Nuclear Lattice EFT: An introduction

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

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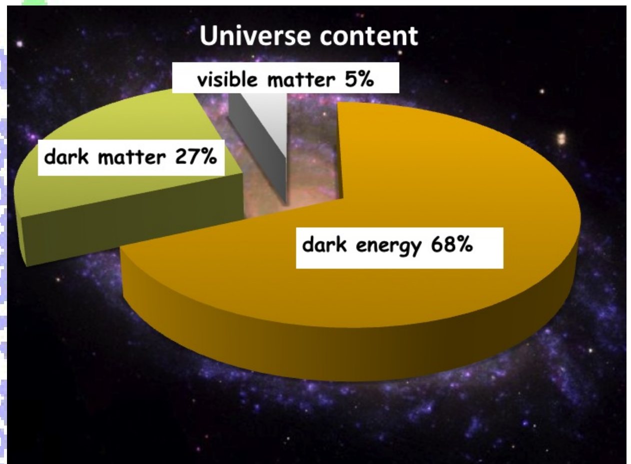
by VolkswagenStftung

CONTENTS

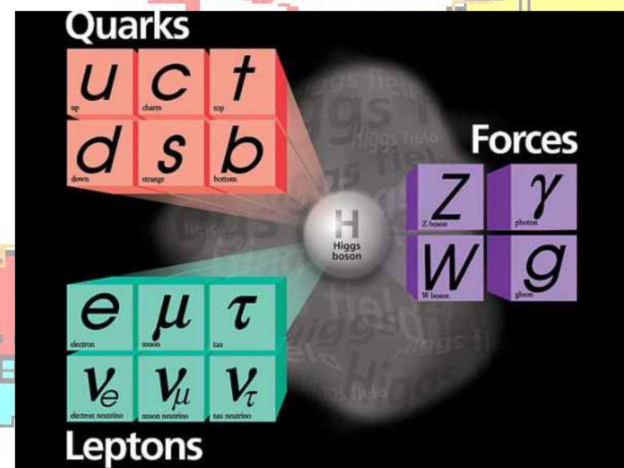
Nuclear physics factbook

WHY NUCLEAR PHYSICS?

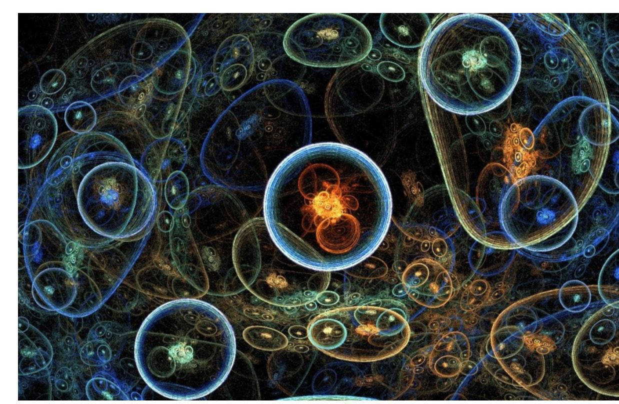
- **The matter we are made off**



- **The last frontier of the SM**



- **Access to the Multiverse**

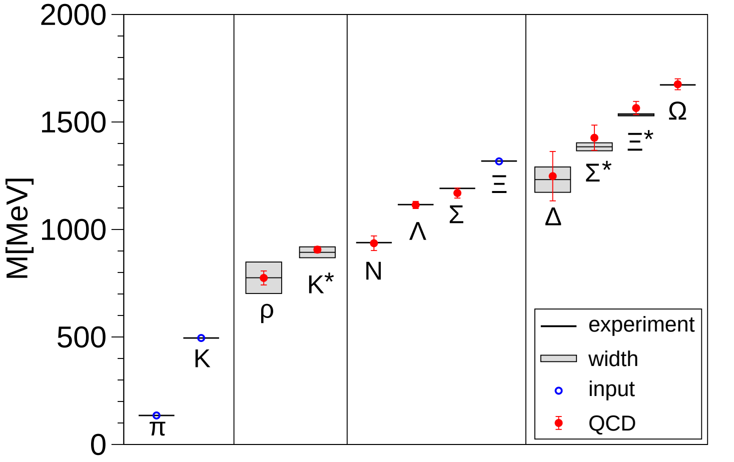


FACETS of STRUCTURE FORMATION in QCD

- quarks and gluons form hadrons

  ⇒ **lattice QCD**

  ⇒ exploring the strong color force

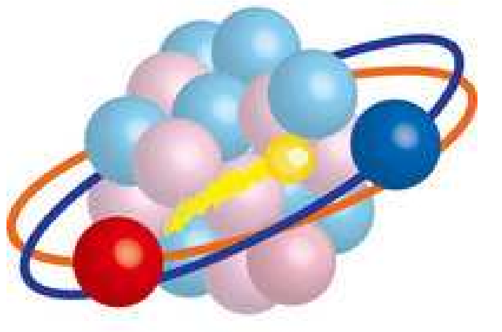


BMW collaboration and others

- nucleons and mesons form nuclei

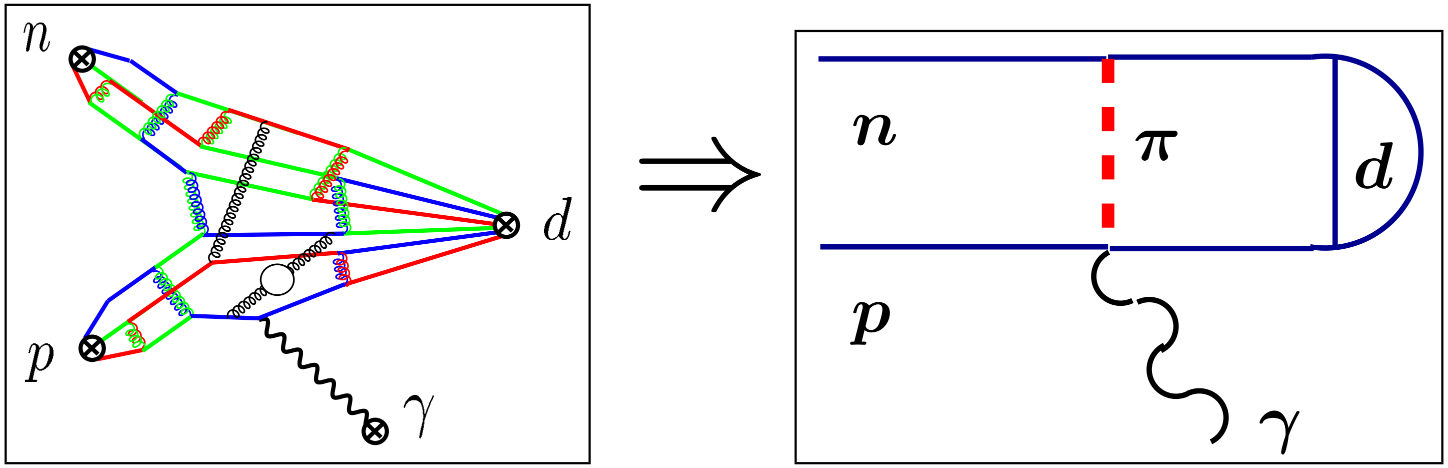
  ⇒ **nuclear physics**

  ⇒ exploring the residual color force



RESIDUAL CHROMODYNAMIC FORCES

- Quarks and gluons are confined within hadrons
- Nuclear forces are the residual forces between colorless objects
- Hadronic energies correspond to a low resolution microscope
- $np \to d\gamma$



wrong d.o.f.s　　　　right d.o.f.s

BASIC FACTS

- At nuclear lengths scales, hadrons are the relevant degrees of freedom (dofs)

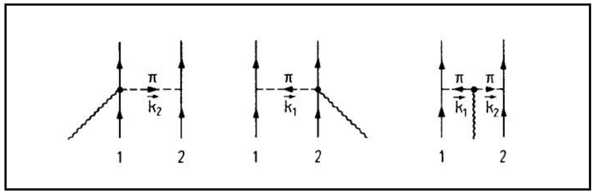
  Ex: Deuteron break-up with 2 MeV photons: $\gamma + d \to n + p$

- Nuclei are made of protons and neutrons & virtual mesons

  Ex: Pion-exchange currents required to get

  the proper $\sigma_{\rm tot}(\gamma + d \to n + p)$

  Brown, Riska, Gari, ...

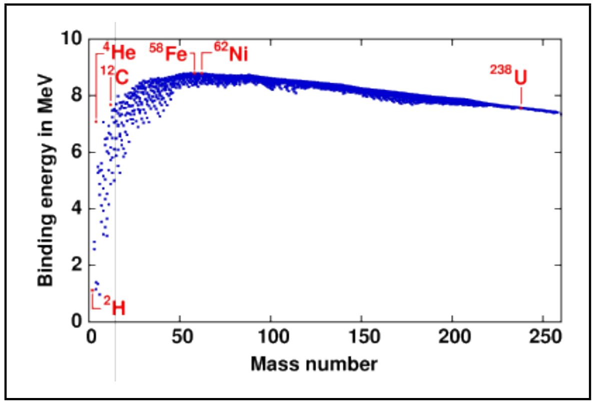


- Nuclear binding energies $\ll$ nuclear masses

  $\to$ non-relativistic problem

  Exercise: average momentum in a nucleus

  with $R = 1.3 A^{1/3}$ fm [hint: Heisenberg]



$\to$ can solve the nuclear A-body problem w/ the Schrödinger equation

BASIC FACTS cont'd

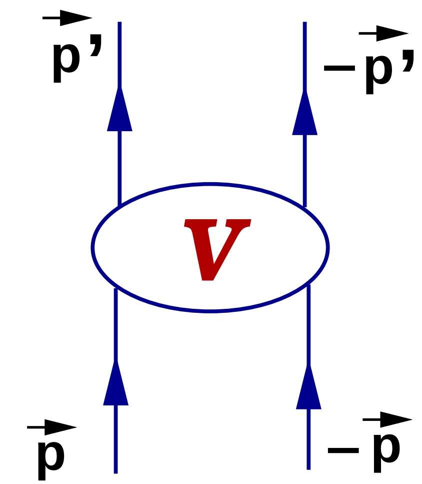
- Nuclear A-body problem w/ the Schrödinger equation

$$
\begin{aligned}
H\Psi_A &= E_A\Psi_A \\
H &= T + V = \sum_A \frac{p_A^2}{2m_N} + V \\
V &= V_{NN} + V_{3N} + V_{4N} + \ldots
\end{aligned}
$$

- Input: V_{NN} from pp and np phase shift analysis
- high precision nucleon-nucleon potentials (CD-Bonn, Nijm I,II, AV18, ...)
- Further input: V_{3N} small, from phenomenological fits/models
- Ab initio calculations based on this are astonishingly precise

Glöckle, Nogga, Witala, Carlson, Phandaripande, Pieper, Wiringa, ...

THE TWO-NUCLEON FORCE: FUNDAMENTALS



- One-pion exchange as the longest range interaction (Yukawa 1935)

$$V_{1\pi}(\vec{q}\,) \propto \vec{\tau}_1 \cdot \vec{\tau}_2 \frac{\vec{\sigma}_1 \cdot \vec{q}\,\vec{\sigma}_2 \cdot \vec{q}}{\vec{q}^{\,2} + M_\pi^2}\,, \quad \vec{q} = \vec{p}\,' - \vec{p}$$

- Parameterize the shorter-range terms in the most general way

available vectors $\vec{\sigma}_1, \vec{\sigma}_2, \vec{q}, \vec{k} = (\vec{p} + \vec{p}\,')/2$ and isovectors $\vec{\tau}_1, \vec{\tau}_2$

$\rightarrow$ hermiticity, isospin conservation, invariance under rotations, space reflection and time reversal yields 10 structures

$$\{1,\ \ \vec{\sigma}_1\cdot\vec{\sigma}_2,\ \ i(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{q}\times\vec{k},\ \ \vec{\sigma}_1\cdot\vec{q}\,\vec{\sigma}_2\cdot\vec{q},\ \ \vec{\sigma}_1\cdot\vec{k}\,\vec{\sigma}_2\cdot\vec{k}\,\} \otimes \{1, \vec{\tau}_1\cdot\vec{\tau}_2\}$$

times scalar functions, to be obtained from a fit to data

- so-called “high-precision” potentials (AV18, CD Bonn, NijmI/II, Reid93)
  - nearly perfect description of pp and np data below ~ 350 MeV
  - need typically about 40 -50 parameters

THE TWO-NUCLEON FORCE: PARTIAL WAVES

- Partial wave basis: $|\vec{p}\rangle \to |p\ell m_\ell\rangle$
- Two-nucleon state: $|p(\ell s)jm_j\rangle$
- Spectroscopic notation: $^{2S+1}L_J$

S = total spin (0,1) (singlet, triplet)
L = angular momentum (0,1,2,...)
$L = 0$ S-wave, $L = 1$ P-wave, $L = 2$ D-wave, ...
$J = L + S$ = total ang. momentum (0,1,2,...)

- Partial-wave decomposition of the potential:

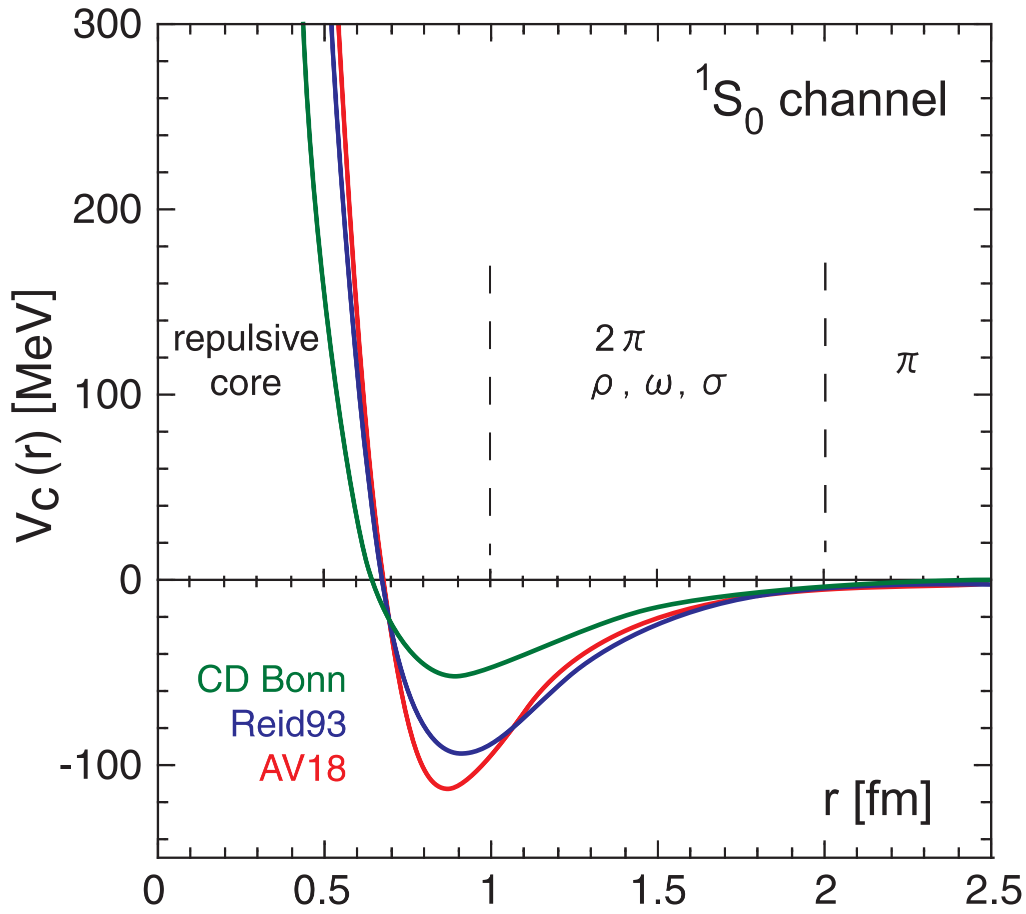
$$\langle p'(l's')j'm_j'|V|p(ls)jm_j\rangle \equiv \delta_{j'j}\delta_{m_j'm_j}\delta_{s's}\, V^{sj}_{l'l}(p',p)$$

$$V^{sj}_{l'l}(p',p) = \sum_{m_l',m_l}\int d\hat{p}'d\hat{p}\,\langle l',m_l';s,m_j-m_l'|j,m_j\rangle\langle l,m_l;s,m_j-m_l|j,m_j\rangle$$
$$\times\; Y^*_{l',m_l'}(\hat{p}')Y_{l,m_l}(\hat{p})\,\langle s(m_j-m_l')|V(\vec{p}',\vec{p})|s(m_j-m_l)\rangle$$

- Exercise: derive the partial-wave S-matrix for uncoupled and coupled channels
- hint: spin-singlet waves are uncoupled, spin-triplet waves are coupled

THE CENTRAL NN POTENTIAL

• consider the central potential ($\mathbf{1} \otimes \mathbf{1}$) in the spin-singlet, S-wave $^1S_0$



• universal features:

long-range one-pion exchange

intermediate-range attraction

short-range repulsion

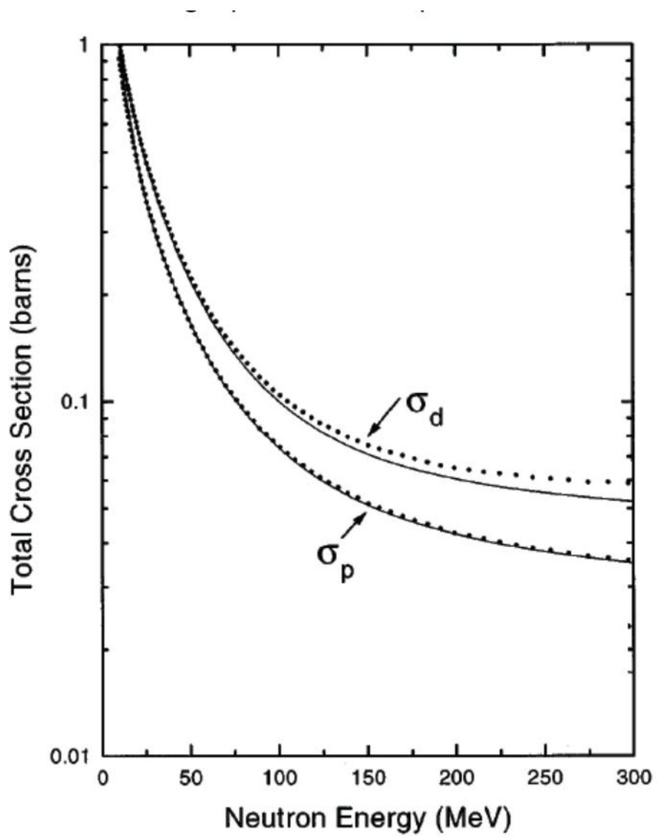
• note, however:

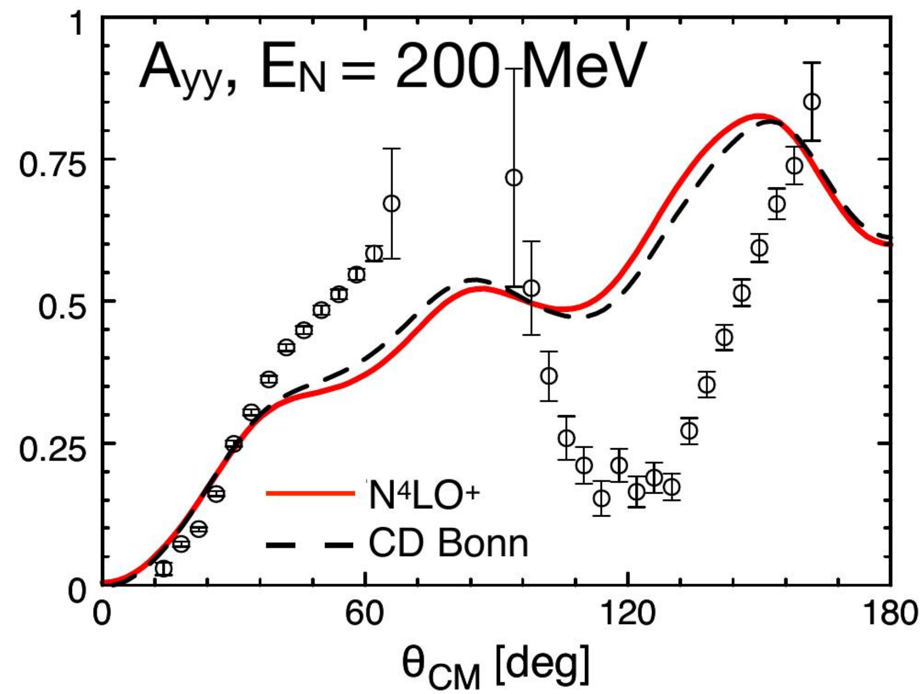
potential is **not an observable**

short-range physics is representation dependent

INDICATIONS of 3-NUCLEON FORCES

- Use high-precision NN potentials → explore three-particle systems
- Perform numerically exact calculations (here: Faddeev-Yakubowsky)
- Total XS for np and nd scattering
- Tensor analying power in Nd scattering



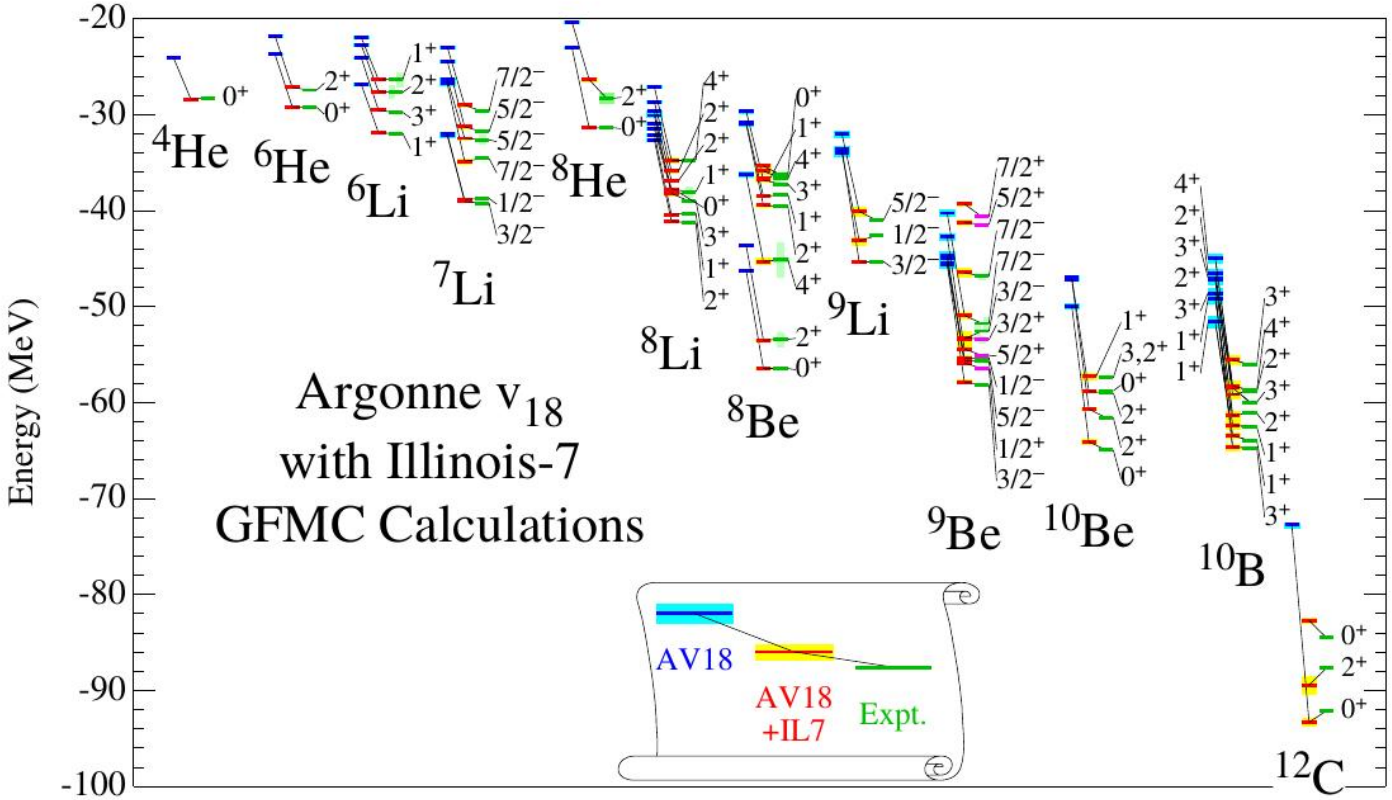


Abfalterer et al., Phys. Rev. Lett. **81** (1998) 57   E. Epelbaum, priv. comm.

QUANTUM MC CALCULATIONS OF NUCLEI

J. Carlson et al., Rev. Mod. Phys. **87** (2015) 1067

- large numerical effort



- a small three-nucleon force is needed!

- but the 2NF and 3NF are not consistent

OPEN ENDS

- Why is there this hierarchy $\boxed{V_{2N} \gg V_{3N} \gg V_{4N}}$?
- Gauge and chiral symmetries difficult to include (meson-exchange currents)

Brown, Riska, Gari, . . .

- Connection to QCD ?

most models have one-pion-exchange, but not necessarily respect chiral symmetry

some models have two-pion exchange reconstructed via dispersion relations from $\pi N \to \pi N$

$\Rightarrow$ We want an approach that

– is linked to QCD via its symmetries
– allows for systematic calc's with a controlled theoretical error
– explains the observed hierarchy of the nuclear forces
– matches nucleon structure to nuclear dynamics
– allows for a lattice formulation / chiral extrapolations
– puts nuclear physics on a sound basis

THE NUCLEAR LANDSCAPE: AIMS & METHODS

- Theoretical methods:

– Lattice QCD: A = 0,1,2, . . . → Detmold, Aoki

– NCSM, Faddeev-Yakubowsky, GFMC, ... :
A = 3 - 16

– coupled cluster, . . .: A = 16 -100

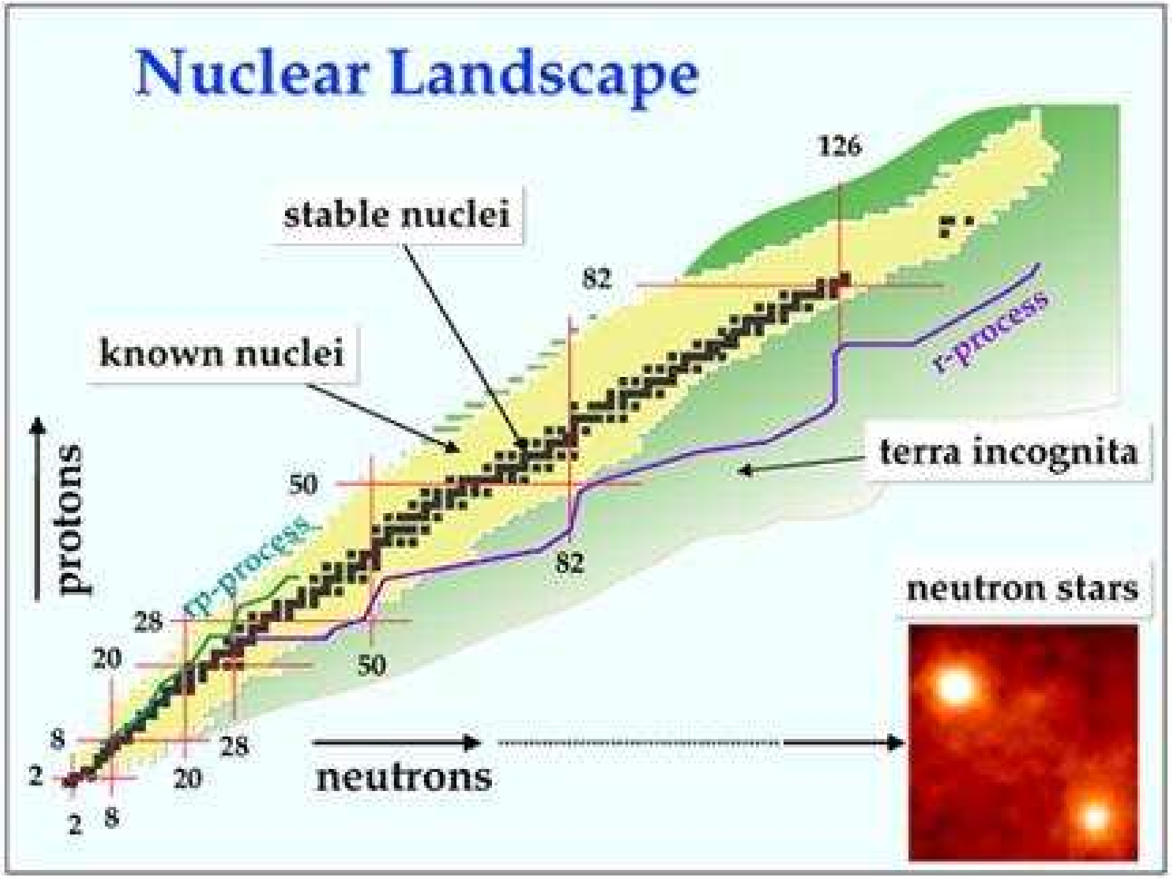
– density functional theory, . . .: $A \geq 100$

- Chiral EFT:

– provides **accurate 2N, 3N and 4N forces**

– successfully applied in light nuclei with A = 2, 3, 4

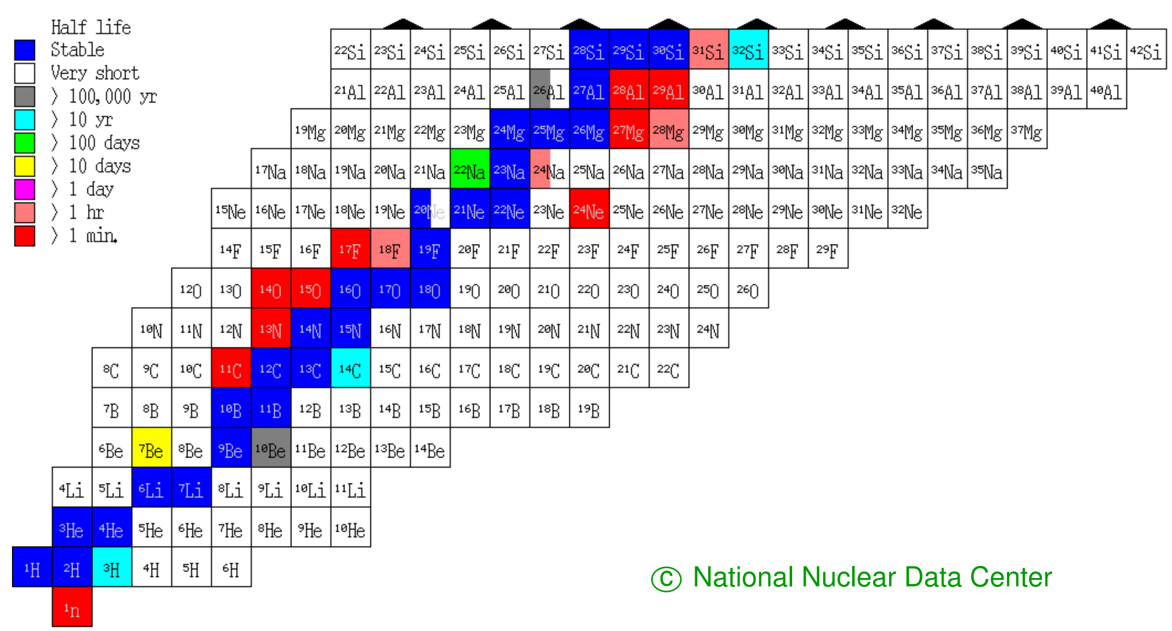
– combine with simulations to get to larger A



⇒ Nuclear Lattice Effective Field Theory

AB INITIO NUCLEAR STRUCTURE and SCATTERING

- Nuclear structure:
  - ⋆ 3-nucleon forces
  - ⋆ limits of stability
  - ⋆ alpha-clustering
  - ⋮



- Nuclear scattering: processes relevant for nuclear astrophysics
  - ⋆ alpha-particle scattering: $^4\mathrm{He} + {^4\mathrm{He}} \to {^4\mathrm{He}} + {^4\mathrm{He}}$
  - ⋆ triple-alpha reaction: $^4\mathrm{He} + {^4\mathrm{He}} + {^4\mathrm{He}} \to {^{12}\mathrm{C}} + \gamma$
  - ⋆ alpha-capture on carbon: $^4\mathrm{He} + {^{12}\mathrm{C}} \to {^{16}\mathrm{O}} + \gamma$
  - ⋮

MANY–BODY APPROACHES

- nuclear physics = notoriously difficult problem: strongly interacting fermions

- define *ab initio*: combine the precise and well-founded forces from *chiral EFT* with a many-body approach

- two different approaches followed in the literature:

  ⋆ combine chiral NN(N) forces with standard many-body techniques

  Dean, Hagen, Navratil, Nogga, Papenbrock, Schwenk, . . .

