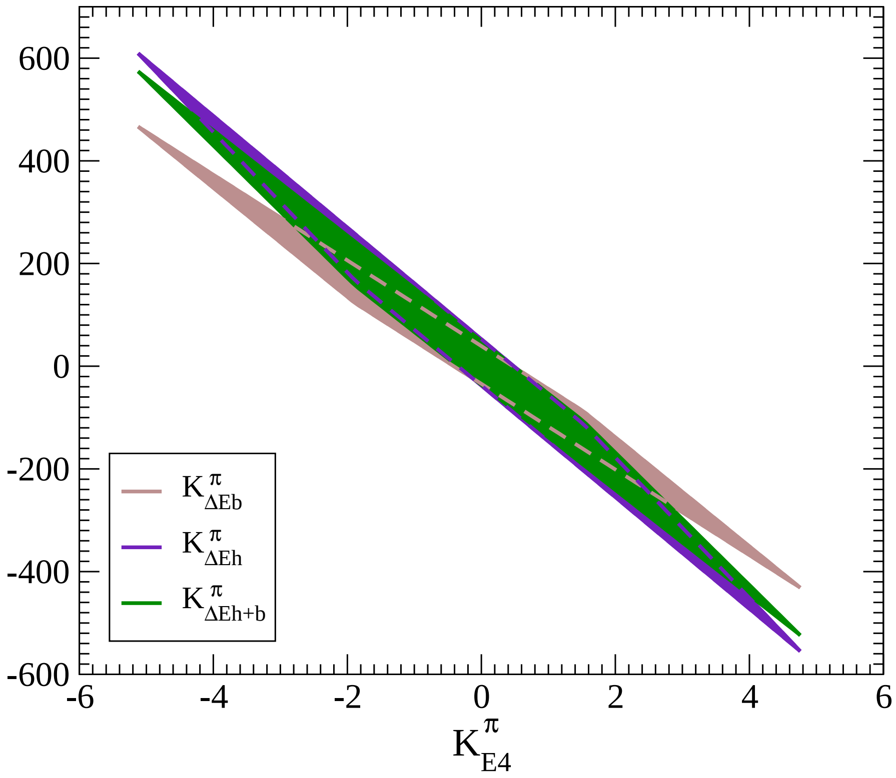
- explicit and implicit pion mass dependences



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

CORRELATIONS

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



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

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

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

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

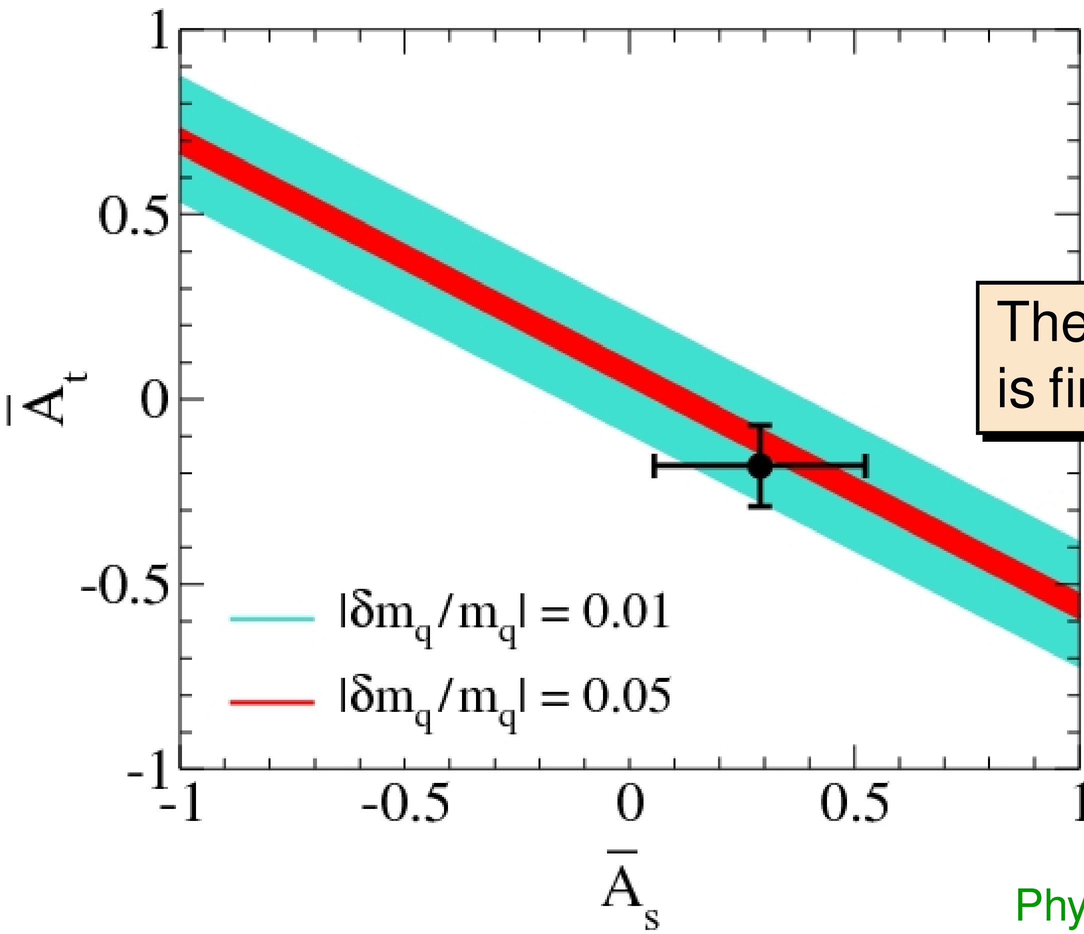
- clear correlations: α-particle BE and the energies/energy differences