  $\longrightarrow$ successful, but problems with cluster states (SM, NCSM,...)

  ⋆ combine chiral forces and lattice simulations methods

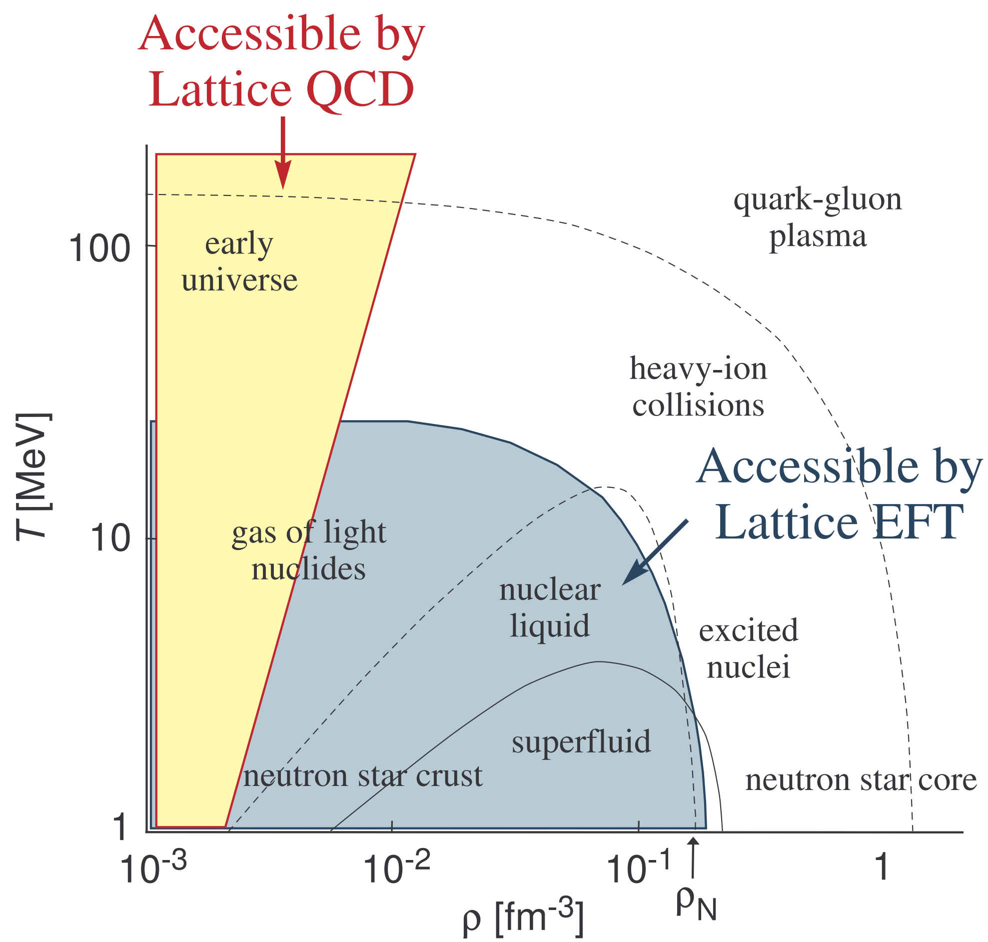
  $\longrightarrow$ this new method is called *nuclear lattice EFT* (NLEFT)

  Borasoy, Epelbaum, Krebs, Lee, Lähde, UGM, Rupak, . . .

  $\longrightarrow$ rest of the lectures

COMPARISON to LATTICE QCD

LQCD	NLEFT
relativistic fermions	non-relativistic fermions
renormalizable th'y	EFT
continuum limit	no continuum limit
(un)physical masses	physical masses
Coulomb - difficult	Coulomb - easy
high T/small ρ	small T/nuclear densities
sign problem severe	sign problem moderate



- similar methods:
  hybrid MC, parallel computing, . . .
  ↪ not treated here

- what I want to discuss within the time limitations:
  - ↪ how to put the chiral EFT on a lattice
  - ↪ scattering on a lattice (**not** the Lüscher approach)
  - ↪ show some assorted results & give some outlook

Chiral EFT in the continuum: A crash-course

for an intro, see: Epelbaum, Prog. Part. Nucl. Phys. **57** (2006) 654

for a review, see: Epelbaum, Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773

A TOY MODEL

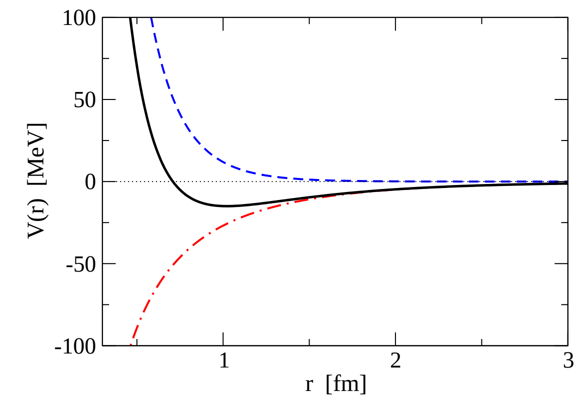
- Consider a toy model with light & heavy boson exchanges

$$V(\vec{q}) = \frac{\alpha_l}{\vec{q}^{\,2} + M_l^2} + \frac{\alpha_h}{\vec{q}^{\,2} + M_h^2} \rightarrow V(\vec{r}) = \underbrace{\frac{\alpha_l}{4\pi r}\mathrm{e}^{-M_l r}}_{\text{long-range}} + \underbrace{\frac{\alpha_h}{4\pi r}\mathrm{e}^{-M_h r}}_{\text{short-range}}$$

– $M_l = 200$ MeV , $M_h = 750$ MeV

– $\alpha_l = -1.5$, $\alpha_h = 10.81$ [attractive, repulsive]

→ S-wave bound state: $E_B = 2.2229$ MeV



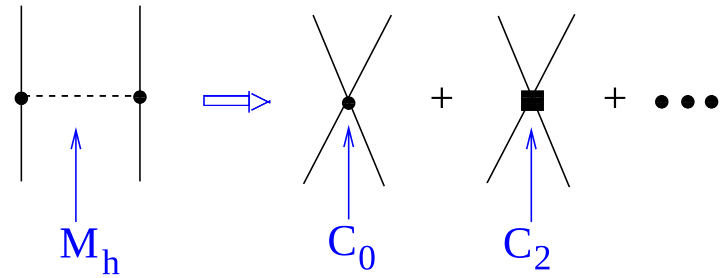
- Effective theory

– at low energy $q \sim M_l \ll M_h$, structure of short-distance potential irrelevant

– represent short-range potential by a series of contact interactions

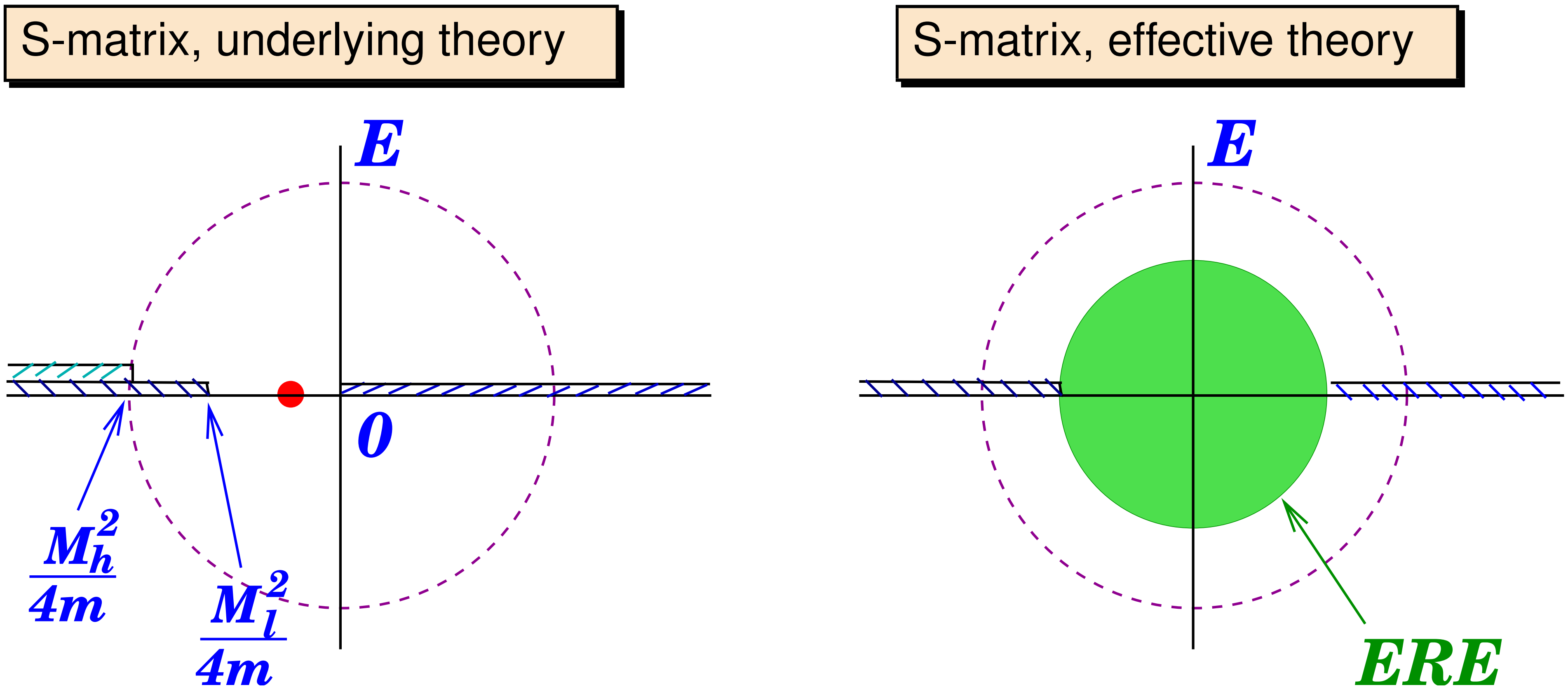
$$\rightarrow \boxed{V_{\rm eff} = V_{\rm long-range} + C_0 + C_2(\vec{p}^{\,2} + \vec{p}^{\,\prime 2}) + \ldots}$$

corresponding to $\frac{1}{M_h^2 - q^2} = \frac{1}{M_h^2} - \frac{q^2}{M_h^4} + \ldots$



TOY MODEL cont'd

- Expectations:



- should work for momenta $|k| \leq \frac{M_h}{2} = 375$ MeV (or $E_{\rm lab} \leq \frac{M_h^2}{2m} \sim 300$ MeV)
- should go beyond the ERE, converges for $|k| \leq \frac{M_l}{2} = 100$ MeV (or $E_{\rm lab} \leq \frac{M_l^2}{2m} \sim 20$ MeV)

[ERE = effective range expansion]

TOY MODEL cont'd

- T-matrix of the effective theory:

weak interaction $|\alpha_{l,h}| \ll 1: \quad \langle f|T|i\rangle \simeq \langle f|V_{\rm eff}|i\rangle$

strong interaction $|\alpha_{l,h}| \geq 1: \quad \langle f|T|i\rangle = \langle f|V_{\rm eff}|i\rangle + \sum_n \frac{\langle f|V_{\rm eff}|n\rangle\langle n|V_{\rm eff}|i\rangle}{E_i - E_n + i\epsilon} + \ldots$

sum diverges, high-momentum physics $\to$ introduce UV cutoff Λ: $M_l \ll \Lambda \sim M_h$

- Fix the $C_i(\Lambda)$ from some low-energy data $\to$ make predictions

- use e.g. the ERE: $k\cot\delta(k) = -\frac{1}{a} + \frac{1}{2} r k^2 + v_2 k^4 + v_3 k^6 + \ldots$

LO: $V_{\rm eff} = V_{\rm long} + C_0 f_\Lambda(p,p') \longrightarrow C_0 \text{ from } a \quad [f_\Lambda(p,p') = \exp(-(p^2+p'^2)/\Lambda^2)]$

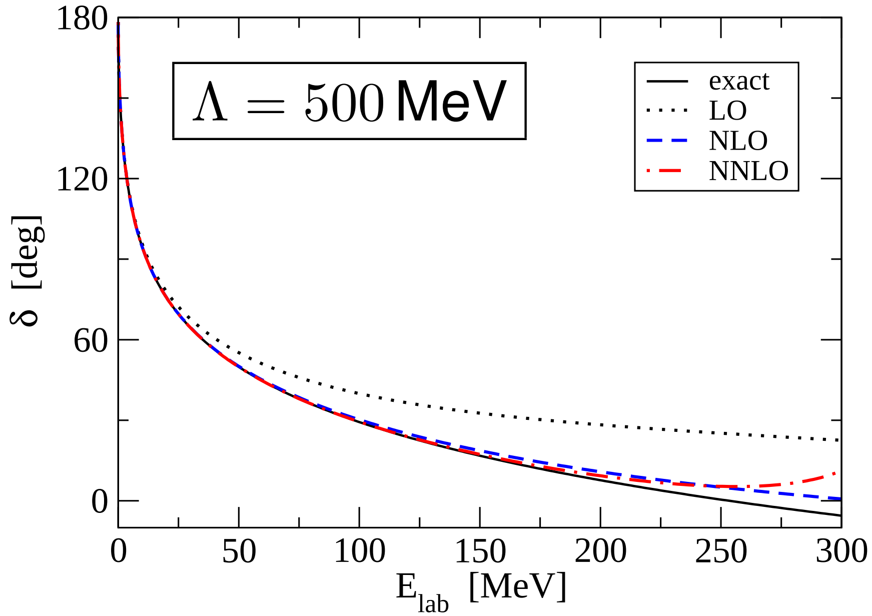
NLO: $V_{\rm eff} = V_{\rm long} + \left[C_0 + C_2(p^2+p'^2)\right] f_\Lambda(p,p') \longrightarrow C_0, C_2 \text{ from } a, r$

NNLO: $V_{\rm eff} = V_{\rm long} + \left[C_0 + C_2(p^2+p'^2) + C_4 p^2 p'^2\right] f_\Lambda(p,p')$

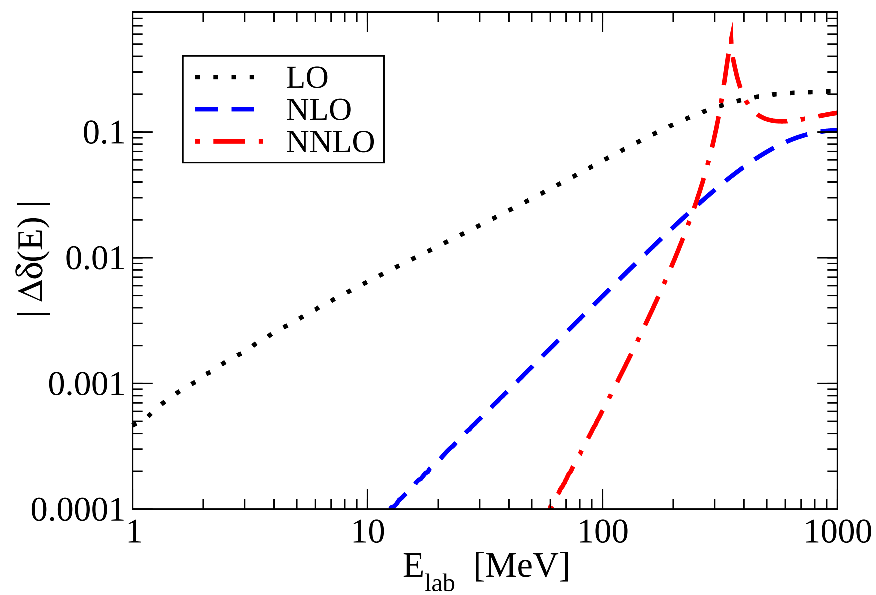
$\longrightarrow C_0, C_2, C_4 \text{ from } a, r, v_2$

TOY MODEL: RESULTS

- Phase shift



- relative error



- error at order n: $\Delta\delta(k) \sim (k/\tilde{\Lambda})^{2n}$, $\tilde{\Lambda} \sim 400$ MeV

  agrees with $\tilde{\Lambda} \sim M_h/2$ [breakdown scale]

- results for the bound state: $E_B = \underbrace{2.1594}_{\text{LO}} + \underbrace{0.0638}_{\text{NLO}} - \underbrace{0.0003}_{\text{NNLO}} = 2.2229$ MeV

TOY MODEL: LESSONS

- Incorporate the *correct long-range force*
- Represent short-range physics by local contact interactions in $\boldsymbol{V}_{\mathbf{eff}}$, respect symmetries
- Introduce an UV cut-off Λ (large enough but not neccessarily ∞)
- Fix LECs from some (low-energy) data and make predictions

$\Rightarrow$ At low energies model-independent and systematically improvable!

- for more details see:

  G.P. Lepage, “How to renormalize the Schrödinger equation”, nucl-th/9706029
- Let’s tackle this from an EFT point of view

EFFECTIVE FIELD THEORY in a NUTSHELL

Weinberg, Gasser, Leutwyler, ...

- Rules to construct an EFT:

> - *scale separation* – what is low, what is high?
> - *active degrees of freedom* – what are the building blocks?
> - *symmetries* – how are the interactions constrained by symmetries?
> - *power counting* – how to organize the expansion in low over high?

- QCD with light quarks (up, down):

$\rightarrow$ low scale $\sim M_\pi \ll$ high scale $\sim M_\rho$

$\rightarrow$ DOFs: pions = Goldstone bosons, nucleons, ... $\rightarrow$ validates Yukawa

$\rightarrow$ **broken chiral symmetry**, PCT, Lorentz, ...

$\rightarrow$ Amp $\sim q^\nu$, $\nu = 4 - N + 2(L - C) + \sum_i V_i \Delta_i$

SCALES IN NUCLEAR PHYSICS

- Natural scales (Yukawa, 1935; QCD)

Long-range one-pion-exchange interaction: $\boldsymbol{\lambda_\pi = 1/M_\pi \simeq 1.5}$ fm

Intermediate range attraction (mostly 2π exchange)

Nucleons don't like to touch, short-distance repulsion $(R \simeq 0.8$ fm)

- But: nuclei exhibit UNNATURAL scales

Large S-wave scattering lengths:

$$\boldsymbol{a_{np}(^1S_0) = -23.8\,\text{fm}\;,\;\; a_{np}(^3S_1) = 5.4\,\text{fm} \gg 1/M_\pi}$$

NB: effective ranges are of natural size

Shallow nuclear binding:

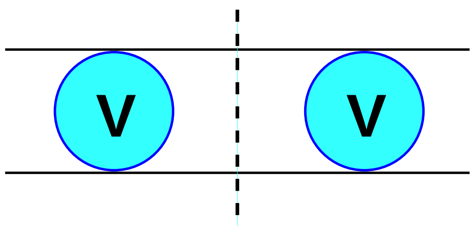
$$\boldsymbol{\gamma = \sqrt{E_D m_N} = 45\,\text{MeV} \ll M_\pi} \quad (\boldsymbol{E_D = 2.22}\,\text{MeV})$$

$\Rightarrow$ the corresponding EFT requires a non-perturbative resummation

CALCULATIONAL SCHEME

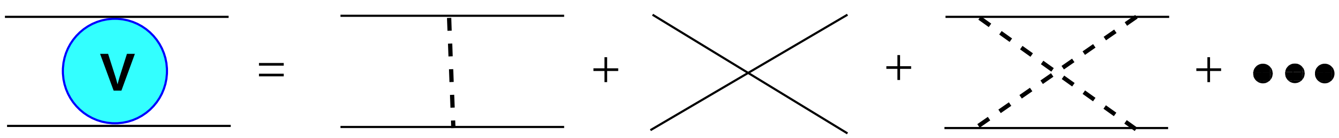
S. Weinberg, Nucl. Phys. **B 363** (1991) 3

- No perturbative description for bound states



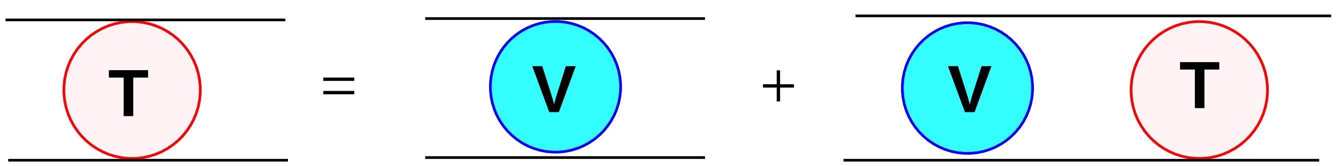
$\Rightarrow$ NN cuts violate perturbative power counting

- Effective potential can be constructed **perturbatively** from chiral EFT



- Solve **non-perturbative** Lippmann-Schwinger/Schrödinger equation

  (requires regularization)



- check convergence for observables *a posteriori*

LIPPMANN-SCHWINGER EQUATION

- compact operator form

$$\boxed{T = V + VG_0T} \qquad G_0 = \text{free two-nucleon propagator}$$

- partial wave representation = projection onto states with orbital angular momentum l, total spin s and total angular momentum j

$$T^{sj}_{l',l}(p',p) = V^{sj}_{l',l}(p',p) + \sum_{l''} \int_0^\infty \frac{dp''(p'')^2}{(2\pi)^3} V^{sj}_{l',l''}(p',p'') \frac{2\mu}{p^2 - p''^2 + i\eta} T^{sj}_{l'',l}(p'',p)$$

  – sometimes also relativistic kinematics used (for comparison w/ PWA)

  – potential also projected on the partial waves

  – potential requires UV regularization $\boxed{V(p,p') \to f_R(p)V(p,p')f_R(p')}$

  – best regulator function: $f_R(\vec{p}^{\,2}) = \exp(-(\vec{p}^{\,2} + M_\pi^2)/\Lambda^2)$

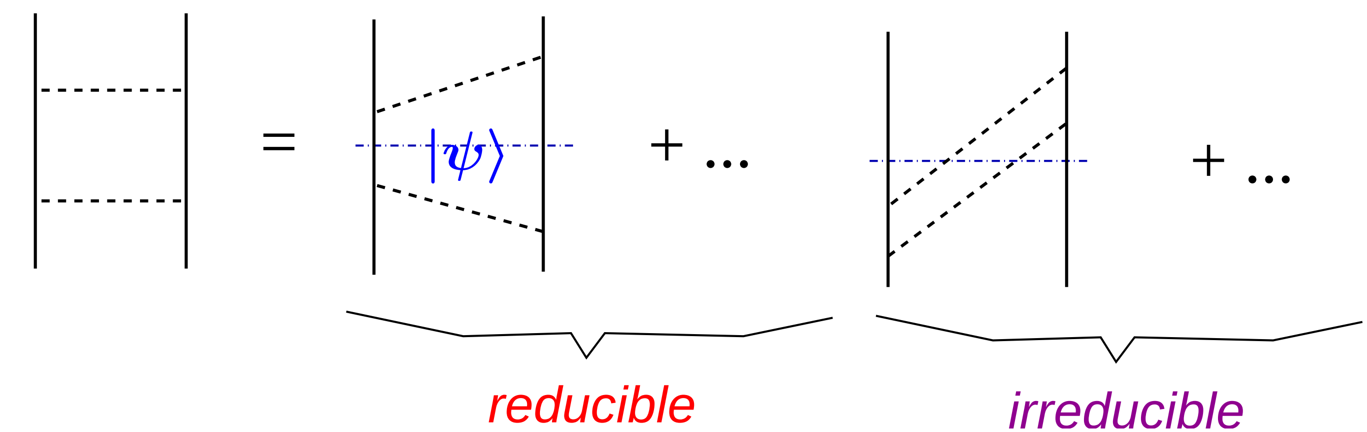
Rijken (1991), Reinert, Epelbaum, Krebs (2017)

  – cut-off Λ to be determined later in the fit

FAILURE of PERTURBATION THEORY

- Enhancement caused by reducible diagrams (IR divergent in the static limit)
- consider time-ordered perturbation theory (let Q be a small parameter)

$$Amp = \langle NN|H_I|NN\rangle + \sum_\psi \frac{\langle NN|H_I|\psi\rangle\langle\psi|H_I|NN\rangle}{E_{NN}-E_\psi} + \ldots$$

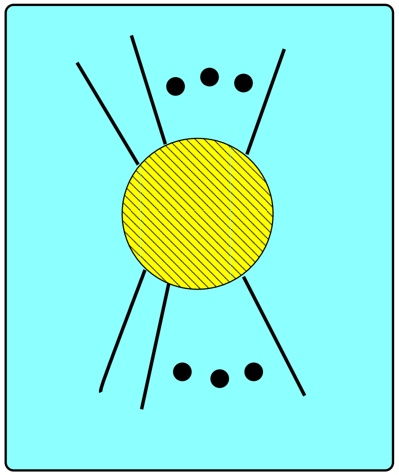


$$\frac{1}{E_{NN}-E_\psi} = \frac{2m_N}{\vec{p}^{\,2}-\vec{q}^{\,2}} \underbrace{\sim \frac{m_N}{Q^2} \gg \frac{1}{Q}}_{\text{enhanced}}\,, \quad \frac{1}{E_{NN}-E_\psi} \underbrace{\sim \frac{1}{M_\pi} \sim \frac{1}{Q}}_{\text{expected}}$$

POWER COUNTING for the EFECTIVE POTENTIAL

Weinberg, Rho, van Kolck, Epelbaum, . . .,

- N-nucleon interactions receives contributions $\sim (Q/\Lambda)^\nu$: (with Q the small momentum/mass)



$$\nu = -2 + 2N + 2(L - C) + \sum_i V_i \Delta_i$$

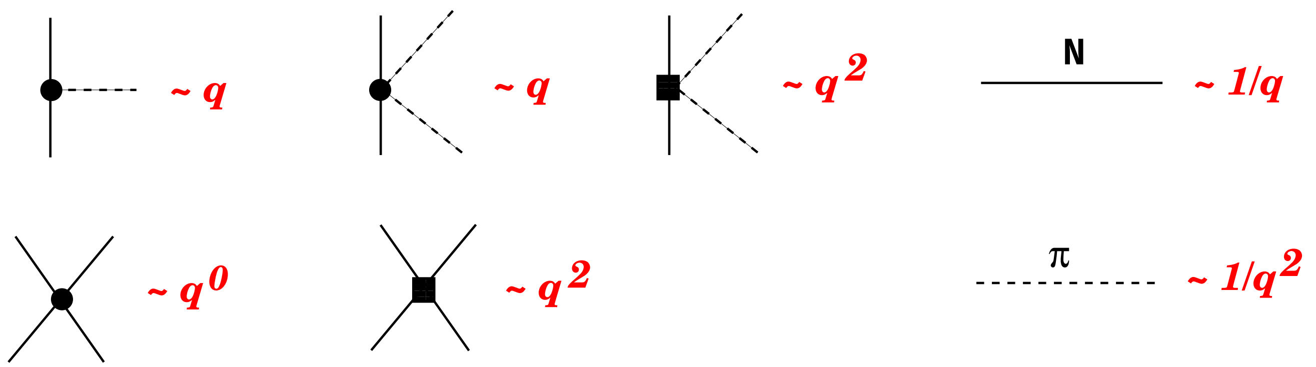
  – N = number of nucleon fields (in- & out-states)
  – L = number of pion loops
  – C = number of connected pieces
  – V_i = number of vertices with the vertex dimension $\Delta_i = d_i + \frac{1}{2} n_i - 2$
    – d_i = number of derivatives or pion mass insertions at the vertex i
    – n_i = number of nucleon fields at the vertex i
    – external sources & virtual photons can easily be included

- central observation: Δ_i (ν) is bounded from below because of chiral symmetry

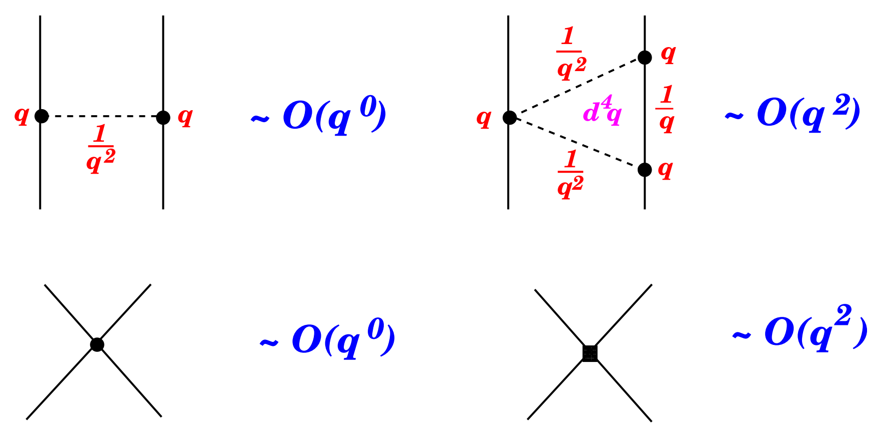
- LO vertices have $\Delta_i = 0 \Rightarrow \nu_{\rm min} = 0$

POWER COUNTING: EXAMPLES

Vertices ***Propagators***



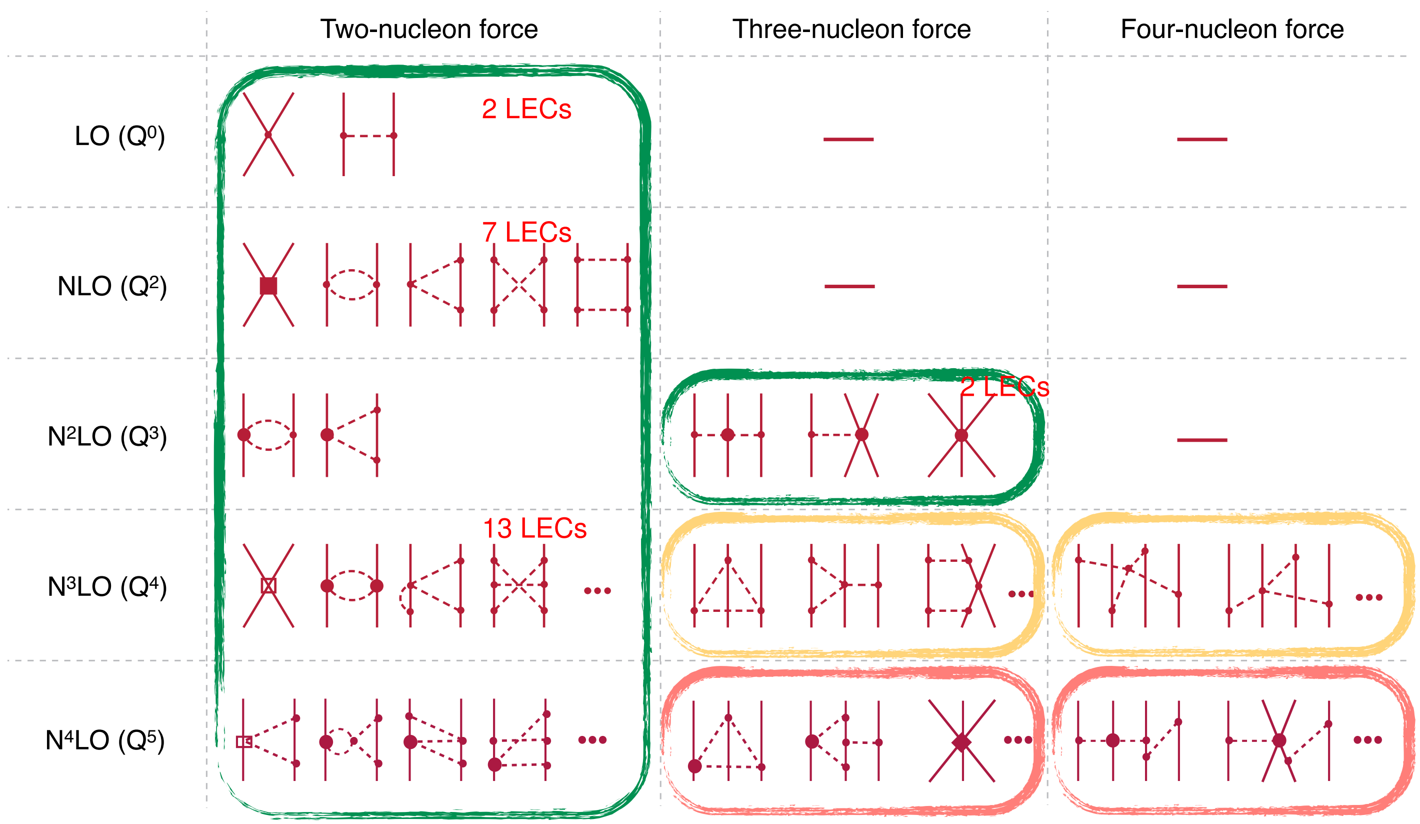
- Examples



NUCLEAR FORCES in CHIRAL NUCLEAR EFT

- expansion of the potential in powers of Q [small parameter]: $\{p/\Lambda_b,\, M_\pi/\Lambda_b\}$
- explains observed hierarchy of the nuclear forces
- extremely successful in few-nucleon systems

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



worked out and applied   worked out and to be applied   calculations in progress

STRUCTURE of the NN POTENTIAL

- LO: one-pion-exchange (OPE) plus contact interactions w/o derivatives **2 LECs**

$$V^{(0)} = -\left(\frac{g_A}{2F_\pi}\right)^2 \vec{\tau}_1 \cdot \vec{\tau}_2 \, \frac{\vec{\sigma}_1 \cdot \vec{q}\, \vec{\sigma}_2 \cdot \vec{q}}{q^2 + M_\pi^2} + C_S + C_T \, \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

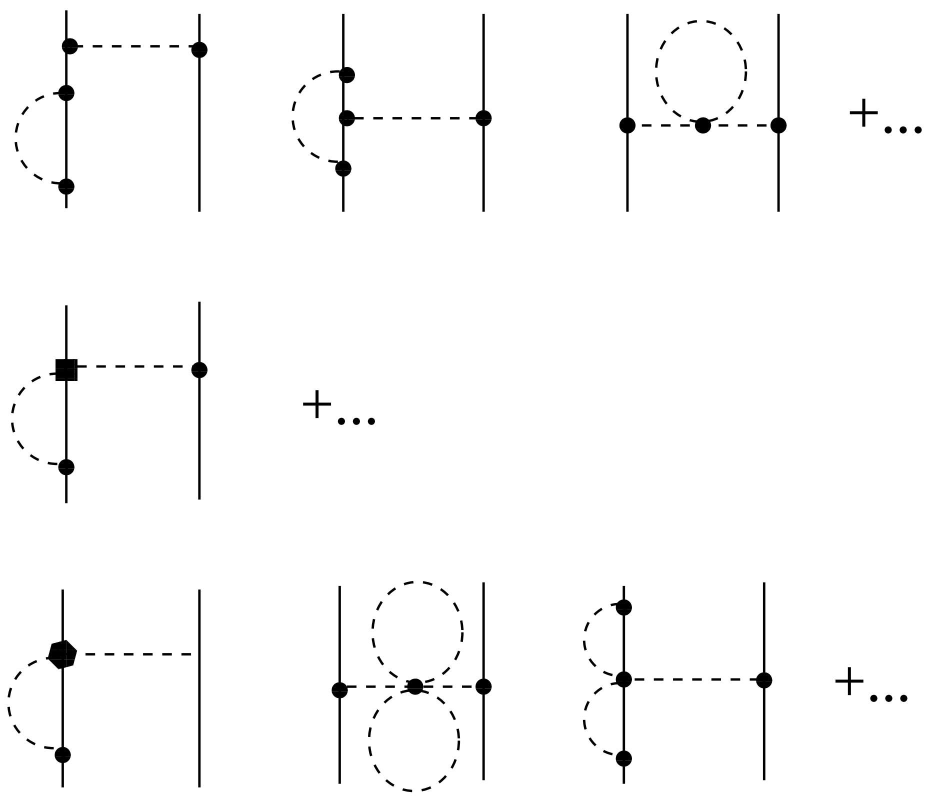
- NLO: renormalization of the one-pion-exchange (OPE)
  plus leading two-pion exchange (TPE)
  plus renormalization of the leading contact interactions
  plus contact interactions w/ 2 derivatives **7 LECs**

- $\mathrm{N^2LO}$: further renormalization of the one-pion-exchange (OPE)
  plus subleading two-pion exchange (TPE) ($\sim$ LECs c_i of the πN sector)

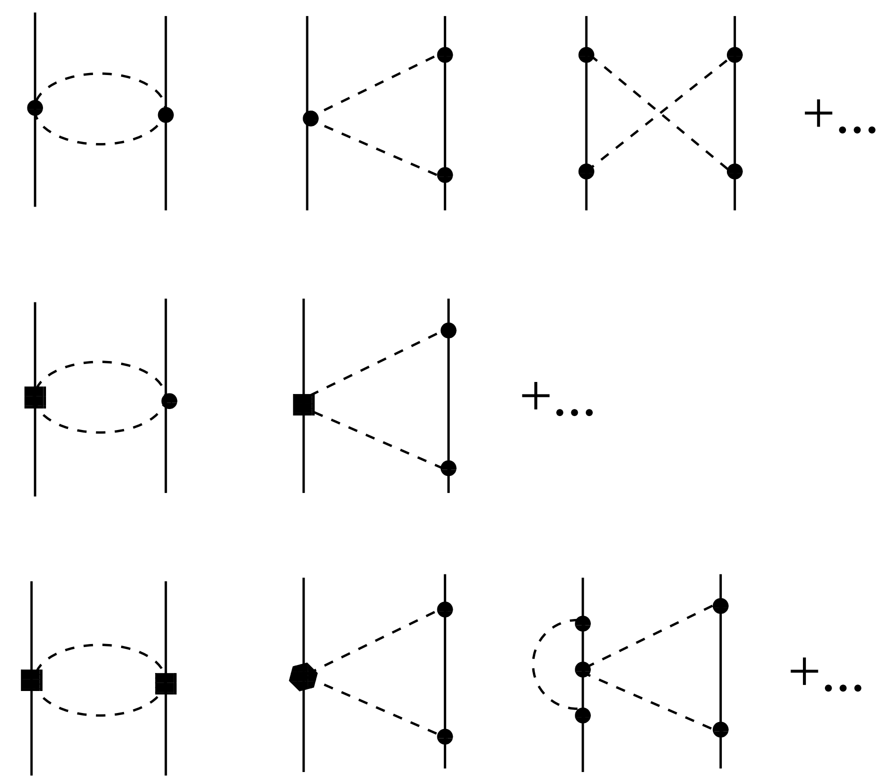
- $\mathrm{N^3LO}$: further renormalization of the one-pion-exchange (OPE)
  plus sub-subleading two-pion exchange (TPE)
  plus leading three-pion exchange (TPE) **(very small)** Kaiser 2000
  plus renormalization of dim. two contact interactions
  plus contact interactions w/ 4 derivatives **13 LECs**

TYPICAL DIAGRAMS

- renormalization of OPEP



- TPEP

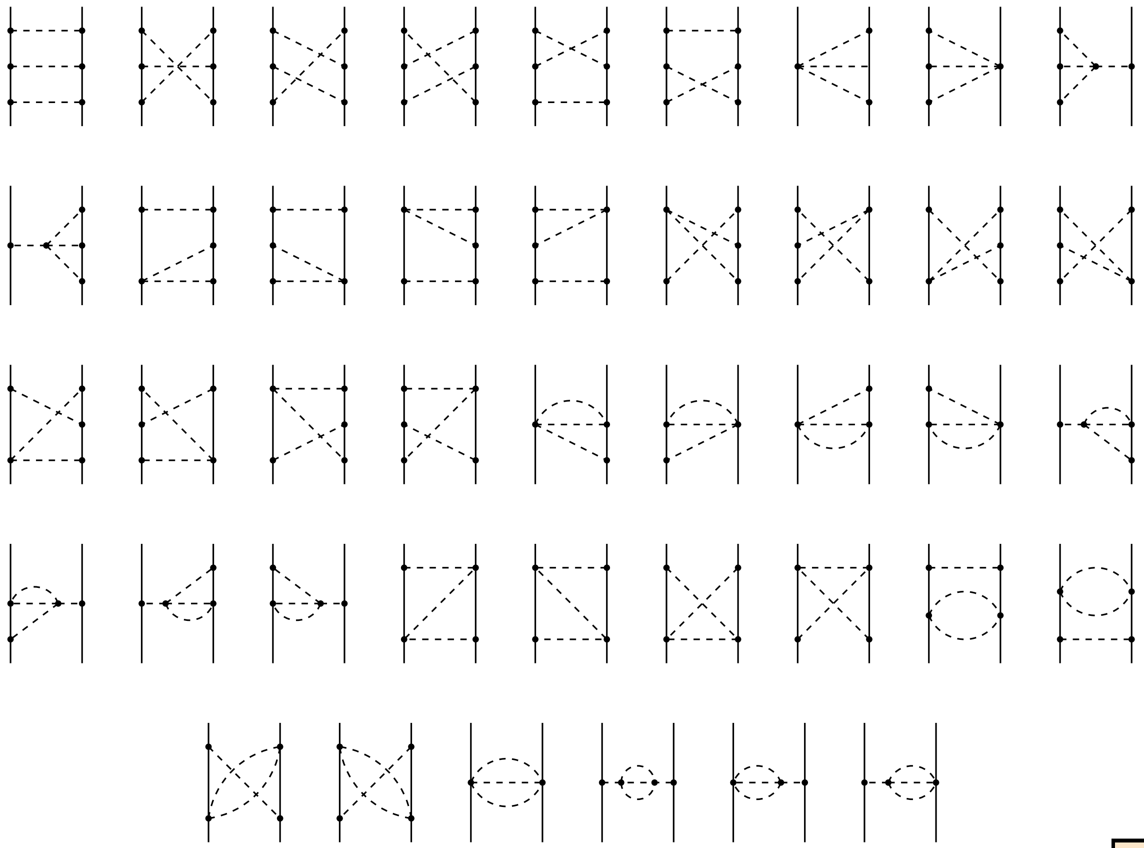


● *dim. 1* ■ *dim. 2* ⬢ *dim. 3*

TYPICAL DIAGRAMS continued

Kaiser, Phys. Rev. C **61** (2000) 014003; C **62** (2000) 024001; C **63** (2001) 044010

- three-pion exchange (starts at N^{3}LO)



$\Rightarrow$ insignificant for $r \geq 1$ fm

SHORT-DISTANCE STRUCTURE of the POTENTIAL

- consider chiral 2π potential $\propto g_A^4$

$$V_{2\pi}^{(2)} = \frac{g_A^4}{32F_\pi^4} \int \frac{d^3l}{(2\pi)^3} \frac{\omega_+^2 + \omega_+\omega_- + \omega_-^2}{\omega_+^3\omega_-^3(\omega_+ + \omega_-)} \left\{ \tau_1^a\tau_2^a \left(\vec{l}^{\,2} - \vec{q}^{\,2}\right)^2 + 6\sigma_1^i(\vec{q}\times\vec{l})^i\,\sigma_2^j(\vec{q}\times\vec{l})^j \right\}$$

with $\omega_\pm = \sqrt{(\vec{q}\pm\vec{l})^2 + 4M_\pi^2}$

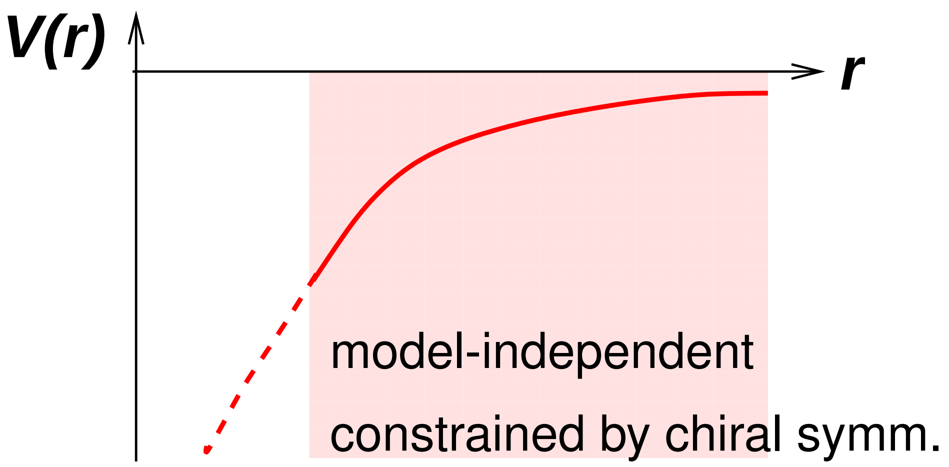
- log and quadratic divergences, absorb in short-range counterterms

$$V_{\rm cont} = (\alpha_1 + \alpha_2\, q^2)\vec{\tau}_1\cdot\vec{\tau}_2 + \alpha_3\,\vec{\sigma}_1\cdot\vec{q}\,\vec{\sigma}_1\cdot\vec{q} + \alpha_4\, q^2\,\vec{\sigma}_1\cdot\vec{\sigma}_2$$

- co-ordinate space representation

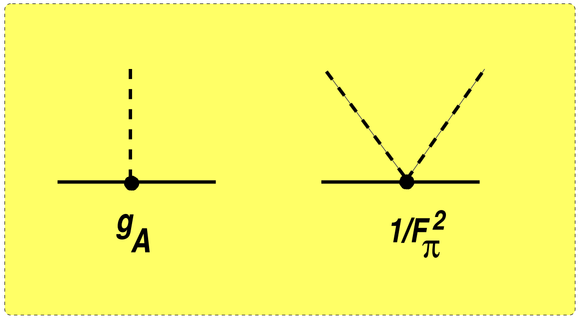
$$V_{2\pi}^{(2)}(q) \to V_{2\pi}^{(2)}(r)$$

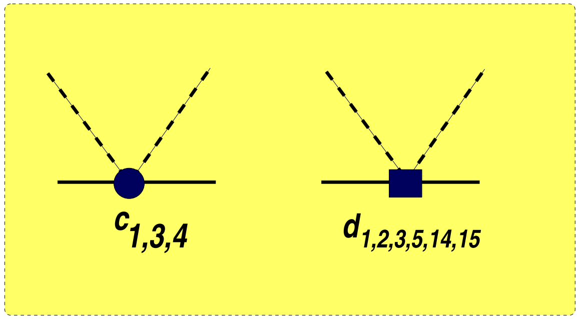
the large-r (long-range) behaviour is uniquely defined and does not depend on the regularization



LOW-ENERGY CONSTANTS

- Pion-nucleon system:





— g_A and F_π precisely known (chiral symmetry)

— dimension 2 & 3 couplings c_i & d_i known

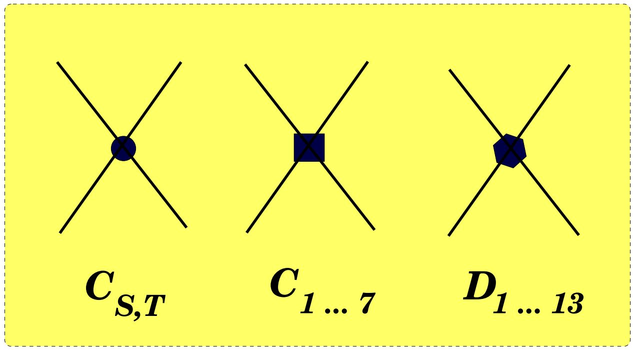
from Roy-Steiner analysis of $\pi N \to \pi N$

Hoferichter, Ruiz de Elvira, Kubis, UGM, Phys. Rept. 625 (2016) 1

— physics understood: resonance saturation

Bernard, Kaiser, UGM, Nucl. Phys. A615 (1997) 483

- Nucleon-nucleon system:



— C_S and C_T: LO 4N couplings Weinberg

— $C_{1,..,7}$: NLO 4N couplings

Ordonez et al., Epelbaum et al.

— $D_{1,..,13}$: N^{3}LO 4N couplings

Epelbaum, Glöckle, Krebs, UGM, Reinert, Entem, Machleidt

⇒ these must be fixed from NN data

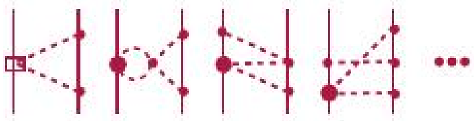
⇒ fit to the low phases (S,P, ...)

. . . and try to understand the physics behind their values

NN FORCES to FIFTH ORDER

Epelbaum, Krebs, UGM, Reinert, Entem, Nosyk, Kaier, Machleidt

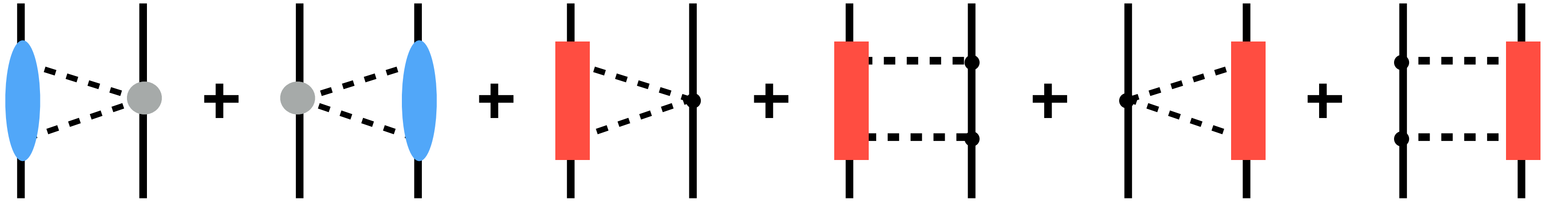
- Many new contributions



- No contact interactions at this order - odd in Q

- New contributions fixed from πN scattering, LECs c_i, d_i, e_i:

Büttiker, Fettes, UGM, Steininger (1998-2000); Krebs, Gasparian, Epelbaum (2012), Hoferichter et al. (2015-2018)



$$\mathcal{L}_{\pi N} = \mathcal{L}_{\pi N}^{(1)} + \mathcal{L}_{\pi N}^{(2)}(c_i) + \mathcal{L}_{\pi N}^{(3)}(d_i) + \mathcal{L}_{\pi N}^{(4)}(e_i)$$

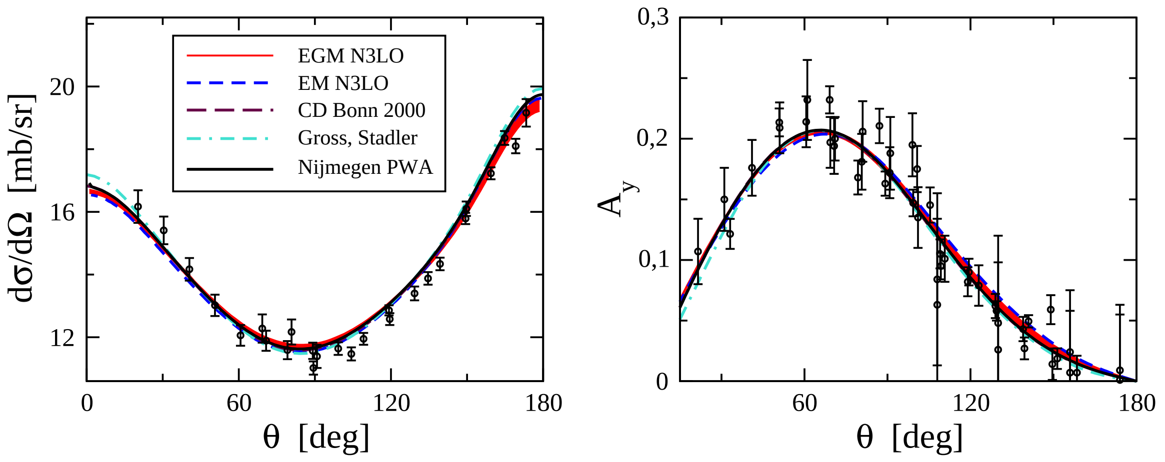
- Three-pion exchange can be neglected

  $\rightarrow$ explicit calculation of the dominant NLO contribution — Kaiser (2001)

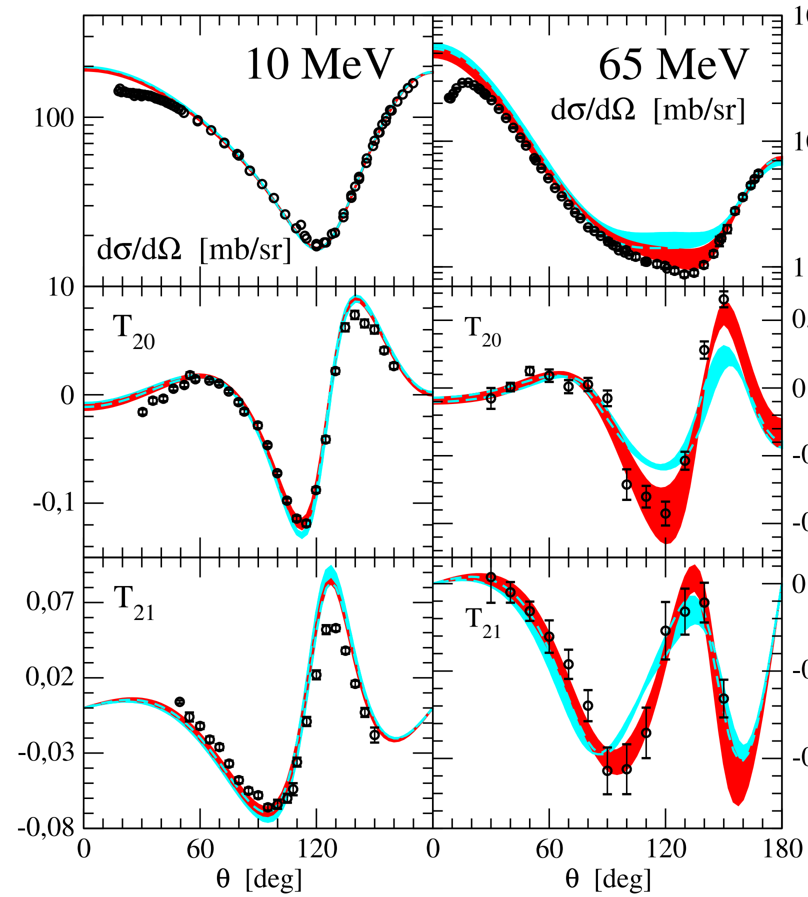
  $\rightarrow$ no influence on phase shifts or deuteron properties

RESULTS at N3LO

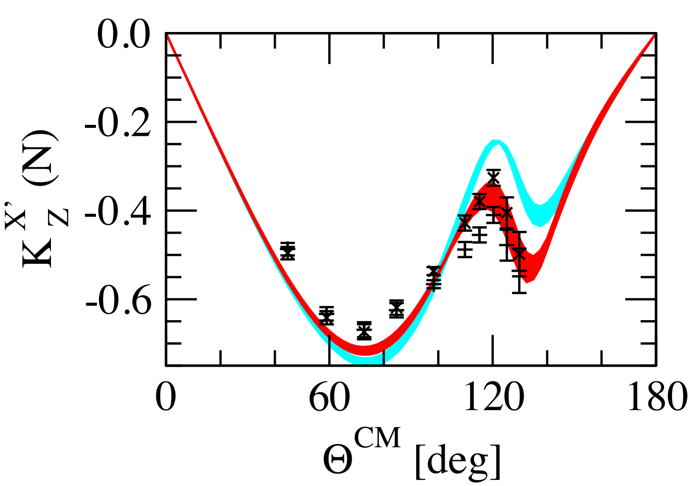
- np scattering



- nd scattering



- pol. transfer in pd scattering



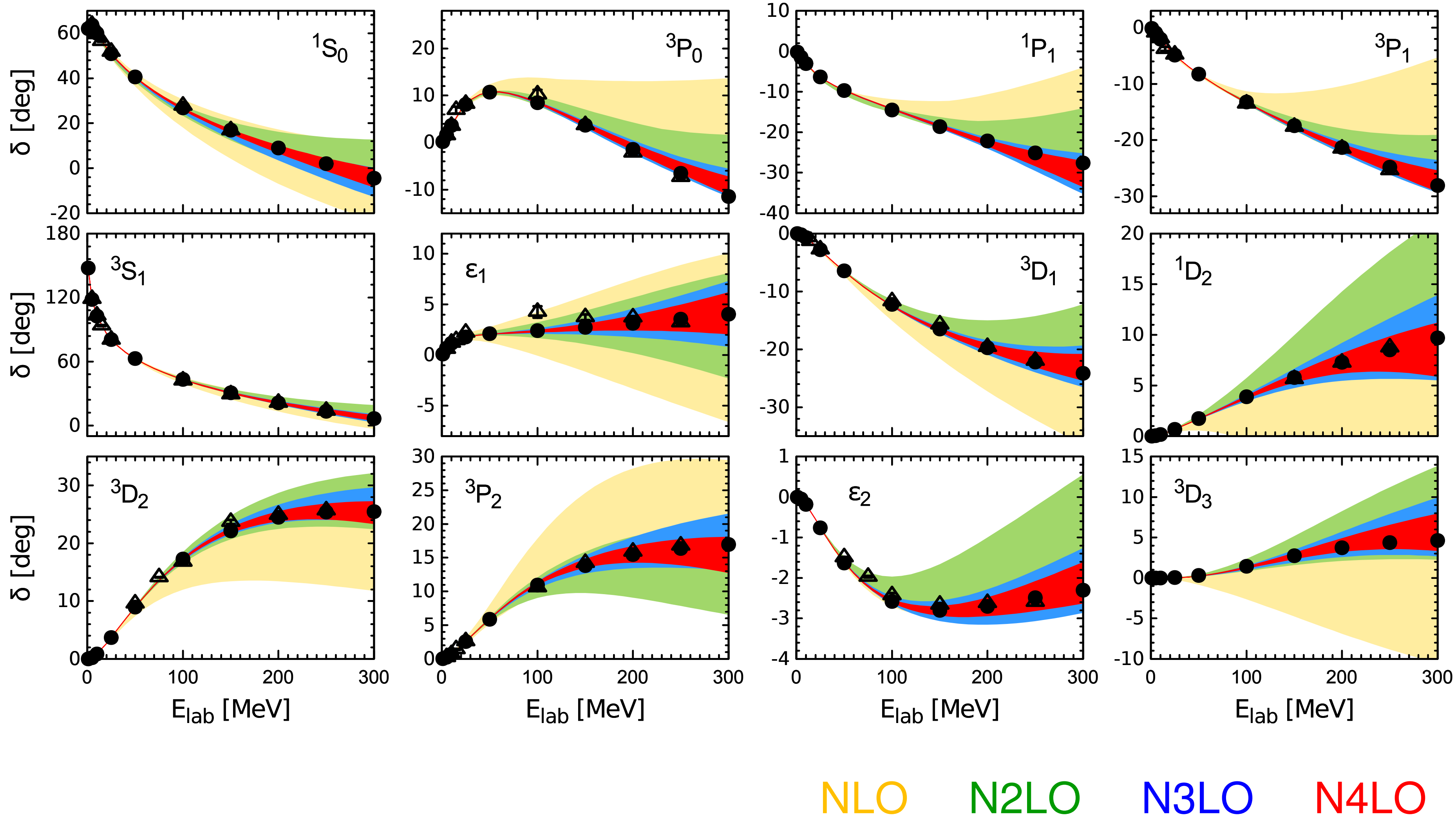
- uncertainties only from cut-off variations!