$\Rightarrow$ 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)

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



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

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

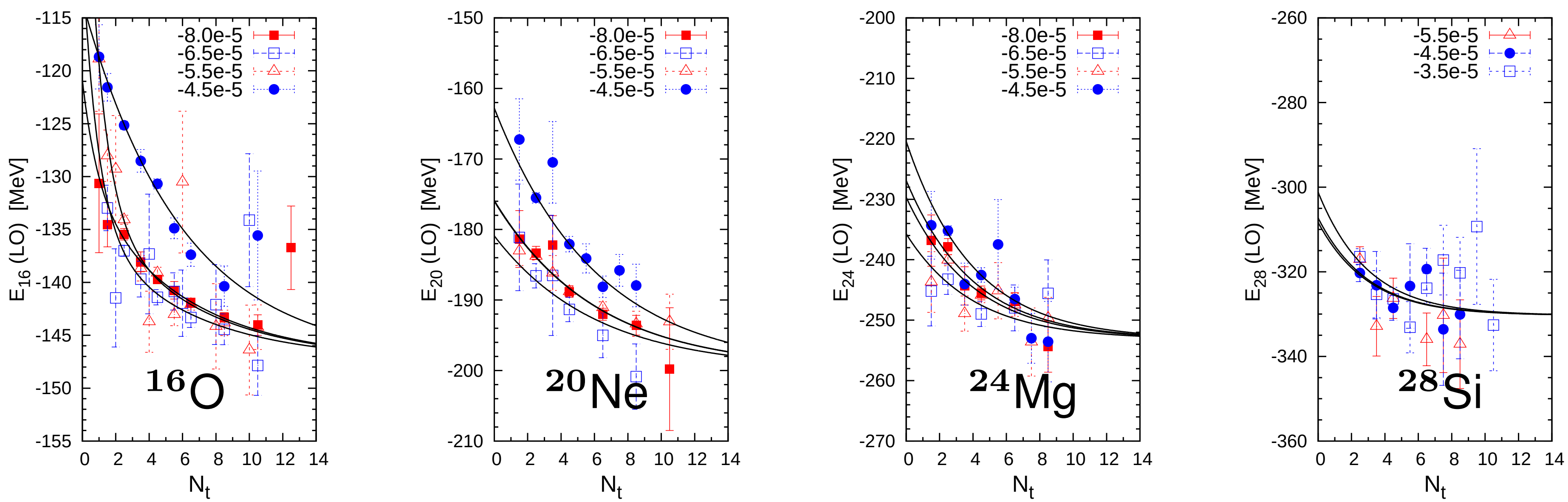
Towards medium-mass nuclei

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



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

REMOVING the OVERBINDING

Lähde et al., 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]