PHASE SHIFTS at N4LO

- N4LO analysis, better error estimates

Epelbaum, Krebs, UGM, Phys. Rev. Lett. **115** (2015) 122301
Entem, Kaiser, Machleidt, Nosyk, Phys. Rev. **C 91** (2015) 014002
Reinert, Krebs, Epelbaum, EPJ **A 54** (2018) 86

- Precision phase shifts with small uncertainties up to $E_{\rm lab} = 300$ MeV



IMPROVED ERROR ESTIMATES

- Various sources of uncertainties, dominated by the orders neglected
- small parameter Q, must deal with the double expansion (momenta/masses):

$$Q = \max\left(\frac{p}{\Lambda_{\rm hard}}, \frac{M_\pi}{\Lambda_{\rm hard}}\right), \qquad \Lambda_{\rm hard} = \text{breakdown scale}$$

- at low momenta ($p < M_\pi$) the error is dominated by the pion mass corrections
- conservative way of estimating the uncertainty: take the maximum of all the differences of the lower orders one has considered for a given observable $X(p)$ at order Q^N [note particular pattern for NN]

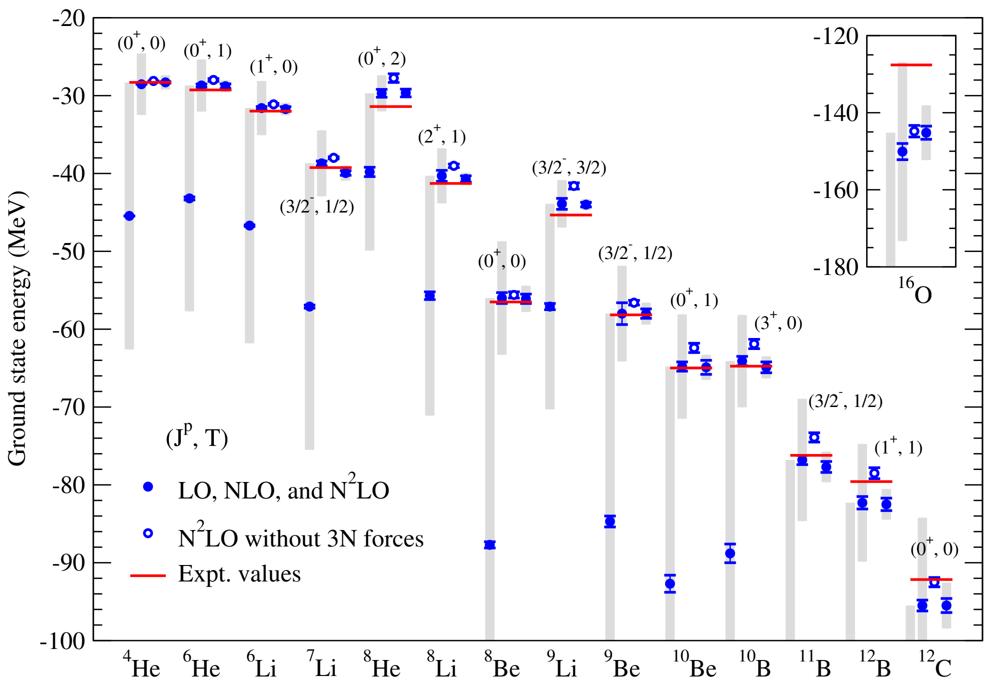
$$\Delta X^N(p) = \max\big(Q^{N+1}\cdot|X^{\rm LO}(p)|, Q^{N-1}\cdot|X^{\rm NLO}(p) - X^{\rm LO}(p)|,$$
$$Q^{N-2}\cdot|X^{\rm N^2LO}(p) - X^{\rm NLO}(p)|, \ldots, Q\cdot|X^{\rm N^NLO}(p) - X^{\rm N^{N-1}LO}(p)|\big)$$

NUCLEI at N2LO

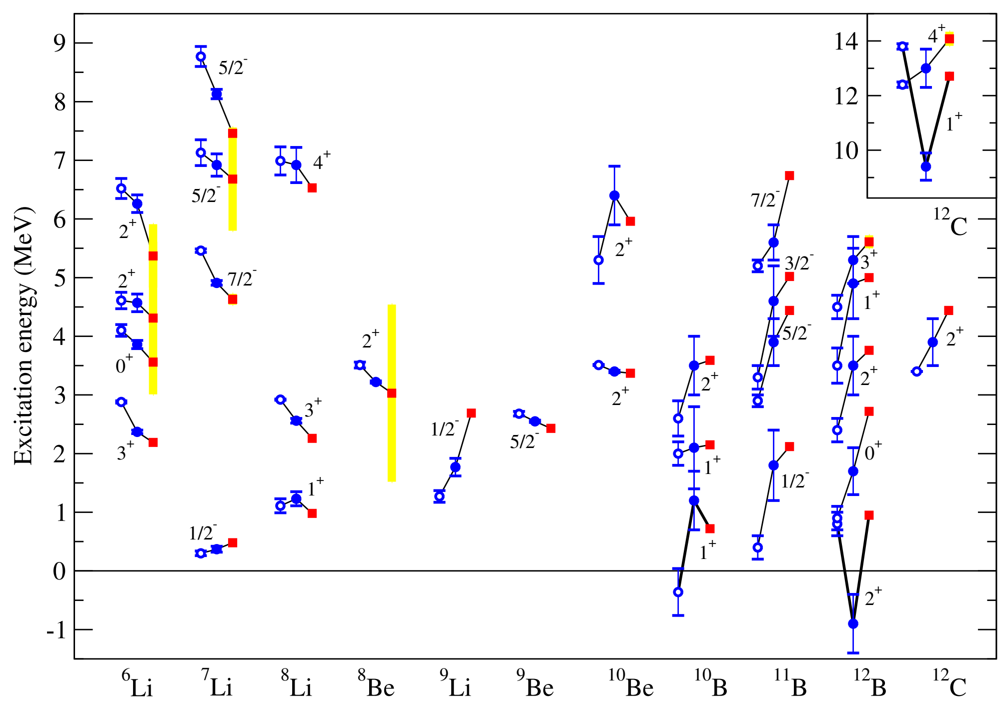
- N2LO analysis, 2NFs + 3NFs consistently included, NCSM

Epelbaum et al. [LENPIC], Phys. Rev. **C99** (2019) 024313

- Ground state energies



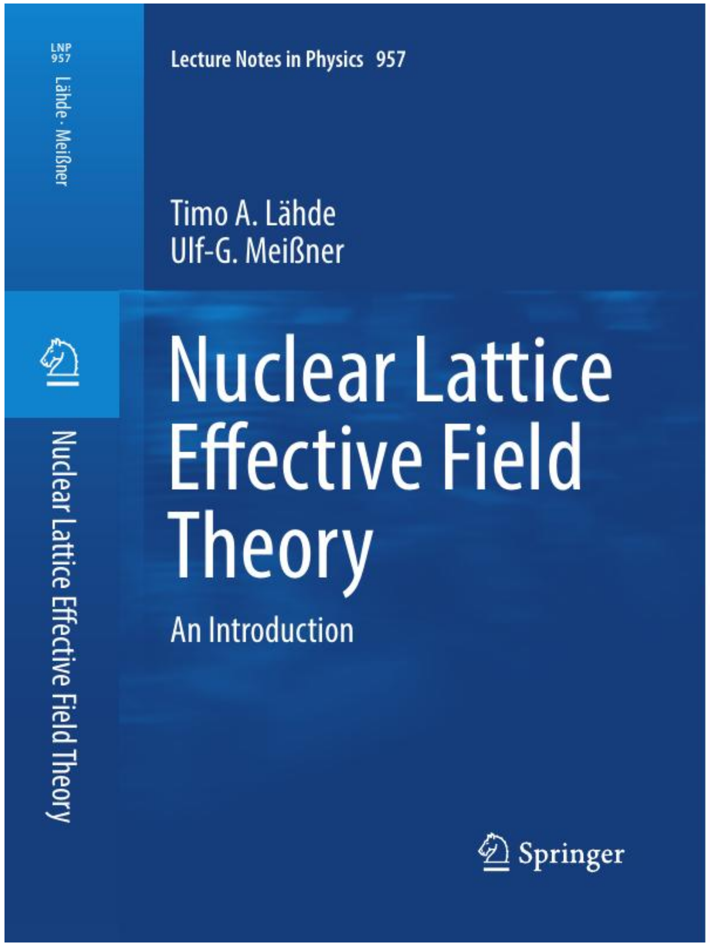
- excitation energies



→ quite reasonable, radii somewhat underpredicted

→ similar to results other groups (TUD, ORNL, Saclay, Sussex, ...)

Chiral EFT on a lattice



T. Lähde & UGM

Nuclear Lattice Effective Field Theory - An Introduction

Springer Lecture Notes in Physics **957** (2019) 1 - 396

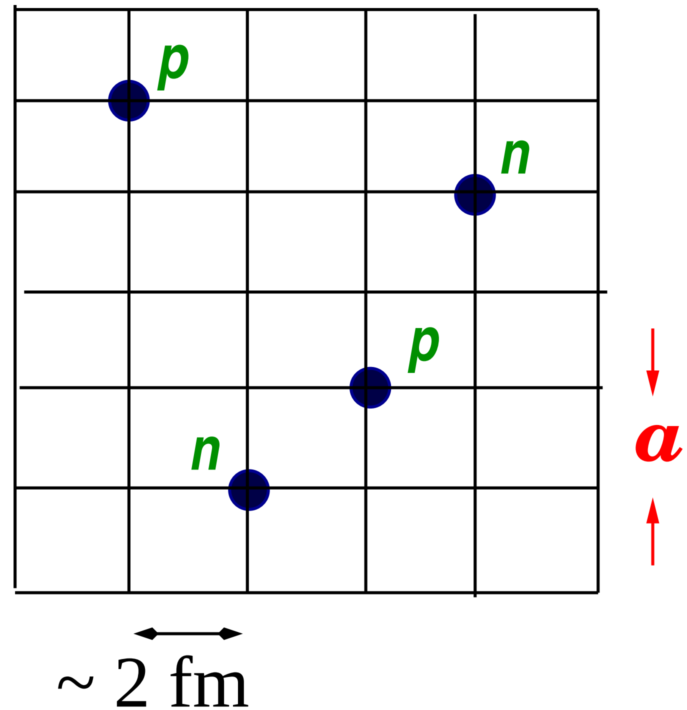
NUCLEAR LATTICE EFFECTIVE FIELD THEORY

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 particles on the sites
- discretized chiral potential w/ pion exchanges
  and contact interactions + Coulomb

  $\rightarrow$ see Epelbaum, Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773
- typical lattice parameters

$$p_{\max} = \frac{\pi}{a} \simeq 314 \text{ MeV [UV cutoff]}$$



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

  E. Wigner, Phys. Rev. **51** (1937) 106; T. Mehen et al., Phys. Rev. Lett. **83** (1999) 931; J. W. Chen et al., Phys. Rev. Lett. **93** (2004) 242302
- physics independent of the lattice spacing for $a = 1 \ldots 2$ fm [@N3LO]

  N. Li et al., Phys. Rev. **C98** (2018) 044002

DISCUSSION of the LATTICE SPACING

- Standard in LQCD is the continuum limit $a \to 0$
- not so in NLEFT: the inverse lattice spacing serves as the UV regulator!
- physical range: $\Lambda = \pi/a$ must be bigger than M_π and smaller than $\Lambda_{\rm hard}$
- this translates into $a \geq 1$ fm and $a \leq 2$ fm

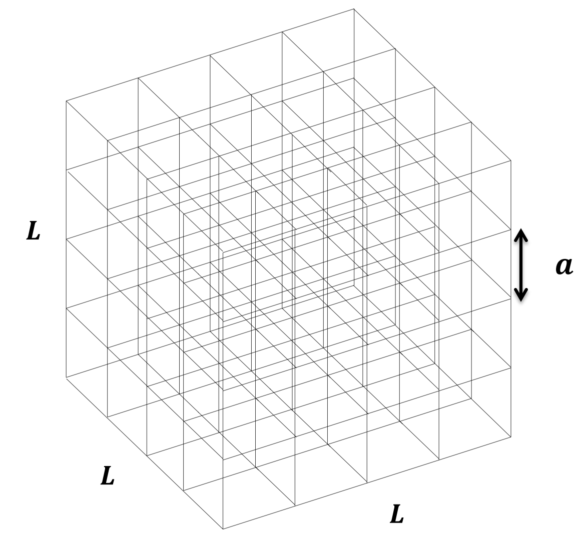
$$\boxed{a \in [1,2]\ \text{fm} \quad \to \quad p_{\rm max} \simeq [300, 600]\ \text{MeV}}$$

- lattice artefacts must be controlled at fixed $a \to$ feasible

  $\hookrightarrow$ will discuss explicit examples later

- alternative approach possible: consider a cut-off EFT with $a \to 0$
  by working with the relativistic path integral and block fields
  for a first try, see Urbach, Montvay, Eur. Phys. J. **A48** (2012) 38

LATTICE NOTATION



- nucleon fields in the isospin basis

- nucleon annihilation/creation ops:

$$a^{(\dagger)}_{0,0} \equiv a_{\uparrow,p},\ a^{(\dagger)}_{1,0} \equiv a_{\downarrow,p},\ a^{(\dagger)}_{0,1} \equiv a_{\uparrow,n},\ a^{(\dagger)}_{1,1} \equiv a_{\downarrow,n}$$

$\to$ labeling **spin** and **isospin**

- spatial & temporal lattice spacing: $a,\, a_t \to \alpha_t \equiv a_t/a$

- lattice size: $L \equiv Na,\, L_t \equiv N_t a_t$ (typically $N = 6-10,\, N_t = 14-18$)

- lattice volume: $V = L^3 \times L_t$

- lattice momenta: $\vec{k} = (k_1, k_2, k_3) \equiv \left(\frac{2\pi}{N}\hat{k}_1, \frac{2\pi}{N}\hat{k}_2, \frac{2\pi}{N}\hat{k}_3\right)$

$\to$ in the first Brillouin zone: $|k_i| < \pi$ and $0 \le |\hat{k}_i| < N/2$

LATTICE NOTATION cont'd

- any derivative operator requires *improvement*, as the simplest representation in terms of two neighboring points is afflicted by the largest discretization errors

$$k_l \equiv \sum_{j=1}^{\nu+1} (-1)^{j+1} \theta_{\nu,j} \sin(jk_l) \; + \mathcal{O}(a^{2\nu+2})$$

$$\frac{k_l^2}{2} \equiv \sum_{j=0}^{\nu+1} (-1)^{j} \omega_{\nu,j} \cos(jk_l) \; + \mathcal{O}(a^{2\nu+2})$$

- no improvement ($\nu = 0$): $\theta_{0,1} = 1, \;\; \omega_{0,0} = 1, \;\; \omega_{0,1} = 1$

- Order a^2 improvement ($\nu = 1$): $\theta_{1,1} = \frac{4}{3}, \; \theta_{1,2} = \frac{1}{6},$

$$\omega_{1,0} = \frac{5}{4}, \; \omega_{1,1} = \frac{4}{3}, \; \omega_{1,2} = \frac{1}{12}$$

- Order a^4 improvement ($\nu = 2$): $\theta_{2,1} = \frac{3}{2}, \; \theta_{2,2} = \frac{3}{10}, \; \theta_{2,3} = \frac{1}{30}$

$$\omega_{2,0} = \frac{49}{36}, \; \omega_{2,1} = \frac{3}{2}, \; \omega_{2,2} = \frac{3}{20}, \; \omega_{2,3} = \frac{1}{90}$$

LATTICE NOTATION cont'd

- definition of the first order spatial derivative:

$$\nabla_{l,(\nu)} f(\vec{n}) \equiv \frac{1}{2} \sum_{j=1}^{\nu+1} (-1)^{j+1} \theta_{\nu,j} \Big[f(\vec{n} + j\hat{e}_l) - f(\vec{n} - j\hat{e}_l) \Big]$$

- second order spatial derivative:

$$\tilde{\nabla}^2_{l,(\nu)} f(\vec{n}) \equiv - \sum_{j=0}^{\nu+1} (-1)^{j} \omega_{\nu,j} \Big[f(\vec{n} + j\hat{e}_l) + f(\vec{n} - j\hat{e}_l) \Big]$$

- has two zeros in per Brillouin zone $\rightarrow$ beneficial feature for tuning NLO coefficients

- improved lattice dispersion relation: $\omega^{(\nu)}(\vec{p}) \equiv \dfrac{1}{\tilde{m}_N} \displaystyle\sum_{j=0}^{\nu+1} \sum_{l=1}^{3} (-1)^j \omega_{\nu,j} \, \cos(j p_l)$

- every quantity in terms of the lattice spacing: $\boxed{\tilde{m}_N \equiv m_N a}$

REMINDER: NUCLEAR FORCES at LO

- Nuclear Hamiltonian: $H = H_0 + V$

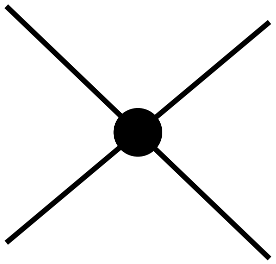
- Chiral expansion of the potential:

$$V = V_{\rm LO}^{\rm cont} + V_{\rm LO}^{\rm OPE} + V_{\rm NLO}^{\rm cont} + V_{\rm NLO}^{\rm TPE} + V_{\rm NNLO}^{\rm TPE} + \ldots$$

- Leading order:

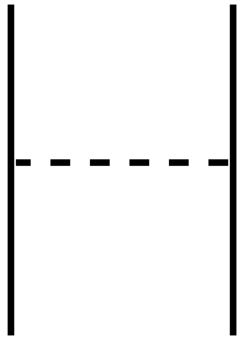
$$V_{\rm LO}^{\rm cont} = C_S + C_T\,(\vec\sigma_1\cdot\vec\sigma_2)$$ [2 LECs]

[on the lattice, $C_I\,(\vec\tau_1\cdot\vec\tau_2)$ is also used]



$$V_{\rm LO}^{\rm OPE} = -\frac{g_A^2}{4F_\pi^2}\,\vec\tau_1\cdot\vec\tau_2\,\frac{(\vec\sigma_1\cdot\vec q\,)\,(\vec\sigma_2\cdot\vec q\,)}{q^{\,2}+M_\pi^2}$$

$\vec q$ = t-channel mom. transfer



LATTICE NOTATION: FREE FIELDS

- Only discuss some bits and pieces
- $O(a^4)$ improved LO free nucleon Hamiltonian:

$$\tilde{H}_{\rm free} = \frac{49}{12\tilde{m}_N}\sum_{\vec{n},i,j} a^\dagger_{i,j}(\vec{n})a_{i,j}(\vec{n}) - \frac{3}{4\tilde{m}_N}\sum_{\vec{n},i,j}\sum_{l=1}^{3}\left[a^\dagger_{i,j}(\vec{n})a_{i,j}(\vec{n}+\hat{e}_l) + a^\dagger_{i,j}(\vec{n})a_{i,j}(\vec{n}-\hat{e}_l)\right]$$
$$+\frac{3}{40\tilde{m}_N}\sum_{\vec{n},i,j}\sum_{l=1}^{3}\left[a^\dagger_{i,j}(\vec{n})a_{i,j}(\vec{n}+2\hat{e}_l) + a^\dagger_{i,j}(\vec{n})a_{i,j}(\vec{n}-2\hat{e}_l)\right]$$
$$-\frac{1}{180\tilde{m}_N}\sum_{\vec{n},i,j}\sum_{l=1}^{3}\left[a^\dagger_{i,j}(\vec{n})a_{i,j}(\vec{n}+3\hat{e}_l) + a^\dagger_{i,j}(\vec{n})a_{i,j}(\vec{n}-3\hat{e}_l)\right]$$

- $O(a^4)$ improved LO free pion action in momentum space:

$$S_{\pi\pi}(\pi'_I) = \frac{1}{2N^3}\sum_{I=1}^{3}\sum_{\vec{k},t}\pi'_I(-\vec{k},t)\,D_\pi^{-1}(\vec{k})\,\pi'_I(\vec{k},t)$$

$$D_\pi(\vec{k})^{-1} = \left[1 + \frac{2\alpha_t}{q_\pi}\sum_{l=1}^{3}\left(-\omega_{2,1}\cos(k_l) + \omega_{2,2}\cos(2k_l) - \omega_{2,3}\cos(3k_l)\right)\right]$$

$$\pi'_I(\vec{n},t) = \sqrt{q_\pi}\,\pi_I(\vec{n},t)\,,\quad q_\pi = \alpha_t(M_\pi^2 + 6\omega_{2,0})$$ rescaled pion fields

LATTICE NOTATION of THE LO HAMILTONIAN

- SU(4) symmetric nucleon density:

$$\rho^{a^\dagger,a}(\vec{n}) \equiv \sum_{i,j=0,1} a^\dagger_{i,j}(\vec{n}) a_{i,j}(\vec{n})$$

- Local spin densitiy:

$$\rho_S^{a^\dagger,a}(\vec{n}) \equiv \sum_{i,j,i'=0,1} a^\dagger_{i,j}(\vec{n}) \left[\sigma_S\right]_{ii'} a_{i',j}(\vec{n}), \ , \quad S = 1,2,3$$

- and similarly for the isospin $\rho_I(\vec{n},t)$ and the spin-isospin $\rho_{S,I}(\vec{n},t)$ densities

$\hookrightarrow$ LO four-nucleon action expressed in terms of these densities:

$$S_{\bar{N}N\bar{N}N} \equiv \frac{\tilde{C}_0 \alpha_t}{2} \sum_{\vec{n},t} \left[\rho(\vec{n},t)\right]^2 + \frac{\tilde{C}_T \alpha_t}{2} \sum_{S=1}^{3} \sum_{\vec{n},t} \left[\rho_S(\vec{n},t)\right]^2$$

- as usual in proper powers of the lattice spacing: $\tilde{C} = C/a^2$

LATTICE NOTATION of THE LO HAMILTONIAN cont'd

- Simulations require **auxiliary fields** aka Hubbard-Stratonovich transformations

  aka Gaussian quadrature:

$$\exp\left(-\frac{\tilde{C}_0\alpha_t}{2}\left[\rho(\vec{n},t)\right]^2\right) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} ds\, \exp\left(-\frac{s^2}{2} + \sqrt{-\tilde{C}_0\alpha_t}\,\rho(\vec{n},t)\, s\right)$$

$$\exp\left(-\frac{\tilde{C}_T\alpha_t}{2}\sum_{S=1}^{3}\left[\rho_S(\vec{n},t)\right]^2\right)$$
$$= \int\left(\prod_{S=1}^{3}\frac{ds_S}{\sqrt{2\pi}}\right)\exp\left(-\sum_{S=1}^{3}\frac{s_S^2}{2} + i\sqrt{\tilde{C}_T\alpha_t}\sum_{S=1}^{3}\rho_S(\vec{n},t)\, s_S\right)$$

- auxiliary field action (just give one example):

$$S_{ss}(s,s_S) = \frac{1}{2}\sum_{\vec{n},t} s^2(\vec{n},t)$$

$$S_{ss\bar{N}N}(s,s_S,\xi^*,\xi) = -\sqrt{-\tilde{C}_0\alpha_t}\sum_{\vec{n},t}\rho(\vec{n},t)s(\vec{n},t) + \ldots$$

LO LATTICE HAMILTONIAN: OPE

- Consider the OPE (One-Pion-Exchange)
- Pion-nucleon coupling at a given time:

$$S_{\pi\bar{N}N}(\pi'_I, a^\dagger, a) = \frac{g_A \alpha_t}{2F_\pi \sqrt{q_\pi}} \sum_{I=1}^{3} \sum_{S=1}^{3} \sum_{\vec{n}} \left[\nabla_{S,(\nu)} \pi'_I(\vec{n}, t)\right] \rho_{S,I}^{a^\dagger, a}(\vec{n})$$

- pions behave as another set (triplet) of auxiliary fields
- we need to express this in terms of the pion-nucleon coupling constant $g_{\pi N}$
- adjust g_A to account for the Goldberger-Treiman discrepancy:

$$g_{\pi N} = \frac{g_A m_N}{F_\pi} \left(1 - \frac{2M_\pi^2 d_{18}}{g_A}\right) \;, \quad \frac{g_{\pi N}^2}{4\pi} = 13.7 \pm 0.1$$

Baru et al., Nucl. Phys. A **872** (2011) 69

$\rightarrow$ use instead of fixing d_{18}: $\boxed{g_A = 1.287}$

DIGRESSION: WIGNER SU(4) SYMMETRY

- Nuclear forces approximately spin- and isospin-independent
- Wigner's super-multiplet theory (1936 ff): Wigner, Phys. Rev. **51** (1937) 106; *ibid* 947
- Analysis in pionless EFT: $\mathcal{L}_2 = -\frac{1}{2}C_0(N^\dagger N)^2 - -\frac{1}{2}C_T(N^\dagger \sigma_i N)^2$
- Wigner trafo: $N \mapsto UN, \quad U = \exp[i\alpha_{\mu\nu}\sigma_\mu\tau_\nu], \quad \sigma_\mu = \{1, \sigma_i\}, \quad \tau_\nu = \{1, \tau_a\}$
  $\alpha_{\mu\nu} = 4 \times 4$ real matrix, $\alpha_{00} = 0$
  $\hookrightarrow$ The C_0 term is invariant under a W.T., the C_T term is not
- in a partial-wave basis: $C(^1S_0) = C_0 - 3C_T\ , \quad C(^3S_1) = C_0 - C_T$

  $\hookrightarrow$ in the Wigner symmetry limit, we have: $C(^1S_0) = C(^3S_1)$

  $\hookrightarrow$ in the Wigner symmetry limit, we thus have: $1/a_{np}^{S=1} = 1/a_{np}^{S=0}$

  $\hookrightarrow$ Wigner symmetry breaking governed by: $\delta = \frac{1}{2}(1/a_{np}^{S=1} - 1/a_{np}^{S=0})$

$$= \frac{1}{2}\left(\frac{1}{36.5\ \mathrm{MeV}} - \frac{1}{8.3\ \mathrm{MeV}}\right)$$

HIGHER ORDERS

- NLO: Leading two-pion exchange and 7 contact terms with 2 derivatives [cont. notation]

$$V_{\rm NLO}^{\rm cont} = C_1 q^2 + C_2 k^2 + \left(C_3 q^2 + C_4 k^2\right)(\vec\sigma_1\cdot\vec\sigma_2) + iC_5 \tfrac{1}{2}(\vec\sigma_1+\vec\sigma_2)\cdot(\vec q\times\vec k) + C_6\,(\vec\sigma_1\cdot\vec q)\,(\vec\sigma_2\cdot\vec q) + C_7(\vec\sigma_1\cdot\vec k)(\vec\sigma_2\cdot\vec k)$$

$\vec k$ = u-channel mom. transfer

$$V_{\rm NLO}^{\rm TPE} = -\frac{\tau_1\cdot\tau_2}{384\pi^2 F_\pi^4} L(q)\Big[4M_\pi^2\left(5g_A^4 - 4g_A^2 - 1\right) + q^2\left(23g_A^4 - 10g_A^2 - 1\right) + \frac{48g_A^4 M_\pi^4}{4M_\pi^2+q^2}\Big] - \frac{3g_A^4}{64\pi^2 F_\pi^4} L(q)\left[(\vec q\cdot\vec\sigma_1)(\vec q\cdot\vec\sigma_2) - q^2(\vec\sigma_1\cdot\vec\sigma_2)\right]$$

- Loop function: $L(q) = \frac{1}{2q}\sqrt{4M_\pi^2+q^2}\,\ln\frac{\sqrt{4M_\pi^2+q^2}+q}{\sqrt{4M_\pi^2+q^2}-q}$
 $\to 1 + \frac{1}{3}\frac{q^2}{4M_\pi^2} + \cdots$ for $q \ll \Lambda$

$\to$ for coarse lattices $a \simeq 2$ fm, the TPE at N(N)LO can be absorbed in the LECs C_i

$\to$ no longer true as a decreases, need to account for the TPE explicitely

- At NNLO, further two-pion exchanges ($\sim c_i$) and leading 3NFs (2 LECs)

$\to$ same book-keeping techniques as shown for LO

COULOMB INTERACTION

- Proton-proton repulsion in coordinate space:

$$\mathcal{A}[V_{\rm em}] = \frac{\alpha_{\rm EM}}{r}\left(\frac{1+\tau_3}{2}\right)_A\left(\frac{1+\tau_3}{2}\right)_B~,~~\alpha_{\rm EM} = e^2/(4\pi) \simeq 1/137$$

- Lattice operator:

$$\tilde{V}_{\rm em} = \frac{1}{2} : \sum_{\vec{n},\vec{n}'} \frac{\alpha_{\rm em}}{R(\vec{n}-\vec{n}')}\,\frac{1}{4}\left[\rho^{a^\dagger,a}(\vec{n}) + \rho^{a^\dagger,a}_{I=3}(\vec{n})\right]\left[\rho^{a^\dagger,a}(\vec{n}') + \rho^{a^\dagger,a}_{I=3}(\vec{n}')\right] :$$

$$R(\vec{n}) = \max(1/2, |\vec{n}|)$$

$\rightarrow$ effect of two protons on the same site **not** observable, $R(\vec{n}) = |\vec{n}|$ absorbed in pp contact term

$\rightarrow$ include pp and nn contact terms to allow for $a_{np} \neq a_{nn} \neq a_{pp}$ & other IB terms

$$\mathcal{A}[V_{nn}] = C_{nn}\left(\frac{1-\tau_3}{2}\right)_A\left(\frac{1-\tau_3}{2}\right)_B~,~~\mathcal{A}[V_{pp}] = C_{pp}\left(\frac{1+\tau_3}{2}\right)_A\left(\frac{1+\tau_3}{2}\right)_B$$

DIGRESSION: A NOTE on the POWER COUNTING

- Isospin breaking through strong ($\sim \epsilon$) and em ($\sim e$) interactions

$$\epsilon = \frac{m_d - m_u}{m_d + m_u} \sim \frac{1}{3}\,, \qquad e = \sqrt{\frac{4\pi}{137.06}} \simeq 0.3$$

- Possible counting: $\epsilon \sim e \sim \frac{Q}{\Lambda}\,, \qquad \frac{e^2}{(4\pi)^2} \sim \frac{Q^4}{\Lambda^4}$

- Coulomb first appears at NLO, consider the S-wave in pp scattering:

$$V_{1\pi}^{(0)}(q) = \left(\frac{g_A}{2F_\pi}\right)^2 \frac{q^2}{q^2 + M_\pi^2} \sim \frac{Q^2}{Q^2 Q^2} \sim Q^{-2} \quad [4\pi \sim \Lambda/Q \text{ in WC}]$$

$$V_{\text{Coulomb}}(q) = \frac{e^2}{q^2} \sim \frac{Q^2}{Q^2} \sim Q^0$$

- one possible way, no rescaling of F_π etc needed in the purely strong sector

- for details, see Epelbaum, Glöckle, UGM, Nucl. Phys. A **747** (2005) 362

EUCLIDEAN TIME PROJECTION

- Euclidean time-projection amplitude for A nucleons (with Eucl. time τ):

$$Z_A(\tau) = \langle \Psi_A | \exp(-\tau H) | \Psi_A \rangle$$

- the trial wave function Ψ_A = Slater determinant for A free nucleons [or ...]

- Transient energy $$E_A(\tau) = -\frac{d}{d\tau} \ln Z_A(\tau)$$

- ground state: $$E_A^0 = \lim_{\tau \to \infty} E_A(\tau)$$

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

$$Z_A^{\mathcal{O}} = \langle \Psi_A | \exp(-\tau H/2)\, \mathcal{O}\, \exp(-\tau H/2)\, | \Psi_A \rangle$$

$$\lim_{\tau \to \infty} \frac{Z_A^{\mathcal{O}}(\tau)}{Z_A(\tau)} = \langle \Psi_A | \mathcal{O} \, | \Psi_A \rangle$$

EUCLIDEAN TIME PROJECTION cont'd

- Common situation: the trial wave function has more than one component
- Examples: excited states or transition between levels
- trial state with $N_{\rm ch}$ channels: $$|\Psi\rangle \equiv \sum_{i=1}^{N_{\rm ch}} c_i |\Psi_i\rangle$$
- with weights c_i like eg. Clebsch-Gordan coefficients
- Eucl. time projection amplitude recieves contributions from $N_{\rm ch}^2$ channels:

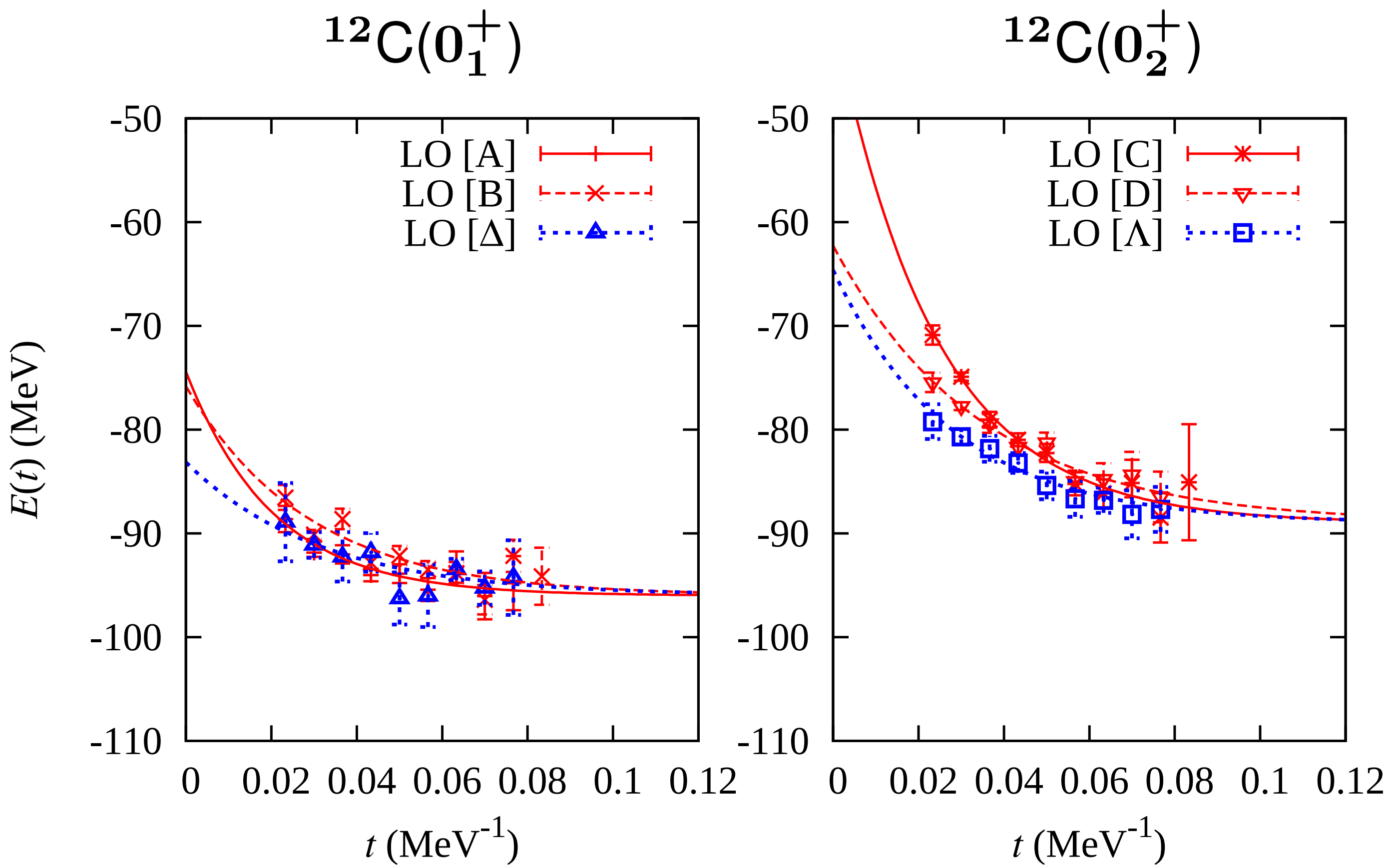
$$Z(t) = \langle\Psi|\exp(-H\tau)|\Psi\rangle = \sum_{i,j}^{N_{\rm ch}} c_i c_j A_{ij}$$

$$A_{ij} = \langle\Psi_i|\exp(-H\tau)|\Psi_j\rangle$$

- quite powerful for excited states, show one example

EUCLIDEAN TIME PROJECTION cont'd

- Ground state and first excited state w/ the same quantum numbers in ^{12}C
- 4 plane-wave and 2 cluster initial states (details later)



- states labelled by their angular momentum (J), parity (P) & level number (n): J_n^P

REMINDER: PATH INTEGRAL and TRANSFER MATRIX

- Path integral representation of the partition function (time proj. amp.):

$$Z = \int D\xi D\xi^* \, \exp\left(-S(\xi^*, \xi)\right) \quad [S = \text{action}]$$

$\hookrightarrow$ most simple to derive the lattice Feynman rules

- Transfer matrix representation: N_t Euclidean time slices

$$Z = \mathrm{Tr}\left\{M^{N_t}\right\} + O(\alpha_t^2)\,, \quad M =: \exp\left(-\alpha_t H(a^\dagger, a)\right):$$

$\hookrightarrow$ most useful to perform the MC simulations

- Outline of the proof: Creutz, Found. Phys. **30** (2000) 487

$$\mathrm{Tr}\left[: f(a, a^\dagger) :\right] = \int D\xi D\xi^* e^{2\xi^*\xi} f(\xi, \xi^*)\,, \quad \xi(n, L_t) = -\xi(n, 0)$$

$$f(\xi, \xi^*) = a_0 + a_1\xi + \bar{a}_1\xi^* + a_{12}\xi^*\xi$$

$$\to \mathrm{Tr}\left[: f(a, a^\dagger) :\right] = 2a_0 + a_{12}$$

that is all one needs...

TRANSFER MATRIX FORMALISM

- Time projection amplitude

  = path-integral over pions & auxiliary fields

$$Z_A(\tau) = \mathcal{N} \int_{-\infty}^{+\infty} \mathcal{D}s \prod_{I=1,2,3} \mathcal{D}s_I \mathcal{D}\pi_I \, \langle \Psi_A | T \exp(-\tau H(s, s_I, \pi_I)) | \Psi_A \rangle$$

$$= \mathcal{N} \int_{-\infty}^{+\infty} \mathcal{D}s \prod_{I=1,2,3} \mathcal{D}s_I \mathcal{D}\pi_I \, \exp(-S_{\pi\pi} - S_{ss}) \, \underbrace{\det \mathcal{M}(\pi_I, s, s_I)}$$

Slater-determinant of single nucleon matrix elements

- **Transfer matrix**:

$$\mathcal{M}(\pi_I, s, s_I) = \langle \psi_{i,X} | M_X^{(L_t-1)} \cdots M_X^{(0)} | \psi_{j,X} \rangle, \;\; X = 1, \ldots, A$$

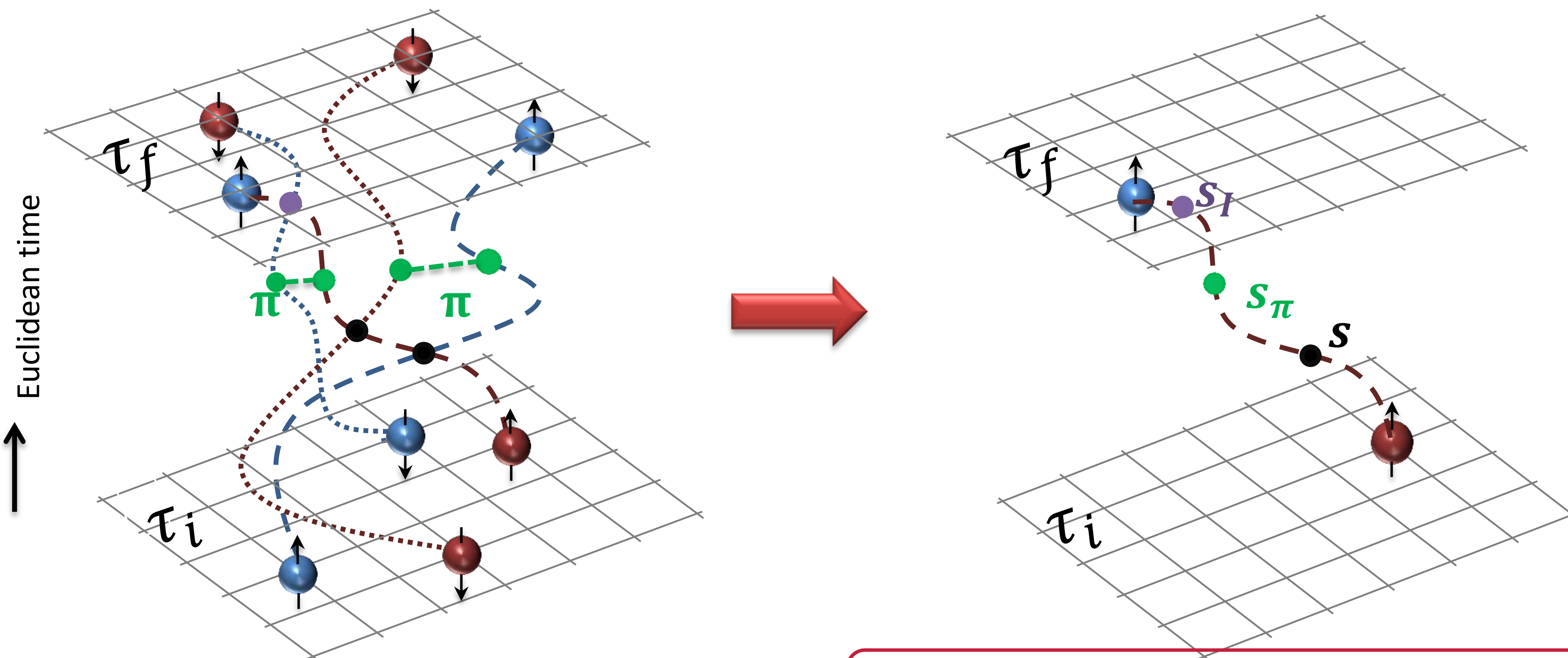
- this is an $A \times A$ matrix

- apply hybrid MC to the fields s, s_I, π_I for the calculation of the path-integral [not covered in these lectures, see chapter 6 of the book]

VISUALIZATION: TRANSFER MATRIX CALCULATION

- Represent interactions and pions by auxiliary fields

  $\rightarrow$ interactions become local, world-lines decouple:



optimally suited for parallel computing!

WIGNER SU(4) SYMMETRY reloaded

- **No** sign problem for spin-isospin saturated nuclei in the W.S. limit!

  J. W. Chen et al., Phys. Rev. Lett. **93** (2004) 242302

- Eucl. time projection amplitude is given by $\det(M)$, where $M_{i,j}$ is the $A \times A$ matrix obtained from the single-nucleon amplitudes

- define $\mathcal{U}[M]$ as the set of unitary matrices such that $U^\dagger M U = M^*$

- it can be shown that $\det(M)$ is positive semi-definite, if there exists an antisymmetric matrix $U \in \mathcal{U}[M]$

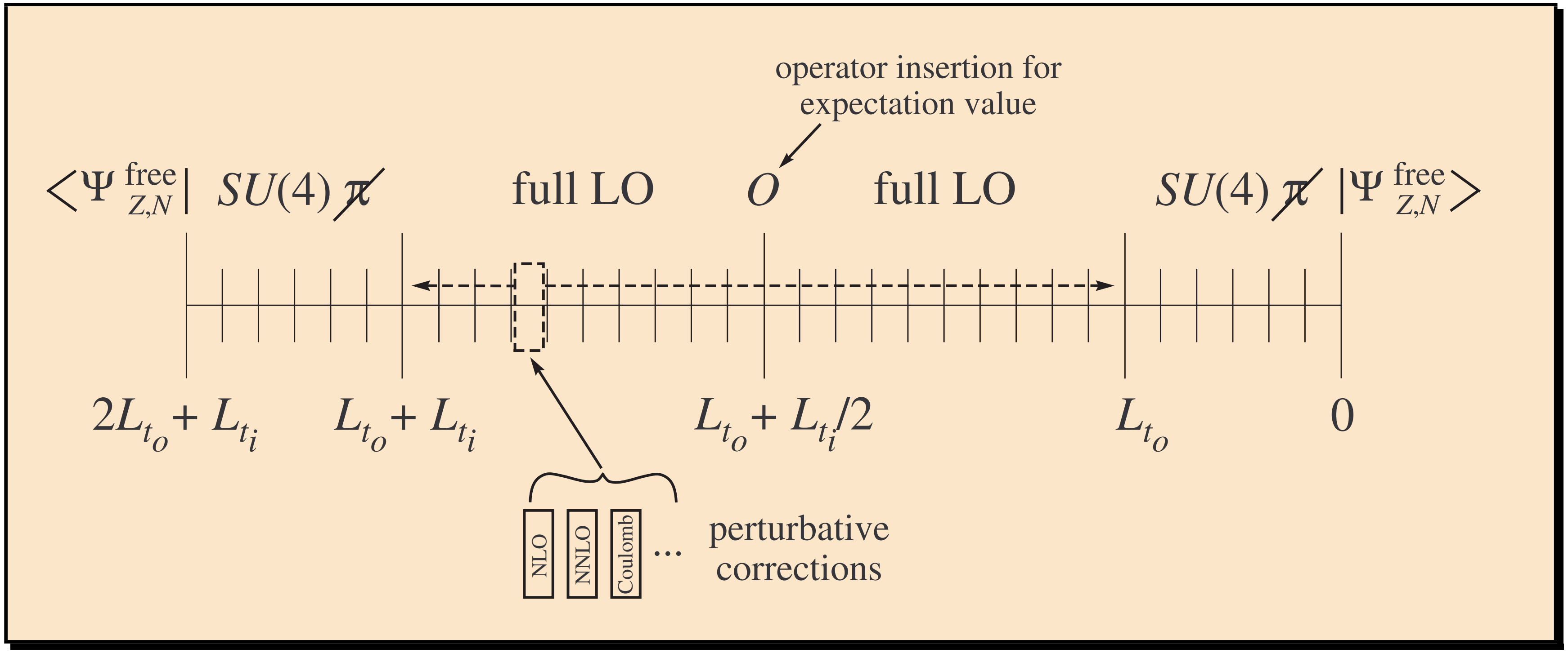
- requires the action of U on the single-particle states $|\psi_i\rangle$ can be represented as an antisymmetric $A \times A$ matrix.

- PMC is free from sign oscillations, whenever the initial single-nucleon states are paired into spin-singlets or isospin-singlets

- breaking through OPE, Coulomb,..., but still an **approximate** symmetry

for details, see chapter 8 of the book

ANATOMY of the TRANSFER MATRIX CALCULATION



– start with pionless SU(4) symmetric theory as approx. inexpensive filter

– then use the full action as exact filter

– then insert the operator under consideration

– continue the filtering procedure to the final time (L_t steps)

– further refined by appropriate smearing procedures (see later)

INITIAL STATES

- Zero momentum standing waves for ^{4}He to define $|\psi_A\rangle = |\psi^{\rm free}_{Z,N}\rangle$

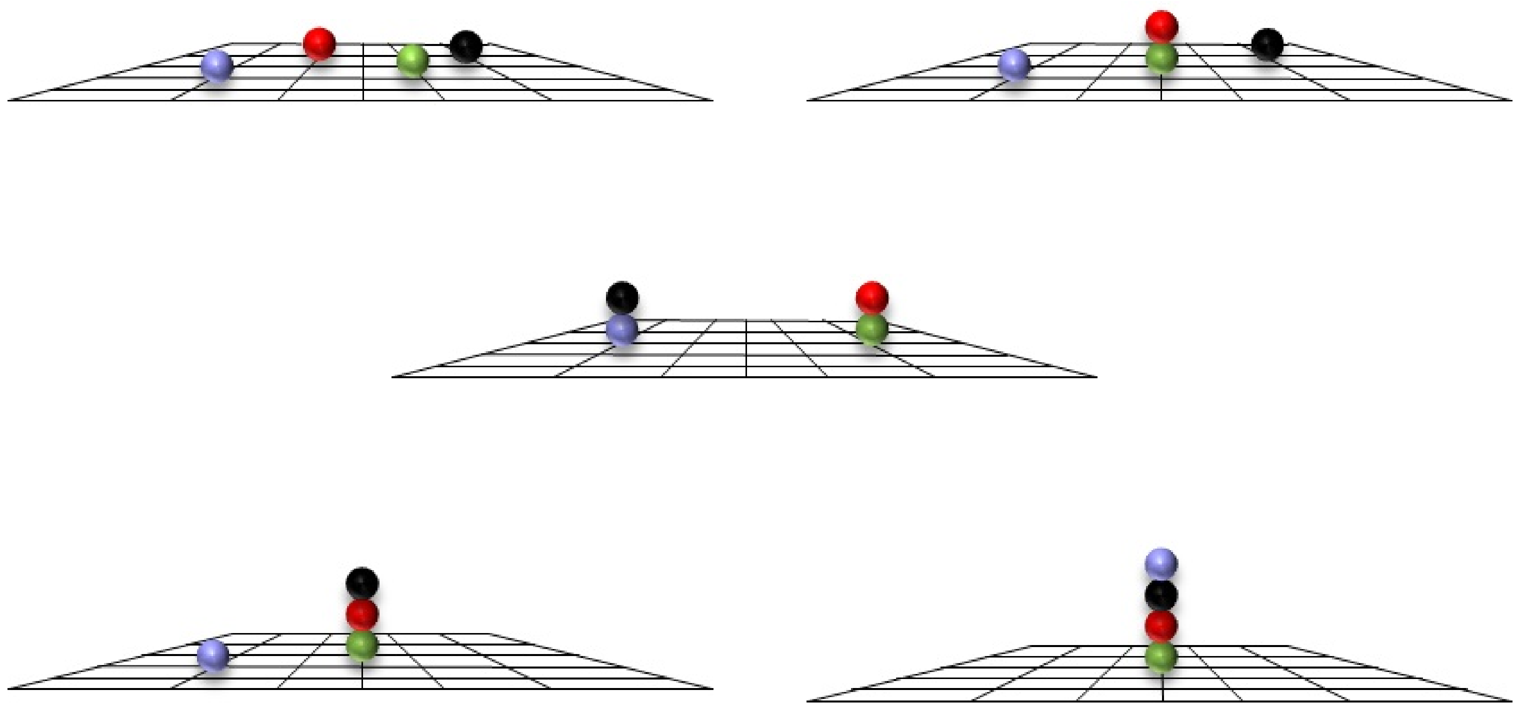
$$\langle 0|a_{i,j}(\vec{n}\,)|\psi_1\rangle = L^{-3/2}\,\delta_{i,0}\delta_{j,1} = |\uparrow, n\,\rangle$$
$$\langle 0|a_{i,j}(\vec{n}\,)|\psi_2\rangle = L^{-3/2}\,\delta_{i,0}\delta_{j,0} = |\uparrow, p\,\rangle$$
$$\langle 0|a_{i,j}(\vec{n}\,)|\psi_3\rangle = L^{-3/2}\,\delta_{i,1}\delta_{j,1} = |\downarrow, n\,\rangle$$
$$\langle 0|a_{i,j}(\vec{n}\,)|\psi_4\rangle = L^{-3/2}\,\delta_{i,1}\delta_{j,0} = |\downarrow, p\,\rangle$$

- Wave packets with small momentum spread for ^{4}He to define $|\psi^{\rm free}_{Z,N}\rangle$

$$\langle 0|a_{i,j}(\vec{n}\,)|\psi_1\rangle = L^{-3/2}\,\sqrt{2}\cos\left(2\pi n_z/L\right)\;\delta_{i,0}\delta_{j,1}$$
$$\langle 0|a_{i,j}(\vec{n}\,)|\psi_2\rangle = L^{-3/2}\,\sqrt{2}\cos\left(2\pi n_z/L\right)\;\delta_{i,0}\delta_{j,0}$$
$$\langle 0|a_{i,j}(\vec{n}\,)|\psi_3\rangle = L^{-3/2}\,\sqrt{2}\cos\left(2\pi n_z/L\right)\;\delta_{i,1}\delta_{j,1}$$
$$\langle 0|a_{i,j}(\vec{n}\,)|\psi_4\rangle = L^{-3/2}\,\sqrt{2}\cos\left(2\pi n_z/L\right)\;\delta_{i,1}\delta_{j,0}$$

- or more complex initial states ...
- Exercise: construct an initial ground state for ^{8}Be

CONFIGURATIONS



⇒ all *possible* configurations are sampled

⇒ preparation of *all possible* initial/final states

⇒ *clustering* emerges *naturally*

INITIAL STATES again

- Alpha-cluster states [cf. Λ and Δ for ^{12}C$(0^+_{1,2})$]

  4 nucleons one one site with a Gaussian radial distribution

$$R_\alpha(r) \sim \exp\left(-\frac{r_d^2}{2\Gamma_\alpha}\right)$$

- with the squared distance r_d^2 given by

$$r_d^2 = \min(x^2, (L-x)^2) + \min(y^2, (L-y)^2) + \min(z^2, (L-z)^2)$$

- and a suitably chosen width parameter Γ_α
- natural choice of Γ_α is given by the rms radius of the α-particle

$r_\alpha \simeq 1.68$ fm Sick (2008)

- other choices: optimize convergence or overlap with the ground state or ...

CLUSTERING INSTABILITY

- Already at LO, the configurations with four nucleons on one site require some massaging
- Consider LO SU(4)-symmetric pionless EFT
- let $E_1^{\rm loc}$ be the expectation value of the single nucleon kinetic energy & $V_2 < 0$
- fix the scattering length, then: $E_1^{\rm loc} \sim -V_2 \sim \frac{\Lambda^2}{2m_N}$
- total energy for 2,3,4 N on one lattice site:

$$E_2^{\rm loc} = 2E_1^{\rm loc} + V_2$$

$$E_3^{\rm loc} = 3E_1^{\rm loc} + 3V_2$$

$$E_4^{\rm loc} = 4E_1^{\rm loc} + 6V_2$$

$$E_A^{\rm loc} = AE_1^{\rm loc} + \binom{A}{2} V_2$$

$\to$ Thomas collapse in the 3N system: 3NF or other stabilizing effect needed

Thomas, Phys. Rev. **47** (1935) 903

CLUSTERING INSTABILITY cont'd

- repeat this exercise with a repulsive 3NF:

$$E_2^{\rm loc} = 2E_1^{\rm loc} + V_2$$
$$E_3^{\rm loc} = 3E_1^{\rm loc} + 3V_2 + V_3$$
$$E_4^{\rm loc} = 4E_1^{\rm loc} + 6V_2 + 4V_3$$

- realistic nuclear forces overbind ^{4}He as long as $\Lambda \lesssim 1.6$ GeV (pionless EFT)

Platter, Hammer, UGM, Phys. Lett. B **607** (2005) 254

- not a useful starting point for NLEFT $\rightarrow$ smearing

- smear the 4N contact interactions with (simplest choice):

$$f(\vec{q}^{\,2}) \propto \exp\left[-b \sum_{l_s=1,2,3} (1 - \cos q l_s)\right]$$

- smearing width b determined from the average effective range: $b \simeq 0.6$ l.u.