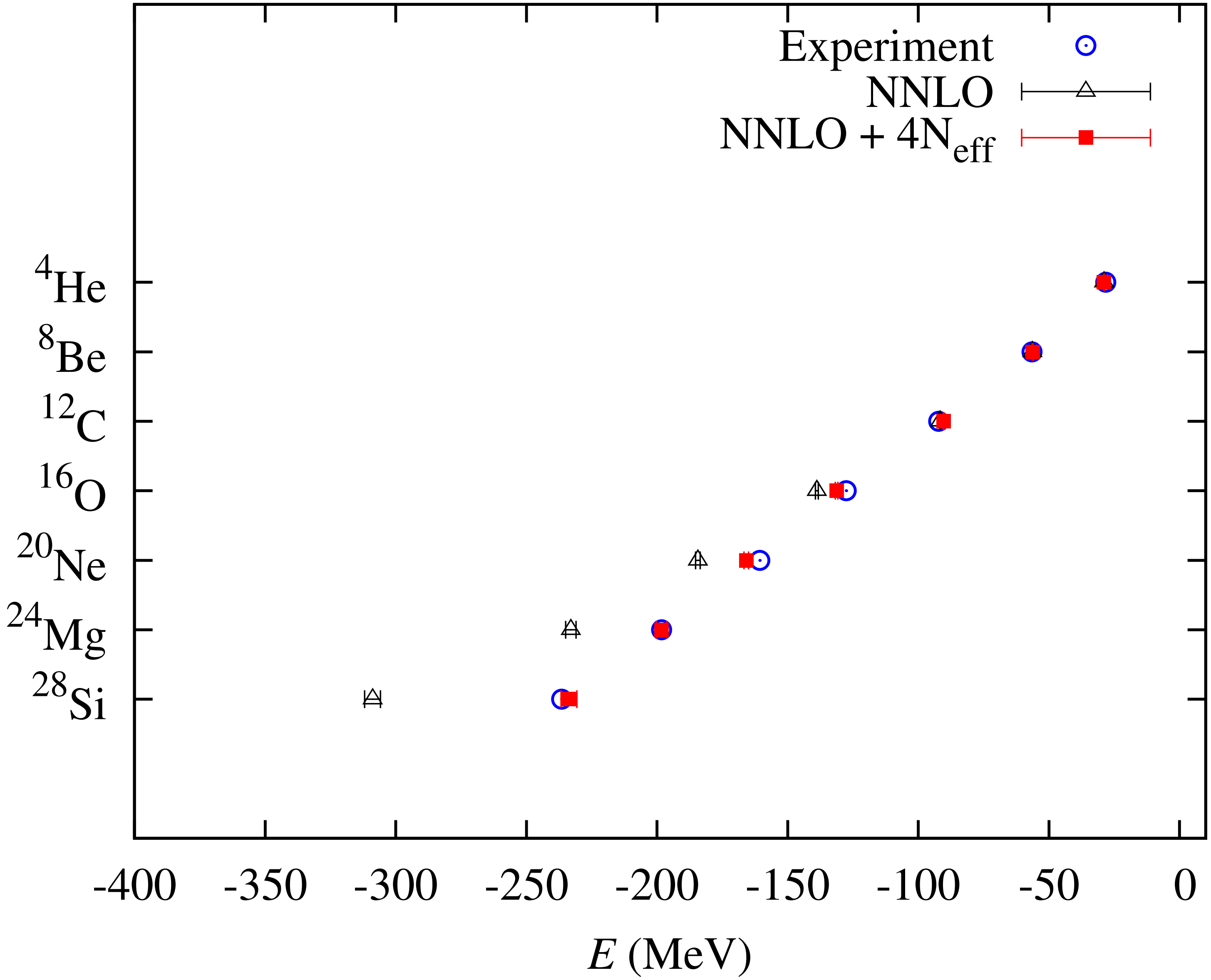
$$V^{(4\mathrm{N_{eff}})} = D^{(4\mathrm{N_{eff}})} \sum_{1\leq(\vec{n}_i-\vec{n}_j)^2\leq 2} \rho(\vec{n}_1)\rho(\vec{n}_2)\rho(\vec{n}_3)\rho(\vec{n}_4)$$

- fix the coefficient $D^{(4\mathrm{N_{eff}})}$ 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



BACK to SQUARE ONE

- Gerry laid the grounds for the

  modern theory of nuclear forces

  the application of these forces
  in modern structure calculations

- see the groundbreaking paper
  from Steven Weinberg

S. Weinberg,
"Nuclear forces from chiral Lagrangians,"
Phys. Lett. B **251** (1990) 288.

the other hand, the four-nucleon potential does involve the nonlinear pion-nucleon couplings as well as the pion self-interaction, through diagrams like those shown in Figure 3. It will be interesting to see whether effects of these multi-nucleon effective potentials can be found in nuclear properties.

I am grateful to H. Georgi for his encouragement, and to G. E. Brown and A. Kerman for enlightening conversations about nuclear forces.

References

1. S. Weinberg, Physica *96A* (1979), 327, and earlier references quoted therein.
2. T. H. R. Skyrme, Proc. Roy. Soc. *A260* (1961), 127; E. Witten, Nucl. Phys. *B160* (1979), 57. Also see ref. 3.
3. For a review, see S.O. Bäckman, G. E. Brown, and J. A. Niskanen, Physics Reports *124*, No. 1 (1985).

⇒ Gerry's legacy will live on

SPARES