SMEARED LO 4N INTERACTIONS

- Consider three different LO actions (suppression of finite cut-off errors)

- LO1: naive discretization $\to$ multi-particle clustering at coarse a

$$\mathcal{A}(V_{\rm LO1}) = C_0 + C_I\,\vec{\tau}_1\cdot\vec{\tau}_2 + \mathcal{A}(V^{\rm OPEP})$$

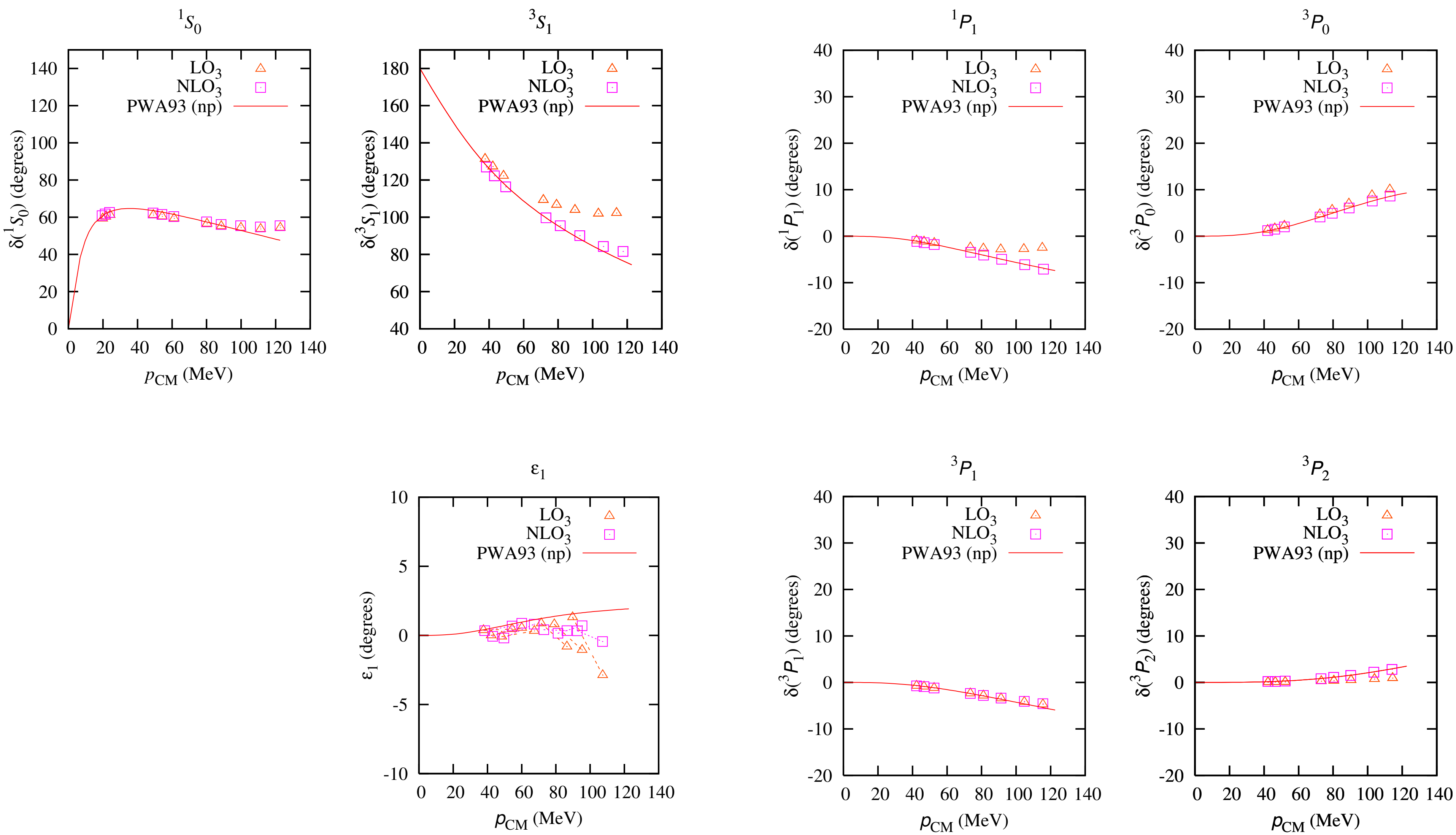
- LO2: Gaussian smearing $\to$ no clustering but too attractive P-waves

$$\mathcal{A}(V_{\rm LO2}) = C_0\,f(\vec{q}^{\,2}) + C_I\,f(\vec{q}^{\,2})\,\vec{\tau}_1\cdot\vec{\tau}_2 + \mathcal{A}(V^{\rm OPEP})$$

- LO3: Gaussian smearing and spin-isopin projections
  (combines advantages of LO1 & LO2)

$$\mathcal{A}(V_{\rm LO3}) = C_{1S0}\,f(\vec{q}^{\,2})\,\overbrace{\left(\frac{1}{4}-\frac{1}{4}\vec{\sigma}_1\cdot\vec{\sigma}_2\right)}^{S=0}\overbrace{\left(\frac{3}{4}+\frac{1}{4}\vec{\tau}_1\cdot\vec{\tau}_2\right)}^{I=1}$$
$$+\,C_{3S1}\,f(\vec{q}^{\,2})\,\underbrace{\left(\frac{3}{4}+\frac{1}{4}\vec{\sigma}_1\cdot\vec{\sigma}_2\right)}_{S=1}\underbrace{\left(\frac{1}{4}-\frac{1}{4}\vec{\tau}_1\cdot\vec{\tau}_2\right)}_{I=0}+\mathcal{A}(V^{\rm OPEP})$$

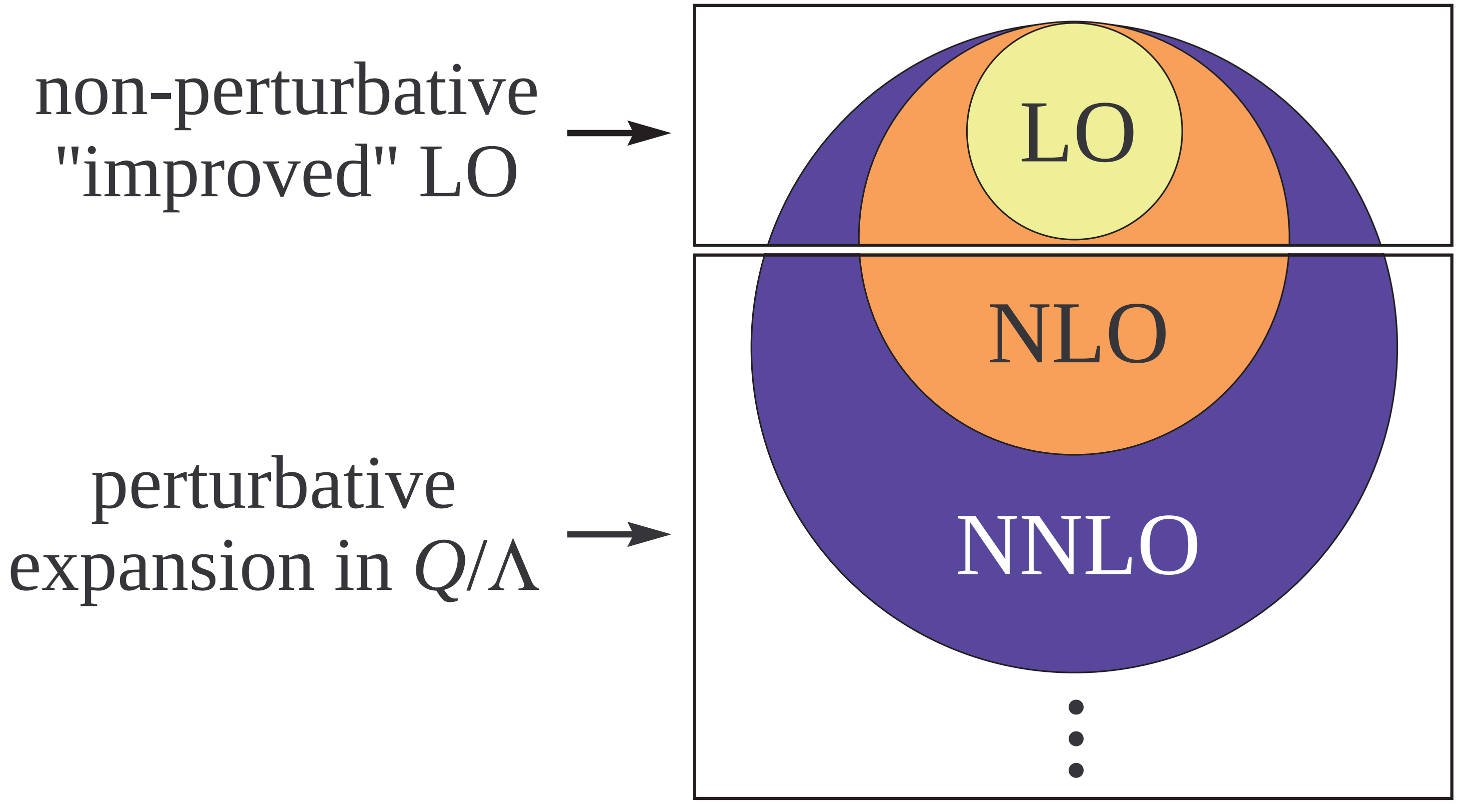
PHASE SHIFTS for LO3



- how to calculate these? → next lecture

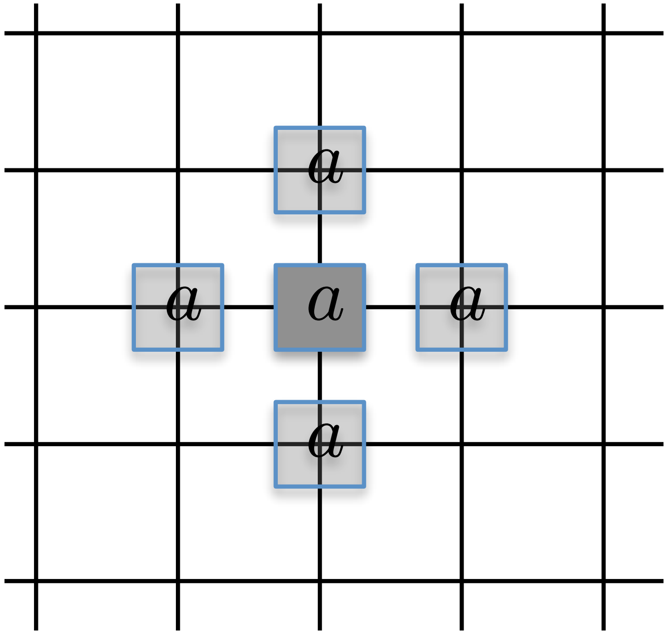
SMEARING EFFECTS

- Added advantage of the 4N smearing: resummation of range corrections



$\Rightarrow$ different types of smearing (OPE, non-local, ...) will be of use later

NON–LOCAL SMEARING



- Local operators/densities:

  $a(\mathbf{n}), a^\dagger(\mathbf{n})$ [$\mathbf{n}$ denotes a lattice point]

  $$\rho_{\rm L}(\mathbf{n}) = a^\dagger(\mathbf{n})a(\mathbf{n})$$

- Non-local operators/densities:

  $\hookrightarrow$ further suppresion of remaining sign oscillations

  $$a^{(\dagger)}_{\rm NL}(\mathbf{n}) = a^{(\dagger)}(\mathbf{n}) + s_{\rm NL}\sum_{\langle \mathbf{n}'\,\mathbf{n}\rangle} a^{(\dagger)}(\mathbf{n}')$$

  $$\rho_{\rm NL}(\mathbf{n}) = a^\dagger_{\rm NL}(\mathbf{n})a_{\rm NL}(\mathbf{n})$$

- where $\sum_{\langle \mathbf{n}'\,\mathbf{n}\rangle}$ denotes the sum over nearest-neighbor lattice sites of $\mathbf{n}$
- the smearing parameter $s_{\rm NL}$ is determined when fitting to the phase shifts
- turns out to be very significant!

ROTATIONAL SYMMETRY BREAKING

- Already mentioned: deal with the lattice spacing artefacts at finite a!
- Example: SO(3) $\to$ SO(3,Z) $\to$ new operators at NLO $O(Q^2)$ [more details later]

$$\sum_{l=1}^{3} q_l^2 \, (\sigma_A)_l \, (\sigma_B)_l \, , \quad (\tau_A \cdot \tau_B) \sum_{l=1}^{3} q_l^2 \, (\sigma_A)_l \, (\sigma_B)_l$$

- terms with total spin $S = 0, 2, 4$. $S = 0$ terms already included in NLO contact operators. Others introduce unphysical mixing such as ${}^3D_3$ into ${}^3S_1 - {}^3D_1$
- introduce two lattice operators

$$\tilde{V}_{R1} = \frac{1}{2}\,\tilde{C}_{R1} : \sum_{S=1}^{3} \sum_{\vec{n}} \left[\nabla_{S,(\nu)} \rho_S^{a^\dagger,a}(\vec{n}) \right] \nabla_{S,(\nu)} \rho_S^{a^\dagger,a}(\vec{n}) :$$

$$\tilde{V}_{R2} = \frac{1}{2}\,\tilde{C}_{R2} : \sum_{S=1}^{3} \sum_{I=1}^{3} \sum_{\vec{n}} \left[\nabla_{S,(\nu)} \rho_{S,I}^{a^\dagger,a}(\vec{n}) \right] \nabla_{S,(\nu)} \rho_{S,I}^{a^\dagger,a}(\vec{n}) :$$

$\to$ adjust the isoscalar combination of these terms to eliminate the unphysical mixing of the ${}^3D_3$ partial wave. The isovector comb. is set to zero (unphys. mixing tiny)

GALILEAN INVARIANCE BREAKING: NN SYSTEM

Li, Elhatisari, Epelbaum, Lu, Lee, UGM, Phys. Rev. C **99** (2019) 064001

- Consider np scattering first with total momentum $\vec{P} = 0$, match to Nijmegen PWA

- then boost to a moving frame with $\vec{P} = (2\pi/L)\vec{k}$

$\Rightarrow$ if the results are different, then there is Galilean invariance breaking →slide

- introduce operators to compensate for GIB (up-to-next-to-next-to-nearest neighbors)

$$V_{\rm GIR} = V^0_{\rm GIR} + V^1_{\rm GIR} + V^2_{\rm GIR}$$

$$V^0_{\rm GIR} = C^0_{\rm GIR} \sum_{\mathbf{n},i,j,i',j'} a^\dagger_{i,j}(\mathbf{n}) a^\dagger_{i',j'}(\mathbf{n}) a_{i',j'}(\mathbf{n}) a_{i,j}(\mathbf{n}$$

$$V^1_{\rm GIR} = C^1_{\rm GIR} \sum_{\mathbf{n},i,j,i',j'} \sum_{|\mathbf{n}'|=1} a^\dagger_{i,j}(\mathbf{n}+\mathbf{n}') a^\dagger_{i',j'}(\mathbf{n}+\mathbf{n}') a_{i',j'}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

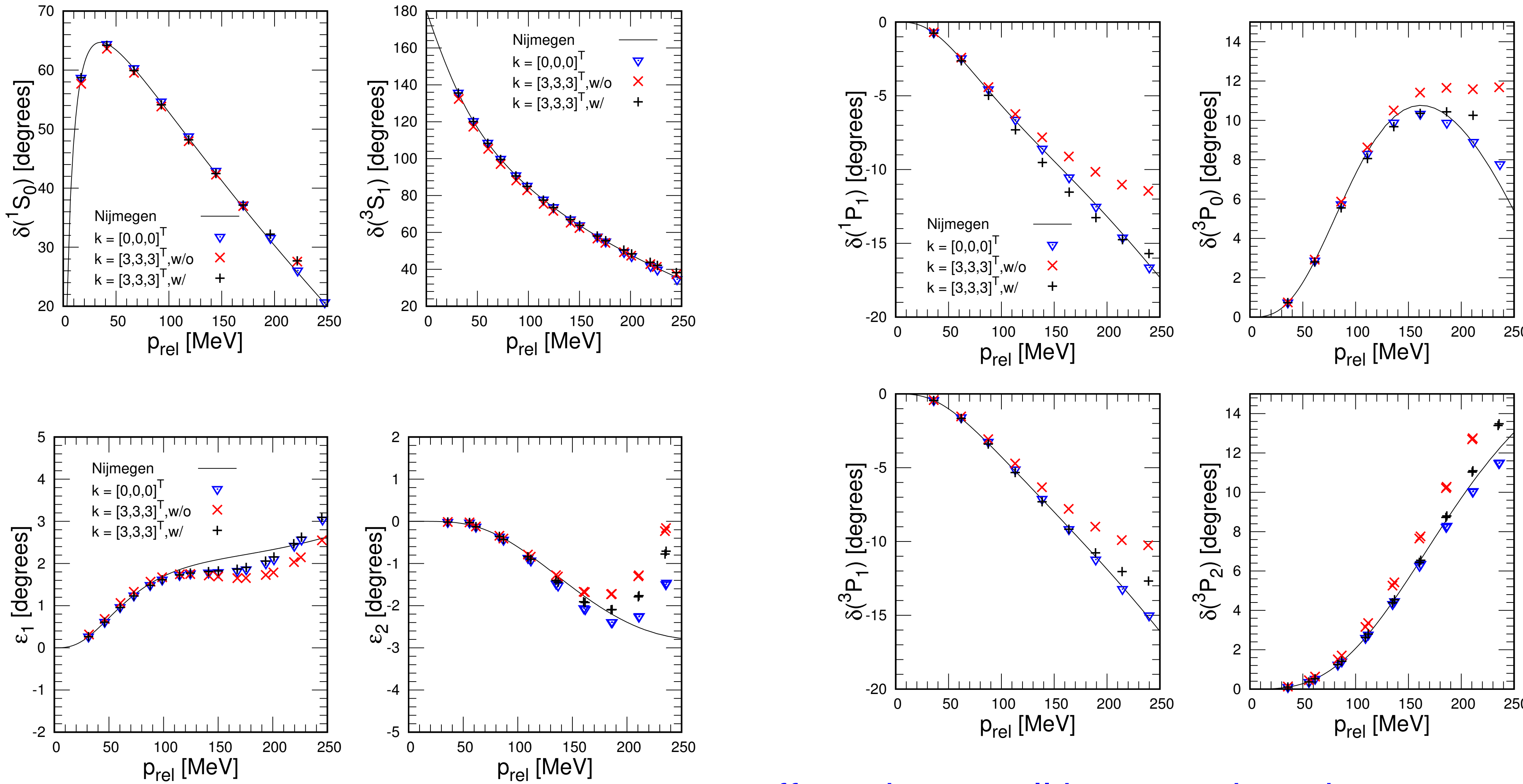
$$V^2_{\rm GIR} = C^2_{\rm GIR} \sum_{\mathbf{n},i,j,i',j'} \sum_{|\mathbf{n}'|=\sqrt{2}} a^\dagger_{i,j}(\mathbf{n}+\mathbf{n}') a^\dagger_{i',j'}(\mathbf{n}+\mathbf{n}') a_{i',j'}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

- restore GI by fixing the coefficients (in each partial wave such that)

$$\boxed{C^0_{\rm GIR} + 6C^1_{\rm GIR} + 12C^2_{\rm GIR} = 0}$$

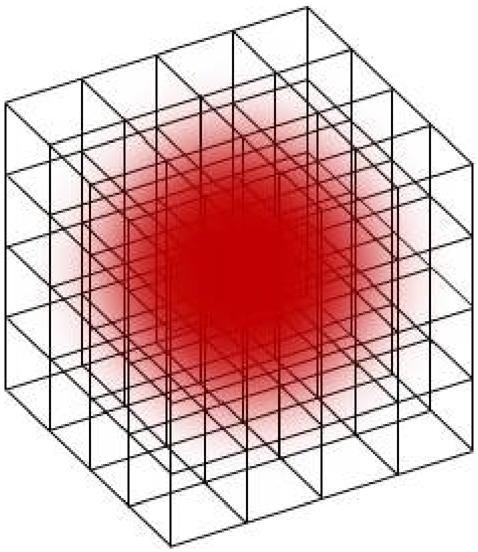
BREAKING and RESTORATION of GALILEAN INV.

- Consider highly smeared N3LO interactions, compare rest-frame $\boldsymbol{k} = [\mathbf{0}, \mathbf{0}, \mathbf{0}]$ with moving frame $\boldsymbol{k} = [\mathbf{3}, \mathbf{3}, \mathbf{3}]$



⇒ effects i.g. small but must be taken care of

CENTER-of-MASS PROBLEM



- AFQMC calculations involve states that are superpositions of many different center-of-mass (com) positions

$$Z_A(\tau) = \langle \Psi_A(\tau) | \Psi_A(\tau) \rangle$$

$$|\Psi_A(\tau)\rangle = \exp(-H\tau/2)|\Psi_A\rangle$$

- but: translational invariance requires summation over all transitions

$$Z_A(\tau) = \sum_{i_{\rm com}, j_{\rm com}} \langle \Psi_A(\tau, i_{\rm com}) | \Psi_A(\tau, j_{\rm com}) \rangle \, , \;\; {\rm com} = {\rm mod}((i_{\rm com} - j_{\rm com}), L)$$

$i_{\rm com}$ $(j_{\rm com})$ = position of the center-of-mass in the final (initial) state

- density distributions of nucleons can not be computed directly, only moments

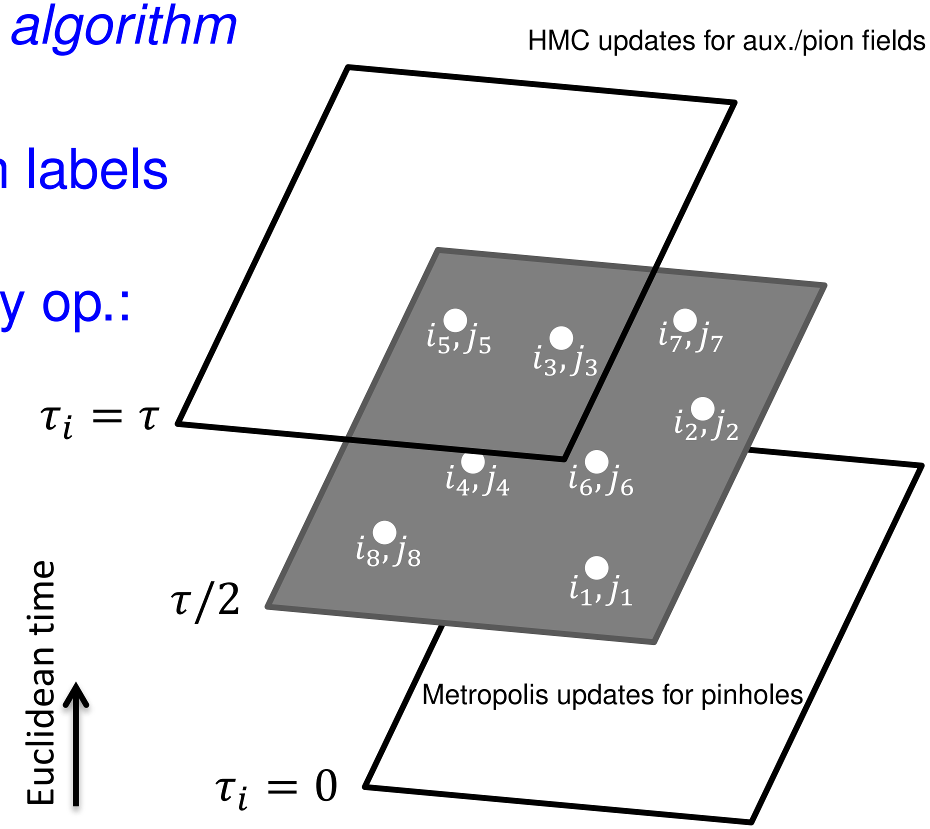
- need to overcome this deficieny

PINHOLE ALGORITHM

- Solution to the CM-problem:
  track the individual nucleons using the *pinhole algorithm*

- Insert a screen with pinholes with spin & isospin labels that allows nucleons with corresponding spin & isospin to pass = insertion of the A-body density op.:

$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A)$$
$$=: \rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$



- MC sampling of the amplitude:

$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A,L_t)$$
$$= \langle \Psi_A(\tau/2)|\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A)|\Psi_A(\tau/2)\rangle$$

- Allows to measure proton and neutron distributions

- Resolution scale $\sim a/A$ as cm position $\mathbf{r}_{\rm cm}$ is an integer $\mathbf{n}_{\rm cm}$ times a/A

Scattering on a lattice

spherical wall method: Borasoy, Epelbaum, Krebs, Lee, UGM, EPJA **34** (2007) 185

auxiliary potential method: Lu, Lähde, Lee, UGM, Phys. Lett. B**760** (2016) 309

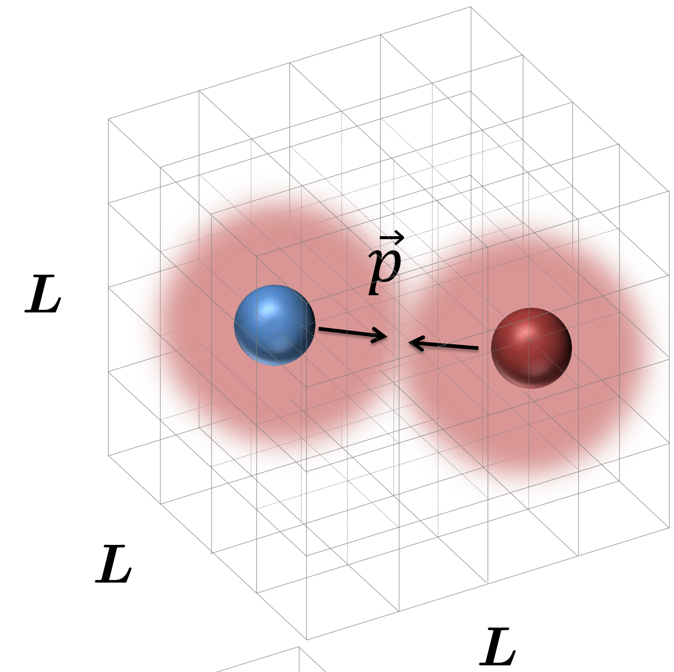
EXTRACTING PHASE SHIFTS on the LATTICE

- Lüscher's method:

  Two-body energy levels below the inelastic threshold on a periodic lattice are related to the phase shifts in the continuum

  Lüscher, Comm. Math. Phys. **105** (1986) 153

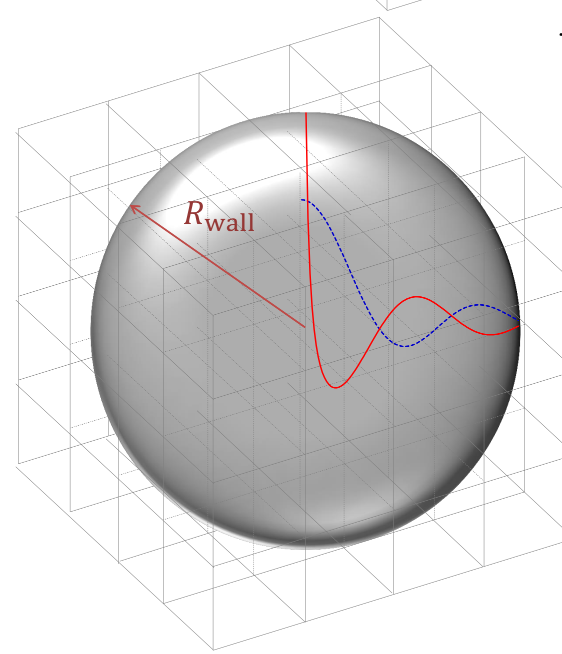
  Lüscher, Nucl. Phys. **354** (1991) 531



- Spherical wall method:

  Impose a hard wall on the lattice and use the fact that the wave function vanishes for $r = R_{\rm wall}$:

$$\psi_\ell(r) \sim [\cos\delta_\ell(p) j_\ell(pr) - \sin\delta_\ell(p) y_\ell(pr)]$$



  Borasoy, Epelbaum, Krebs, Lee, UGM, EPJA **34** (2007) 185

  Carlson,Pandharipande, Wiringa, NPA **424** (1984) 47

SCATTERING in a FINITE VOLUME

Lüscher, Comm. Math. Phys. **104** (1986) 177; **105** (1986) 153; Nucl. Phys, B **354** (1991) 531

- cubic lattice: rotation group SO(3) broken to SO(3,Z)

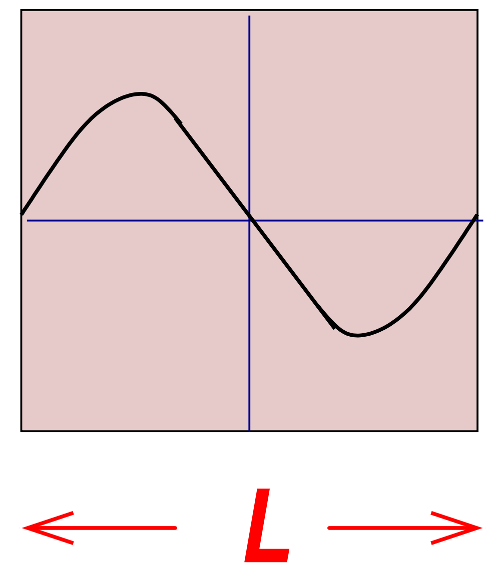
- 5 irreducible representations (A_1, T_1, E, T_2, A_2) include definite J modulo 4

- Lüscher's formula for phase shifts $(LM_{\rm light} \gg 1)$

$$\exp(2i\delta_0) = \frac{Z_{00}(1;q^2) + i\pi^{3/2}q}{Z_{00}(1;q^2) - i\pi^{3/2}q}$$

$$q = 2\pi n/L\,, \quad n \in \mathbb{Z}^3$$

$$Z_{00}(s;q^2) = \frac{1}{\sqrt{4\pi}} \sum_{n\in\mathbb{Z}^3} \frac{1}{(n^2-q^2)^s}$$



- standard method in lattice QCD, see e.g. NPLQCD on hadron-hadron scattering

Beane, Orginos, Savage, Int. J. Mod. Phys. E **17** (2008) 1517

- however: problems w/ partial-wave mixing & higher p.w., need a different formalism

SO(3,Z) REPRESENTATIONS

• Irreducible SO(3,Z) representations

	J_z (mod 4)	$Y_{L,M}(\theta,\phi)$
A_1	0	$Y_{0,0}$
T_1	0, 1, 3	$\{Y_{1,0}, Y_{1,1}, Y_{1,-1}\}$
E	0, 2	$\left\{Y_{2,0}, (Y_{2,-2}+Y_{2,2})/\sqrt{2}\right\}$
T_2	1, 2, 3	$\left\{Y_{2,1}, (Y_{2,-2}-Y_{2,2})/\sqrt{2}, Y_{2,-1}\right\}$
A_2	2	$\left\{(Y_{3,2}-Y_{3,-2})/\sqrt{2}\right\}$

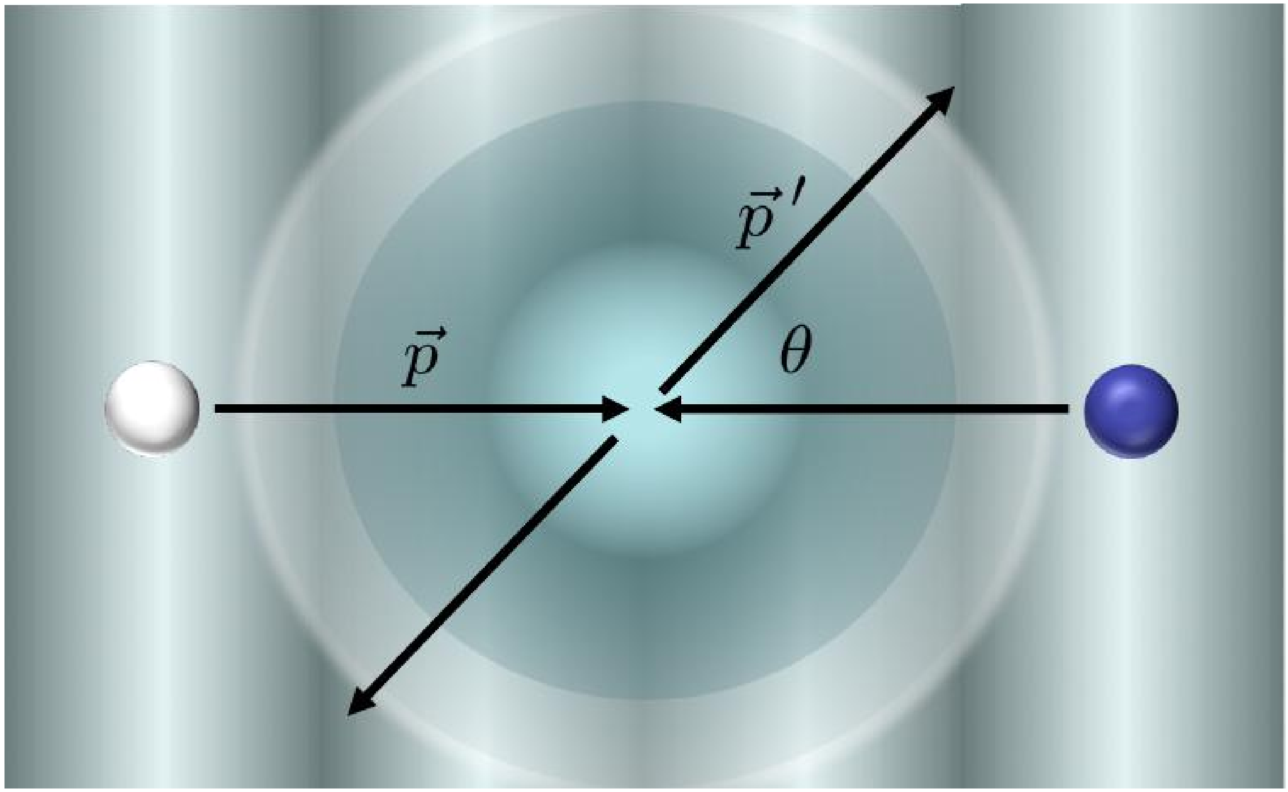
• SO(3,Z) decompositions

SO(3)	SO(3,Z)
$J=0$	A_1
$J=1$	T_1
$J=2$	$E\oplus T_2$
$J=3$	$T_1\oplus T_2\oplus A_2$

SO(3)	SO(3,Z)
$J=4$	$A_1\oplus T_1\oplus E\oplus T_2$
$J=5$	$T_1\oplus T_1\oplus E\oplus T_2$
$J=6$	$A_1\oplus T_1\oplus E\oplus T_2\oplus T_2\oplus A_2$
$J=7$	$T_1\oplus T_1\oplus E\oplus T_2\oplus T_2\oplus A_2$

REMINDER: SCATTERING THEORY I

- Two-body scattering theory in the center-of-mass (CMS) frame:



- Incoming and outgoing waves:

$$\psi(\vec{r}) \xrightarrow[r\to\infty]{} \exp(i\vec{p}\cdot\vec{r}) + f(\vec{p}\,',\vec{p})\frac{\exp(ipr)}{r}$$

REMINDER: SCATTERING THEORY II

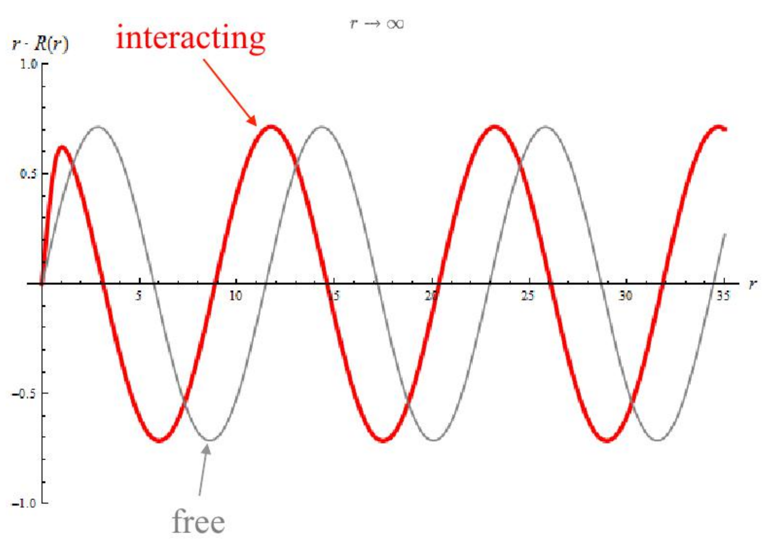
- Time-indepedent Schrödinger equation $\longrightarrow$ spherical waves

$$\psi(r,\theta,\phi) = R(r)\Phi(\theta,\phi)\ , \quad \Phi(\theta,\phi) = Y_{L,M}(\theta,\phi)$$

- all possible integers such that: $|M| \leq L$

$\longrightarrow$ radial equation: $u(r) = r \cdot R(r)$

$$-u''(r) + \left[2\mu V(r) + \frac{L(L+1)}{r^2}\right] u(r) = 2\mu E \cdot u(r)$$



$$r\cos\delta_L(p) j_L(pr) - r\sin\delta_L(p) y_L(pr) \underset{r\to\infty}{\longrightarrow} \sin[pr - \pi L/2 + \delta_L(p)]$$

$$r\, j_L(pr) \underset{r\to\infty}{\longrightarrow} \sin[pr - l\pi/2]$$

REMINDER: SCATTERING THEORY III

- S-matrix from the phase shift:

$$\sin[pr - \pi L/2 + \delta_L(p)]$$

$$= \frac{1}{2i}\left\{e^{i[pr-\pi L/2+\delta_L(p)]} - e^{-i[pr-\pi L/2+\delta_L(p)]}\right\}$$

$$= \frac{1}{2i}e^{-i\delta_L(p)}\left\{\underbrace{e^{2i\delta_L(p)}}_{S_L(p)} e^{i(pr-\pi L/2)} - e^{-i(pr-\pi L/2}\right\}$$

- Partial wave decomposition of the scattering amplitude:

$$\psi(\vec{r}) \underset{r\to\infty}{\longrightarrow} \exp(i\vec{p}\cdot\vec{r}) + f(\vec{p}\,',\vec{p})\frac{\exp(ipr)}{r}$$

$$f(\vec{p}\,',\vec{p}) = \sum_{L=0}^{\infty} f_L(p) P_L(\cos\theta)$$

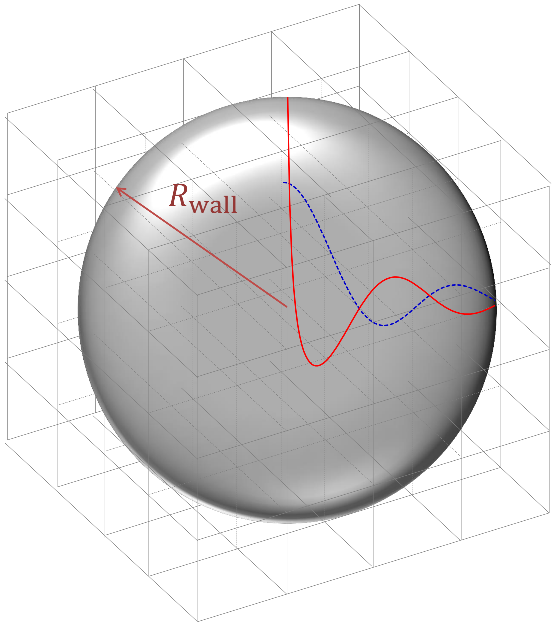
$$f_L(p) = \frac{-i}{2p}\left[e^{2i\delta_L(p)} - 1\right] = \frac{1}{p[\cot\delta_L(p) - i]}$$

[partial wave mixing can also be dealt with in more complex cases]

SPHERICAL WALL METHOD

- Spherical wall method: place a wall at sufficiently large $R = R_{\rm wall}$

$$V(\vec{n}_1 - \vec{n}_2) \to V(\vec{n}_1 - \vec{n}_2) + V_{\rm wall}\theta(|\vec{n}_1 - \vec{n}_2| - \tilde{R}_{\rm wall})$$

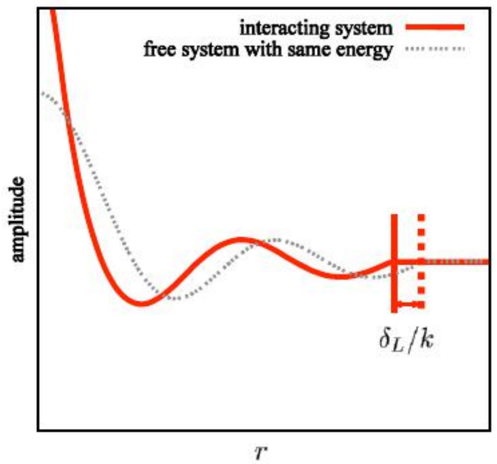


- standing wave allows to extract phase shifts δ_L and mixings ϵ_L

- uncoupled singlet partial waves:

$$\Psi(\vec{r}) = [\cos\delta_L j_L(kr) - \sin\delta_L y_L(kr)]Y_{L,m}(\theta,\phi)$$

$$\Psi(R) = 0 \Rightarrow \boxed{\tan\delta_L = \frac{j_L(kR)}{y_L(kR)}}$$



- coupled triplet waves: more involved

- see chapter 5 of the book

MEASURING PHASE SHIFTS on the LATTICE I

- Toy model: attractive Gaussian potential w/ central & tensor forces

  reproduces continuum phase shifts accurately

  extra copies of the 2-particle interaction
  due to periodic b.c. removed

  much better than standard boxes

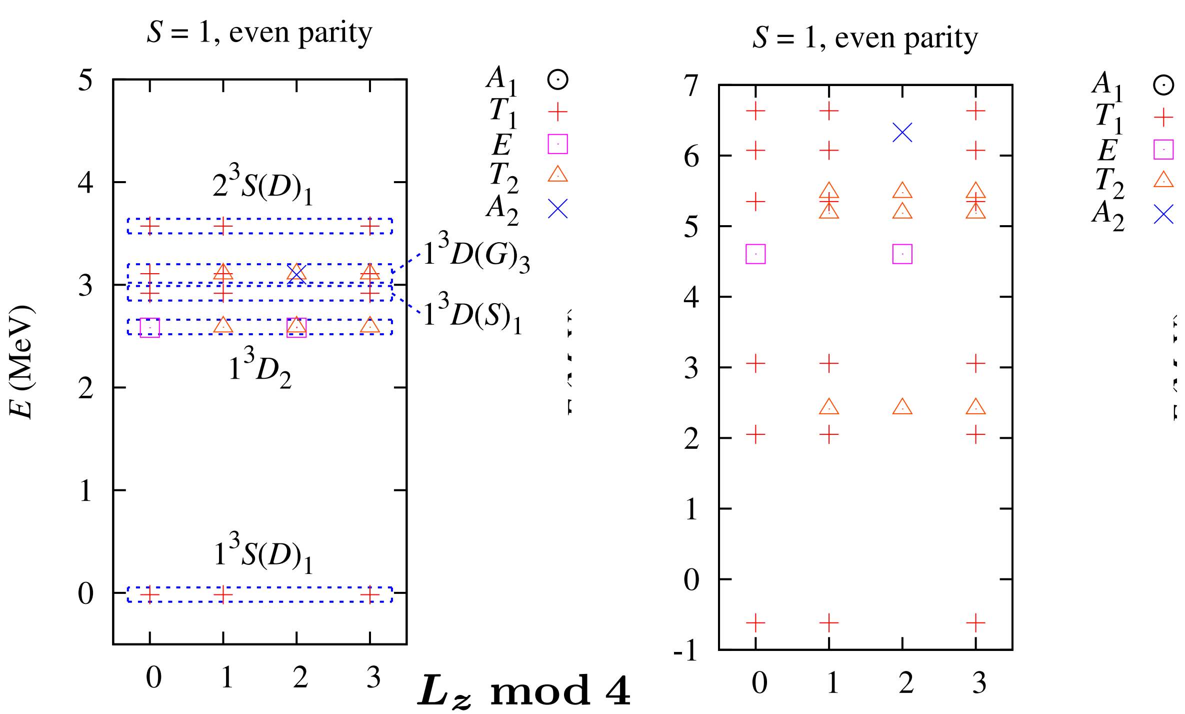
$$V(r) = C\left\{1 + \frac{r^2}{R_0^2}\,S_{12}(\hat{r})\right\}\exp\left(-\frac{1}{2}\frac{r^2}{R_0^2}\right)$$

$$S_{12}(\hat{r}) = 3(\hat{r}\cdot\vec{\sigma}_1)(\hat{r}\cdot\vec{\sigma}_2) - \vec{\sigma}_1\cdot\vec{\sigma}_2$$

$$C = -2\,\text{MeV},\quad R_0 = 0.02\,\text{MeV}^{-1}$$

$$m = 938.92\,\text{MeV}$$

$$R = 10 + \epsilon \qquad \text{vs} \qquad V = 12^3$$

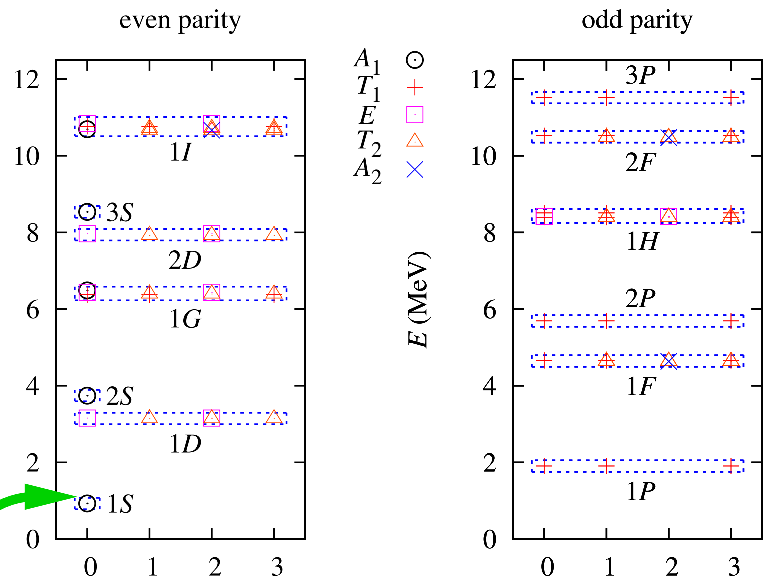


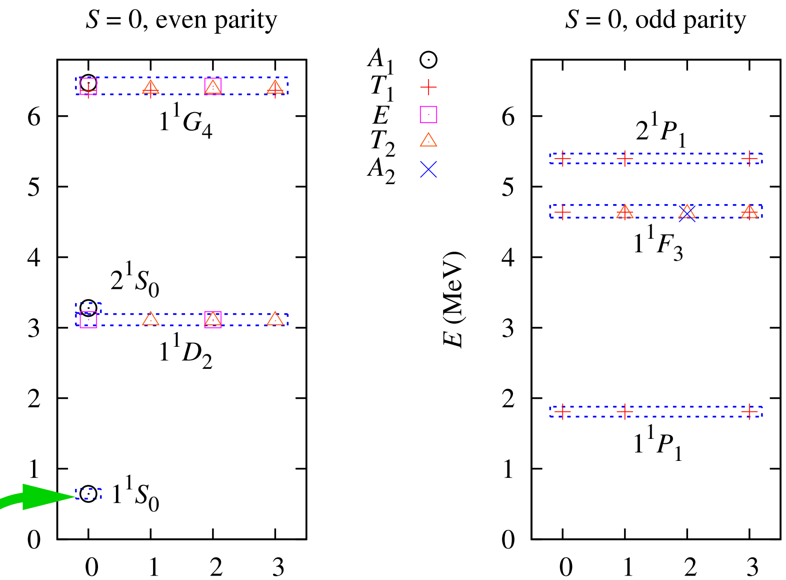
$\Downarrow$

a shallow bound-state in the $^3S_1$-$^3D_1$ channel with a binding energy of -0.155 MeV

MEASURING PHASE SHIFTS on the LATTICE II

- Free particle spectrum for $R = 10 + \epsilon$
- Interacting spectrum for $S = 0$





L_z mod 4

1^1S_0 energy = 0.9280 MeV

$\Downarrow$

$k_{\rm free} = 29.52$ Mev, $j_0(k_{\rm free}R) = 0$

$\Downarrow$

$$R = \frac{\pi}{k_{\rm free}} = 0.1064\,\text{MeV}^{-1}$$

1^1S_0 energy = 0.6445 MeV

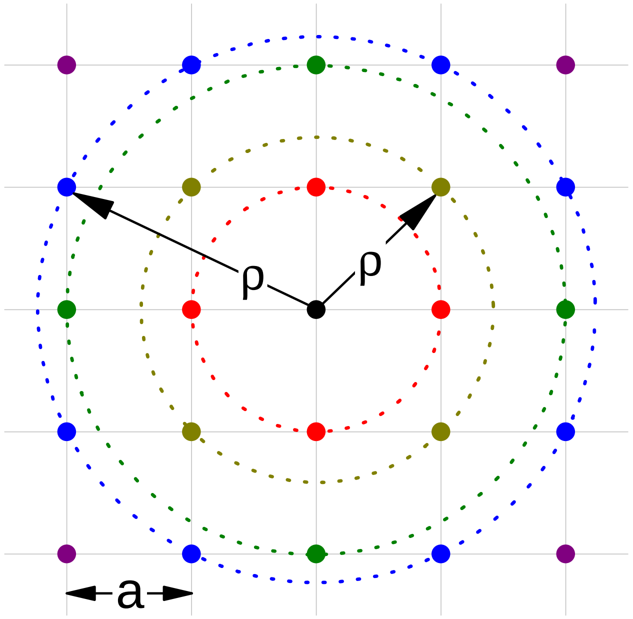
$\Downarrow$

$k = 24.60$ MeV

$\Downarrow$

$$\delta(^1S_0) = \tan^{-1}\left[\frac{j_0(kR)}{y_0(kR)}\right] = 30^\circ$$

RADIAL HAMILTONIAN METHOD



- Consider $|\vec{r}\rangle \otimes |S_z\rangle$: a two-body quantum state with separation $\vec{r}$ and z-component of total spin S_z
- Define radial lattice coordinates (ρ, φ) by grouping equidistant mesh points
- Construct radial wave functions with total angular momentum (J, J_z):

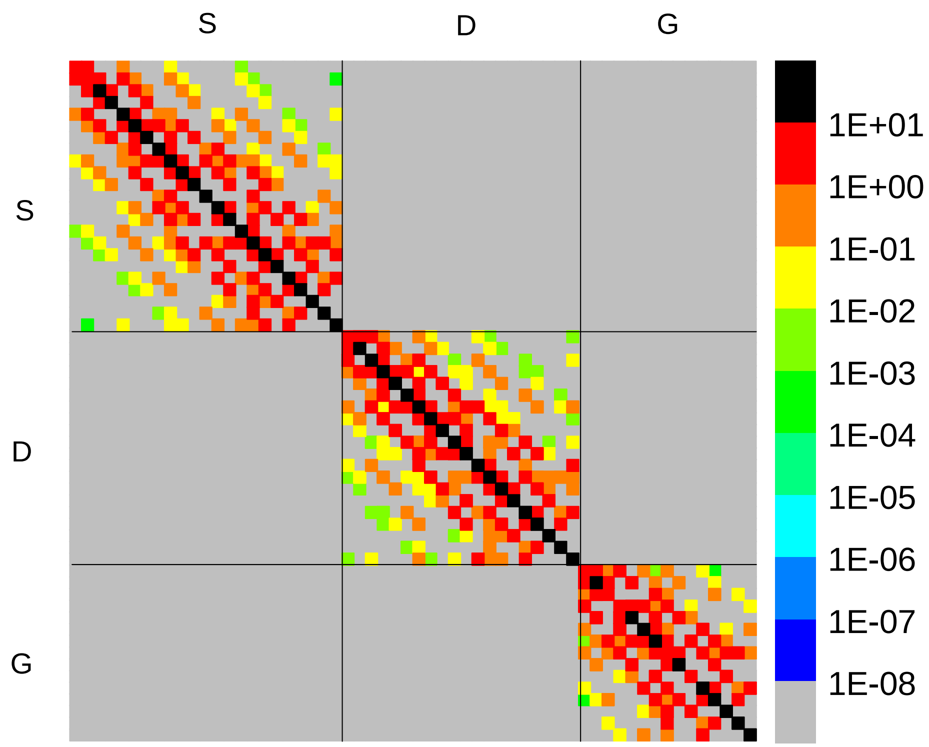
$$|m\rangle^{(J),(J_z)}_{(L)} = \sum_{\vec{n},L_z,S_z} \underbrace{C^{J,J_z}_{L,L_z,S,S_z}}_{\text{CG coeffs}} \underbrace{Y_{L,L_z}(\hat{n})}_{\text{sph. harmonics}} \times \underbrace{\delta_{\rho_m,|\vec{n}|}}_{\text{radial shell}} |\vec{n}\rangle \otimes |S_z\rangle$$

- not exactly good quantum numbers, denoted by (J) etc
- pick out all lattice points for which $\rho_m = |\vec{n}|$
- the $|m\rangle^{J,J_z}_{L}$ form a complete (but non-orthonormal) basis $\rightarrow$ compute norm matrices

RADIAL HAMILTONIAN METHOD continued

- Rotational symmetry breaking disappears as $a \to 0$, how much is left at finite a?

- study our toy model w/ the tensor force switched off:



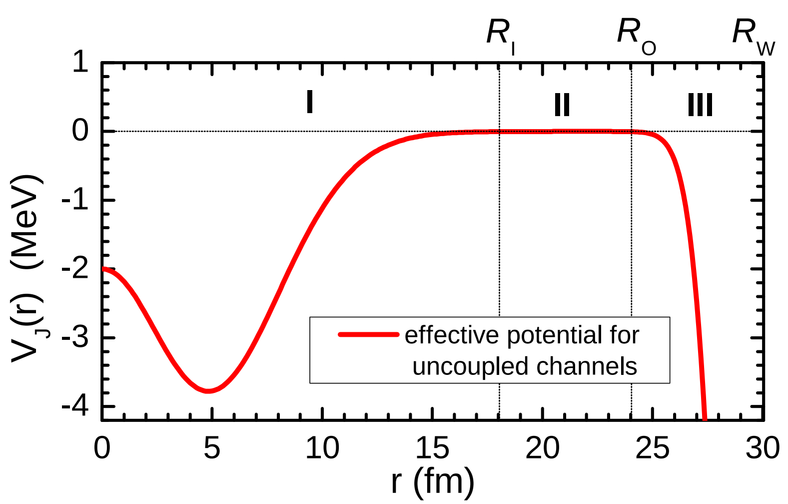
- magnitude of unphysical mixing matrix elements is greatly suppressed

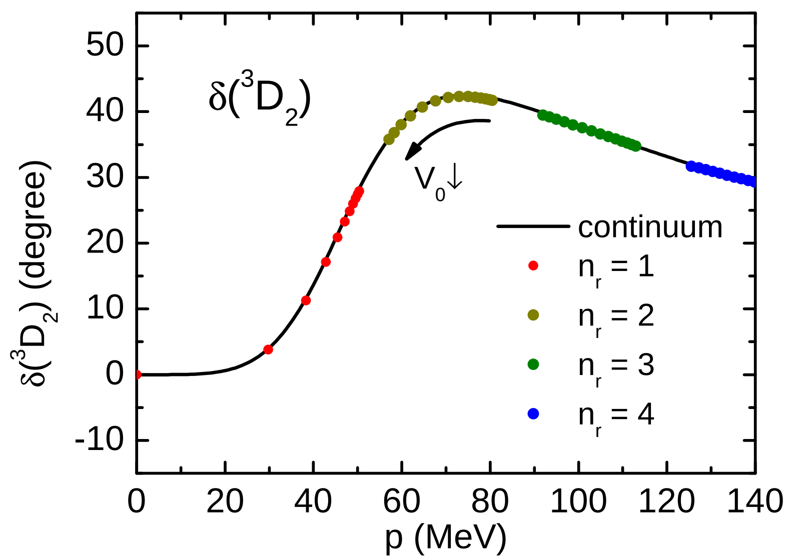
AUXILIARY POTENTIAL METHOD

- Simple sph. wall: small energies require large volumes, accuracy limited
- Improved method: auxiliary potential $\rightarrow$ shift energy levels

$$V_{\rm aux} = V_0 \exp\left[-(r-R_W)^2/a^2\right] \;, \quad R_0 \le r \le R_W$$

- Single channel potential ($V_0 = -25$ MeV)
- typical phase shift





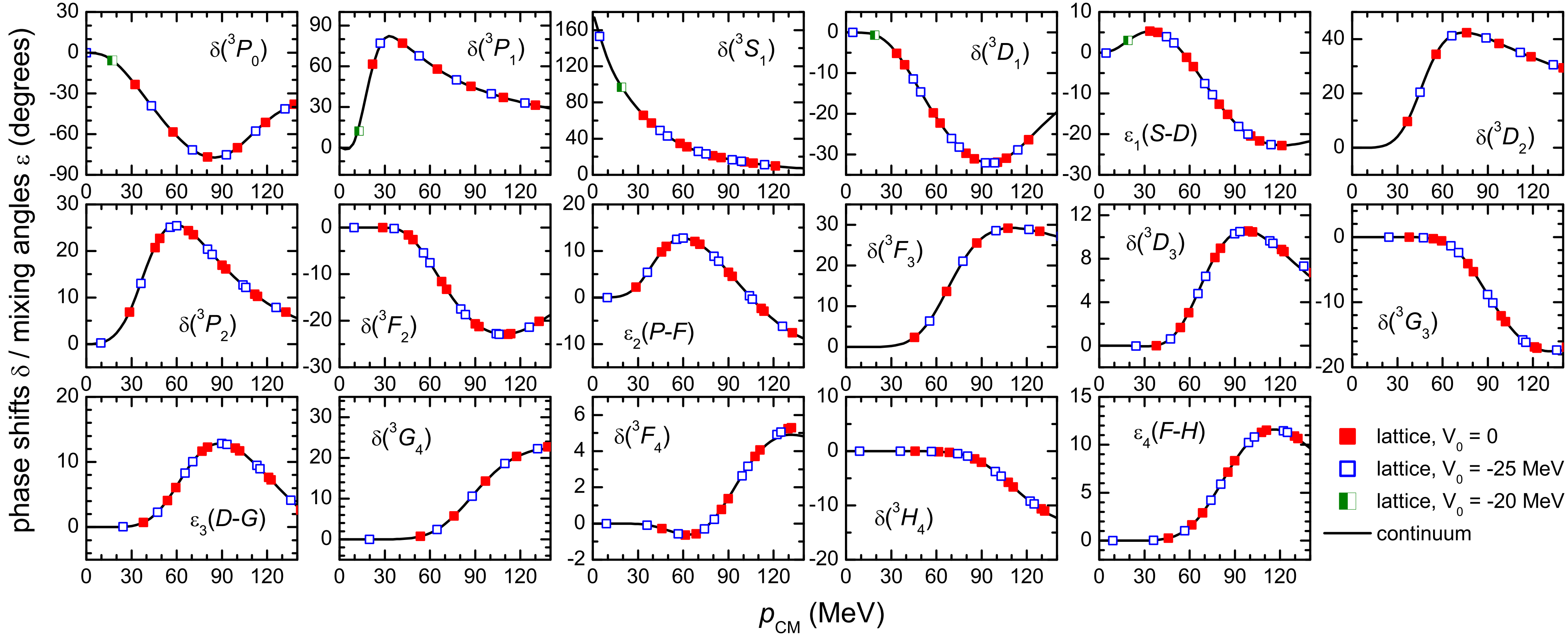
- Extension to coupled channels requires time-reversal symmetry breaking

$\hookrightarrow$ details see in the above reference or in the book

AUXILIARY POTENTIAL METHOD: RESULTS

Lu, Lähde, Lee, UGM, Phys. Lett. **B 760** (2016) 309

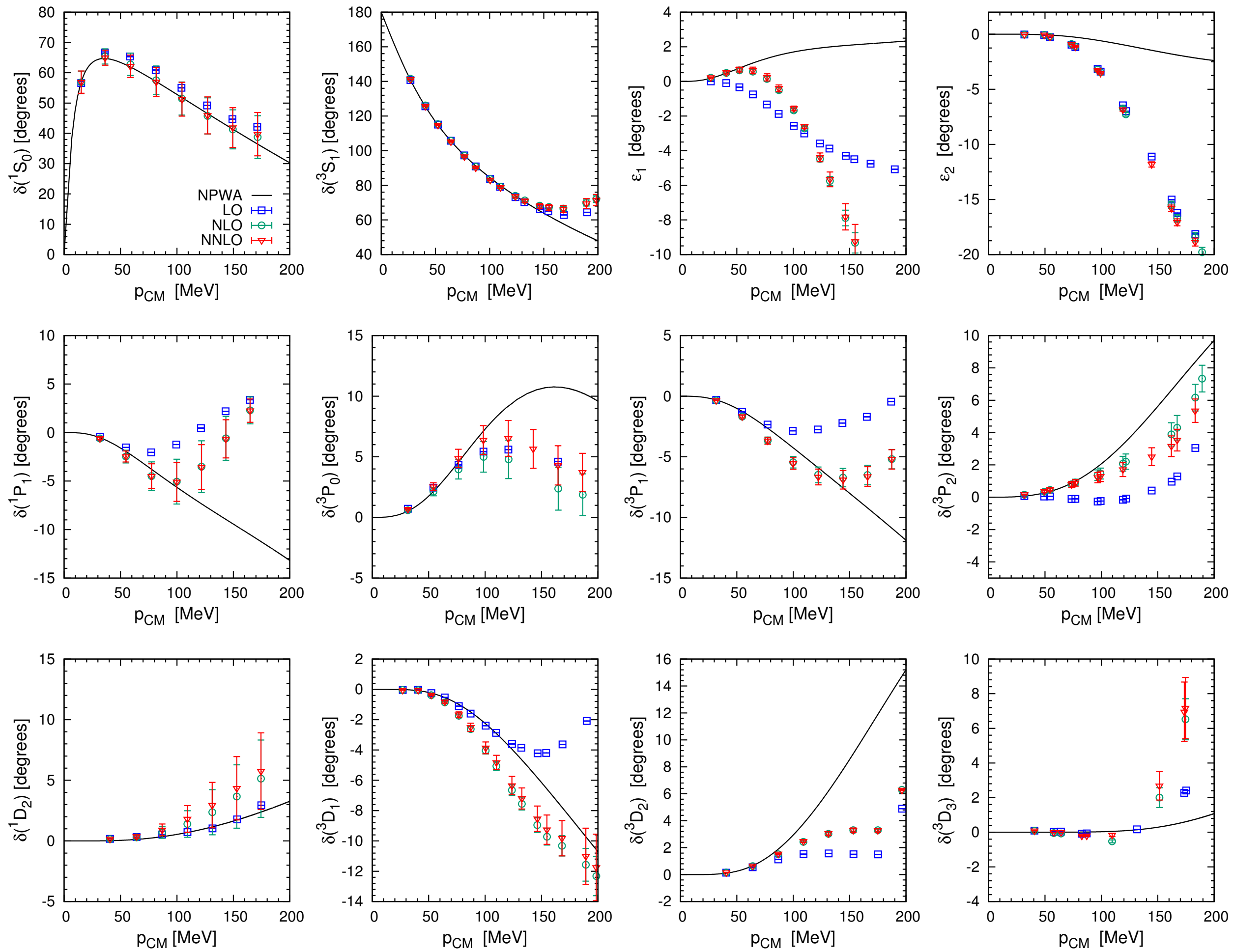
- same toy model with $R_I = 9.02a, R_0 = 12.02a, R_W = 15.02a$ and $U_0 = 20.0$ MeV
- continuum results from solving the LS equation



NLEFT PHASE SHIFTS at N2LO

Alarcon et al., Eur. Phys. J. **A53** (2017) 83

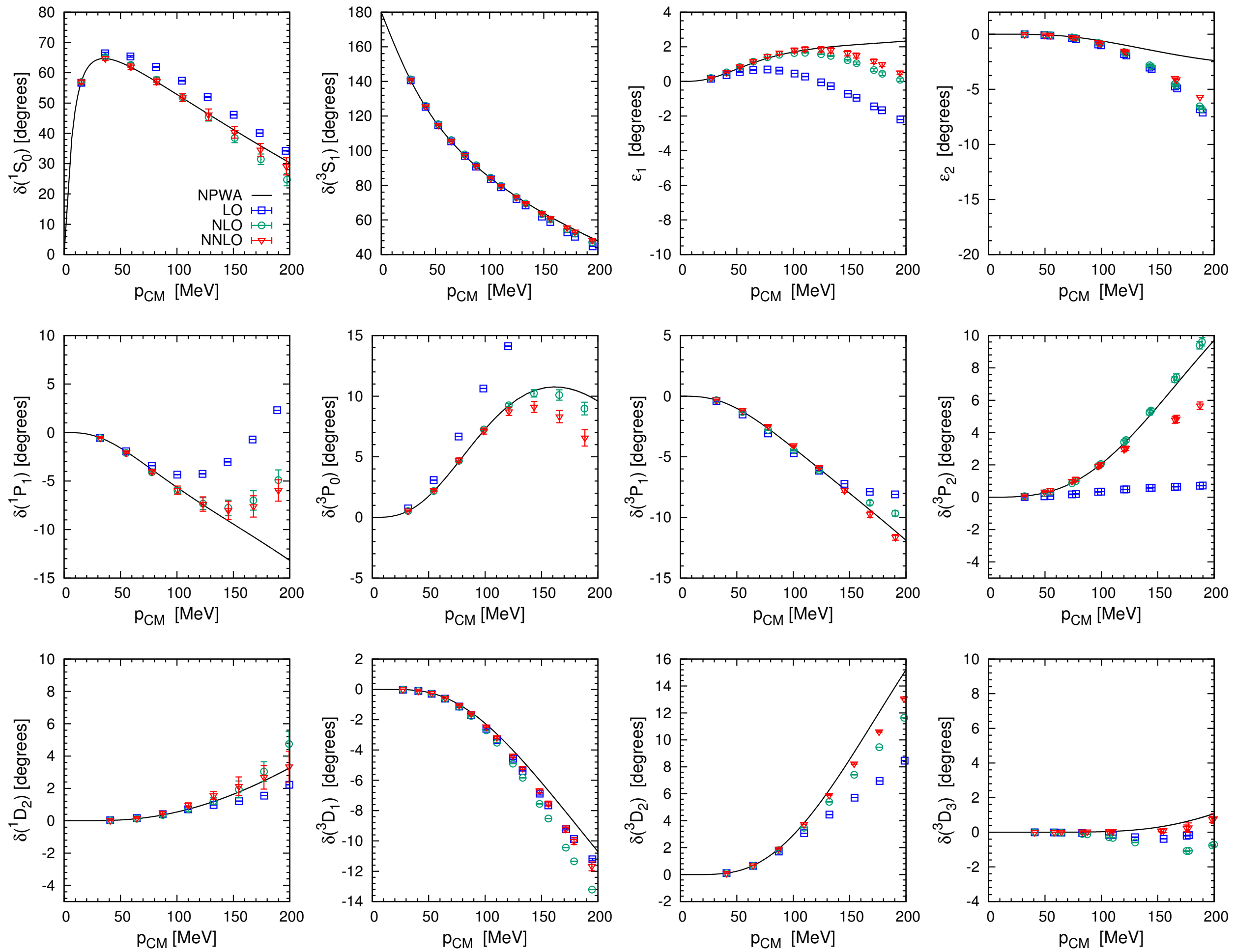
- Consider np scattering for $a = 1.97$ fm – a coarse lattice



NLEFT PHASE SHIFTS at N2LO

Alarcon et al., Eur. Phys. J. **A53** (2017) 83

- Consider np scattering for $a = 0.98$ fm – a fine lattice

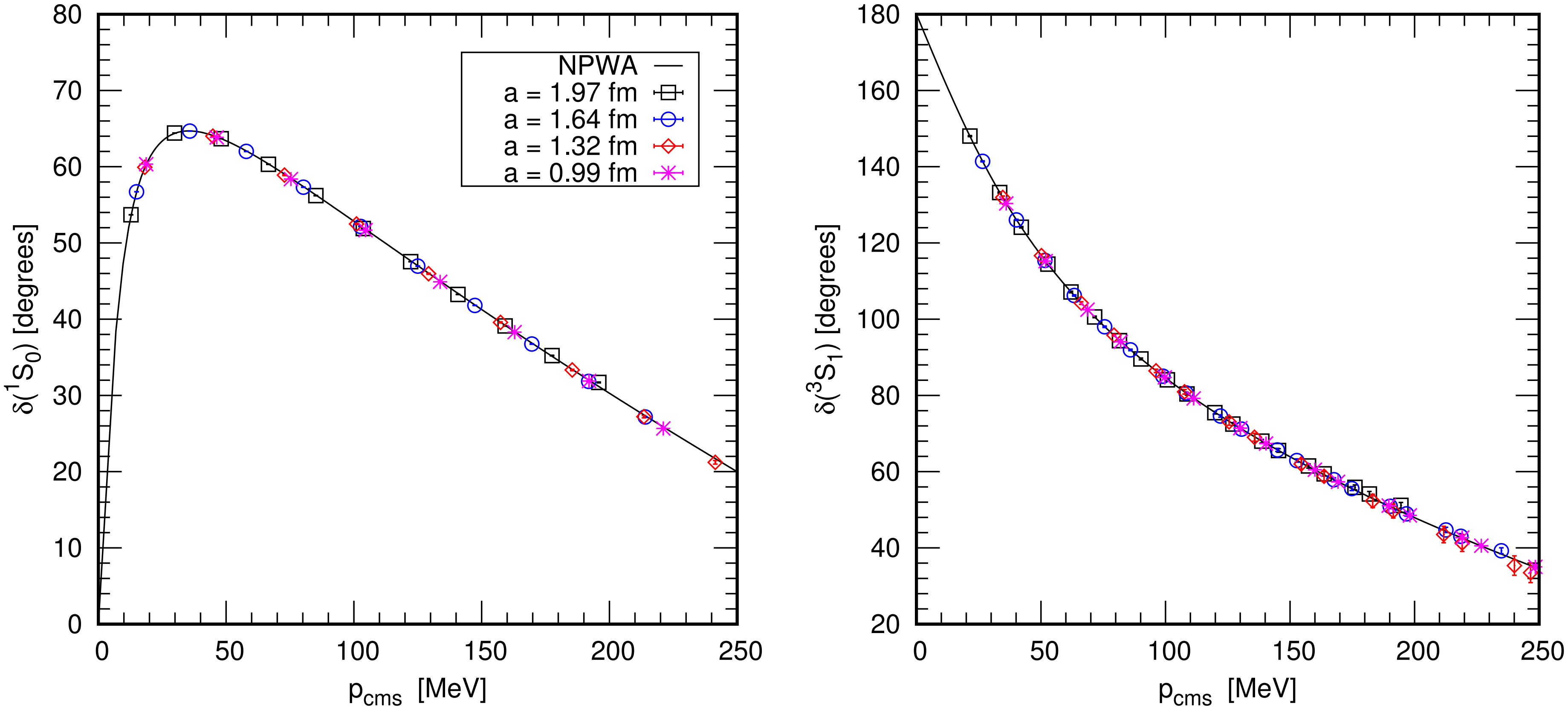


- some residual lattice spacing dependence

NLEFT PHASE SHIFTS at N3LO

Li et al., Phys. Rev. **C98** (2018) 044002

- Consider np scattering for $a = 0.99 - 1.97$ fm – S-waves

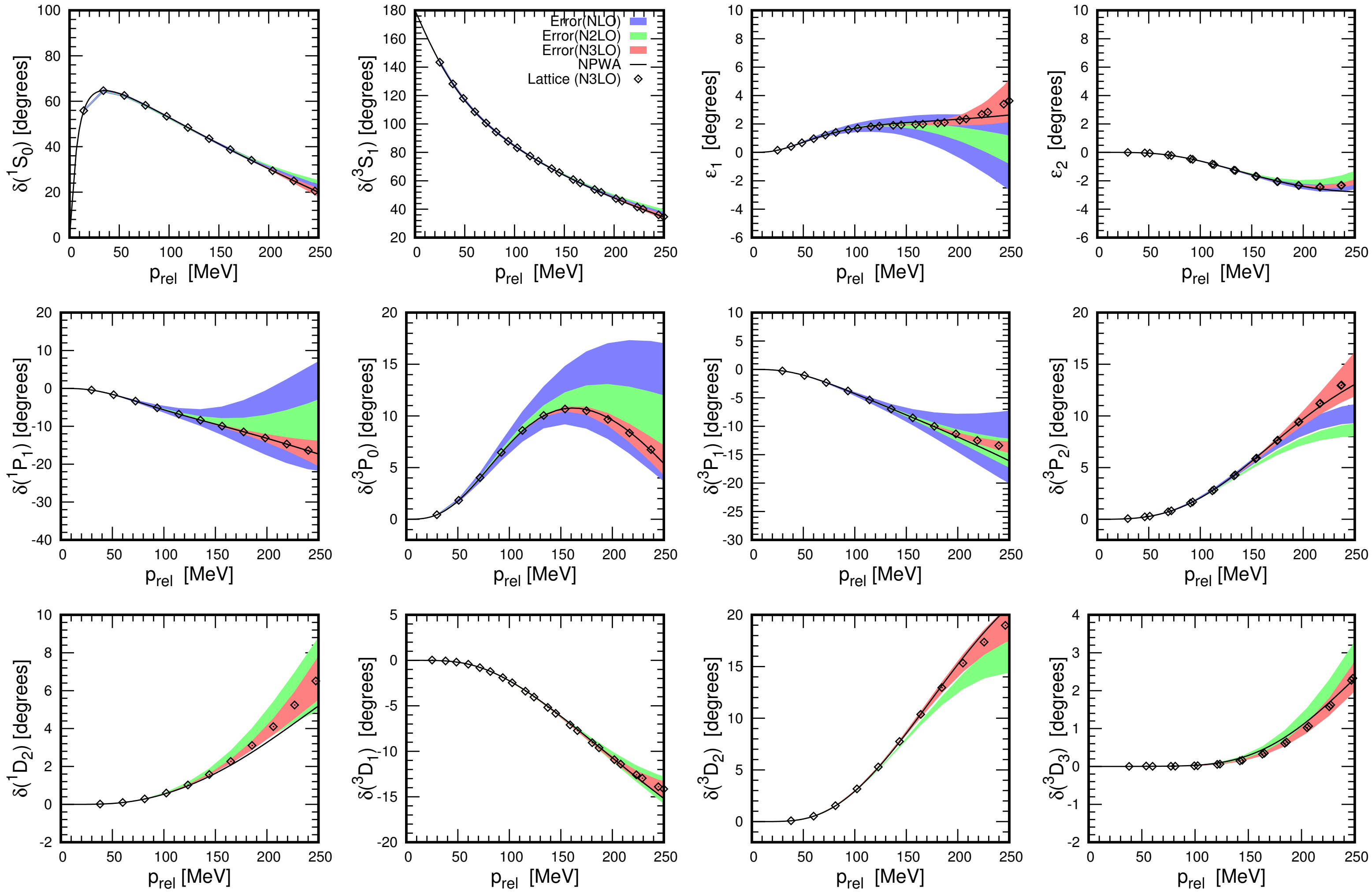


- **no more** lattice spacing dependence

NLEFT PHASE SHIFTS at N3LO

Li et al., Phys. Rev. **C98** (2018) 044002

- np scattering for $a = 1.97$ fm with error bands $\rightarrow$ small at N3LO



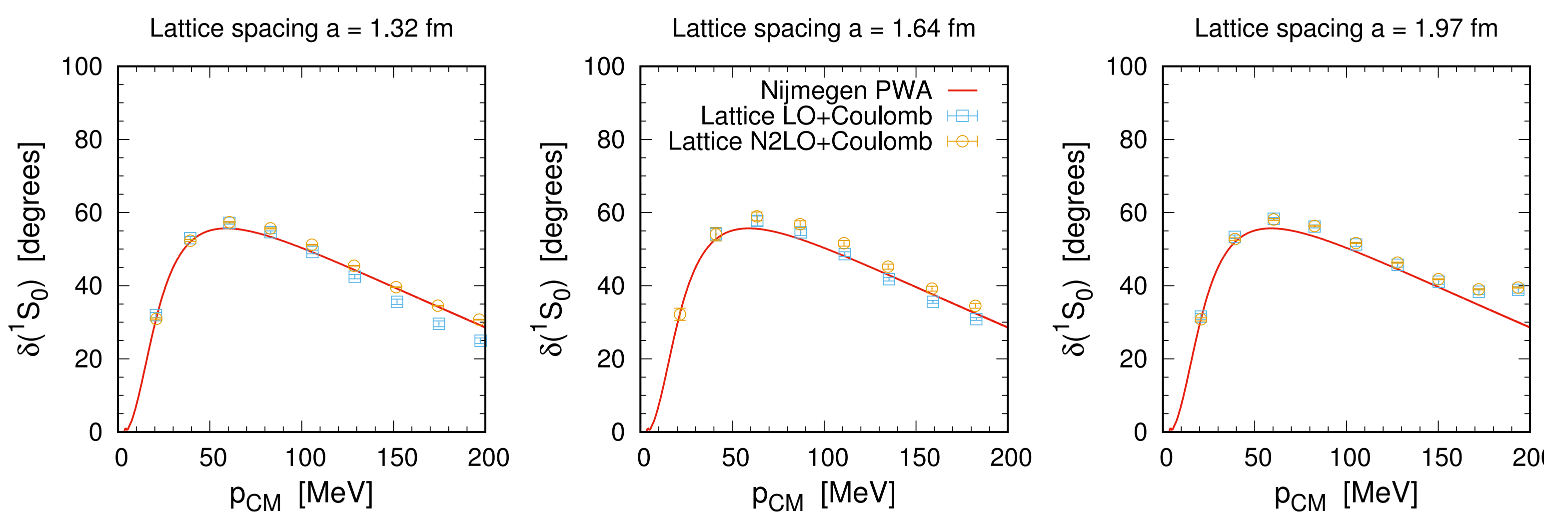
PROTON-PROTON SCATTERING at N2LO

Klein, Elhatisari, Lee, UGM, Eur. Phys. J. A**54** (2018) 121

- well-established formalism, substitute the Bessel and von Neumann functions by the respective Coulomb functions in terms of $\eta = \alpha_{\rm EM}/(2m_p)$:

$$j_\ell(pr) \to F_\ell(\eta, pr)\ ,\quad y_\ell(pr) \to G_\ell(\eta, pr)$$

- results at LO and N2LO for various lattice spacings:

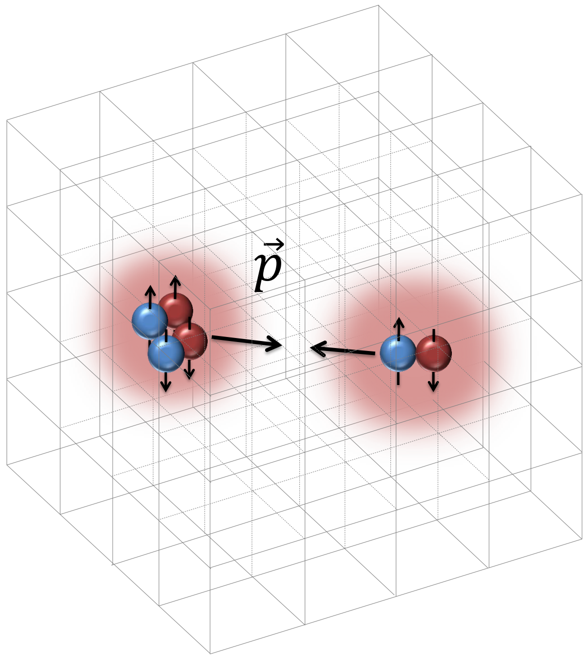


- fine descriptions, improved at N3LO
- for details on the formalism, see chapter 5 of the book

NUCLEUS-NUCLEUS SCATTERING on the LATTICE

- Processes involving α-particles and α-type nuclei comprise a major part of stellar nucleosynthesis, and control the production of certain elements in stars e.g. $\alpha+{}^{12}\text{C}\to{}^{16}\text{O}+\gamma$

- Ab initio calculations of scattering and reactions suffer from computational scaling with the number of nucleons in the clusters (exponential or factorial)



NLEFT computational scaling $\Rightarrow$ $(A_1 + A_2)^2$

Rupak, Lee, Phys. Rev. Lett. **111** (2013) 032502
Pine, Lee, Rupak, Eur. Phys. J. A **49** (2013) 151
Elhatisari, Lee, Phys. Rev. C **90** (2014) 064001
Rokash et al., Phys. Rev. C **92** (2015) 054612
Elhatisari, Lee, UGM, Rupak, Eur. Phys. J. A **52** (2016) 174

ADIABATIC PROJECTION METHOD

- Basic idea to treat scattering and inelastic reactions:
  split the problem into two parts

First part:
use Euclidean time projection to construct an *ab initio* low-energy cluster Hamiltonian, called the **adiabatic Hamiltonian**

Second part:
compute the two-cluster scattering phase shifts or reaction amplitudes using the adiabatic Hamiltonian

ADIABATIC PROJECTION METHOD II

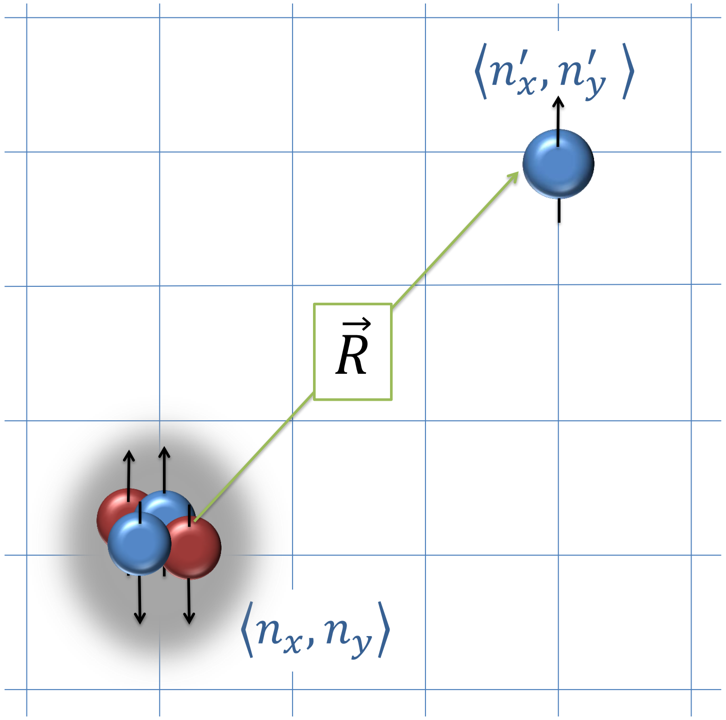
- Construct a low-energy effective theory for clusters

- Use initial states parameterized by the relative separation between clusters

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r} + \vec{R}\rangle \otimes \vec{r}$$

- project them in Euclidean time with the chiral EFT Hamiltonian H

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$



$\rightarrow$ "dressed cluster states" (polarization, deformation, Pauli)

- The adiabatic projection in Euclidean times gives a systematically improvable description of the low-lying scattering states

- In the limit of large Euclidean time, the description becomes exact

ADIABATIC HAMILTONIAN

- Construct the adiabatic Hamiltonian from the dressed cluster states:

$$[H_\tau]_{\vec{R}\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

- States are i.g. not normalized, require *norm matrix*:

$$[N_\tau]_{\vec{R}\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

- construct the full adiabatic Hamiltonian:

$$[H_\tau^a]_{\vec{R}\vec{R}'} = \sum_{\vec{R}_n\vec{R}_m} \left[N_\tau^{-1/2}\right]_{\vec{R}\vec{R}_n} \left[H_\tau\right]_{\vec{R}_n\vec{R}_m} \left[N_\tau^{-1/2}\right]_{\vec{R}_m\vec{R}'}$$

$\rightarrow$ The structure of the adiabatic Hamiltonian is similar to the Hamiltonian matrix used in recent ab initio NCSM/RGM calculations

Navratil, Quaglioni, Phys. Rev. C **83** (2011) 044609
Navratil, Roth, Quaglioni, Phys. Lett. B **704** (2011) 379
Navratil, Quaglioni, Phys. Rev. Lett. **108** (2012) 042503

SCATTERING CLUSTER WAVE FUNCTIONS

- During Euclidean time interval τ_ε, each cluster undergoes spatial diffusion:

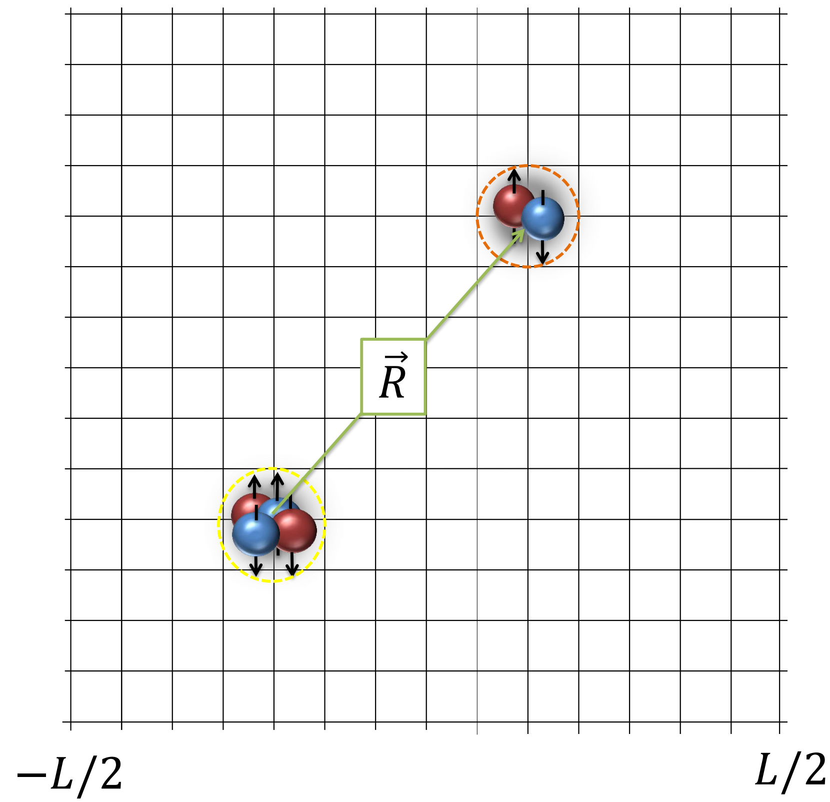
$$d_{\varepsilon,i} = \sqrt{\tau_\varepsilon / M_i}$$

- Only non-overlapping clusters if

$$|\vec{R}| \gg d_{\varepsilon,i} \quad \Rightarrow \quad |\vec{R}\rangle_{\tau_\varepsilon}$$

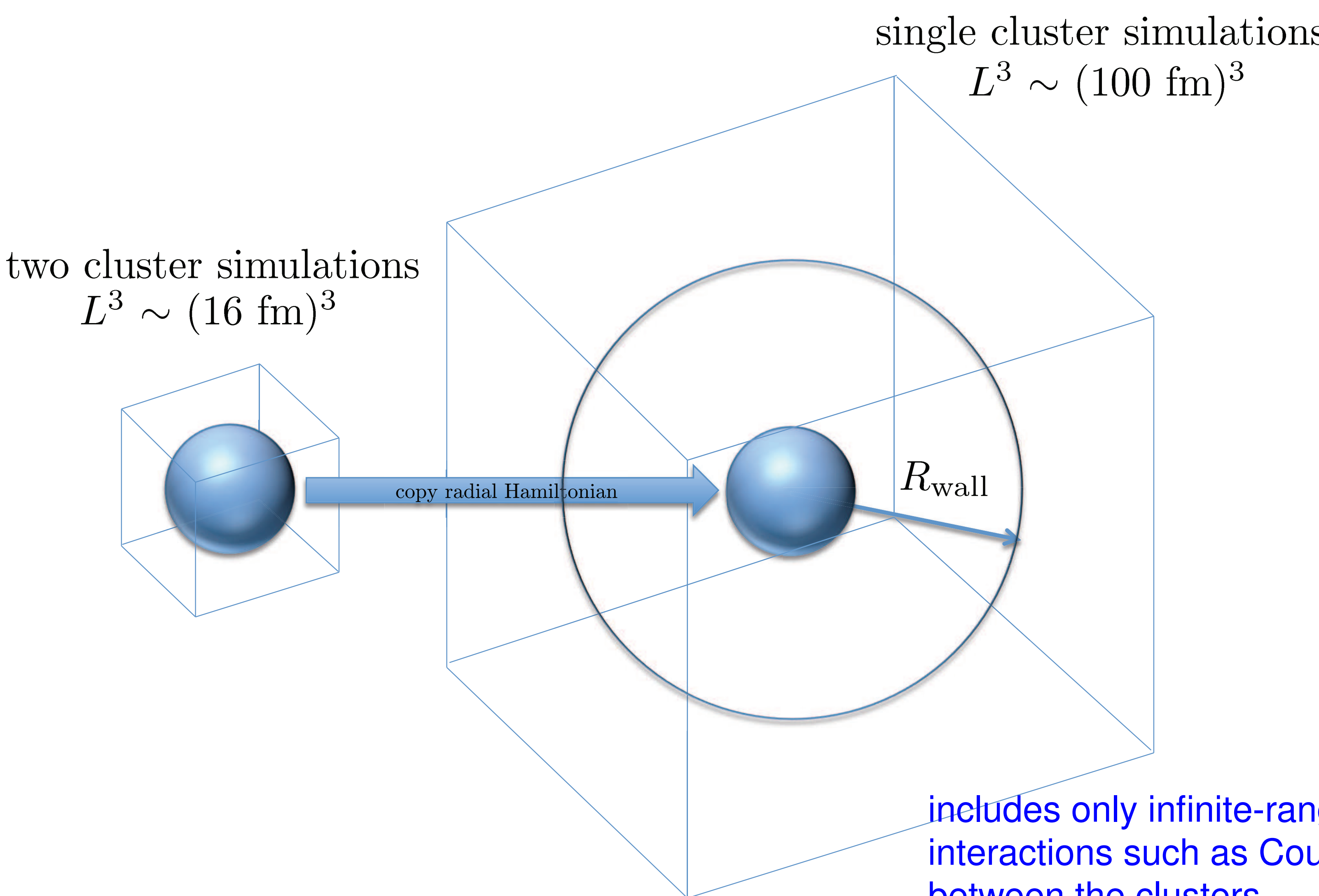
- Defines asymptotic region, where the amount of overlap between clusters is less than ε

$$|\vec{R}| > R_\varepsilon$$



$\Rightarrow$ In the asymptotic region we can describe the system in terms of an effective cluster Hamiltonian (the free lattice Hamiltonian for two clusters) plus infinite-range interactions (like the Coulomb int.)

ADIABATIC HAMILTONIAN plus COULOMB



includes only infinite-range interactions such as Coulomb between the clusters

TESTING the ADIABATIC HAMILTONIAN

- Consider fermion-dimer scattering (Fermion = $|\uparrow\rangle$, dimer = $|\uparrow\rangle \times |\downarrow\rangle$)
- Fermion mass = m_N
- $V(\vec{r} - \vec{r}') = c_0 \delta^{(3)}(\vec{r} - \vec{r}')$, c_0 tuned to the deuteron B.E.
- Microscopic Hamiltonian scaling:

  $L^{3(A-1)} \times L^{3(A-1)}$

- Adiabatic Hamitltonian scaling:

  $L^3 \times L^3$

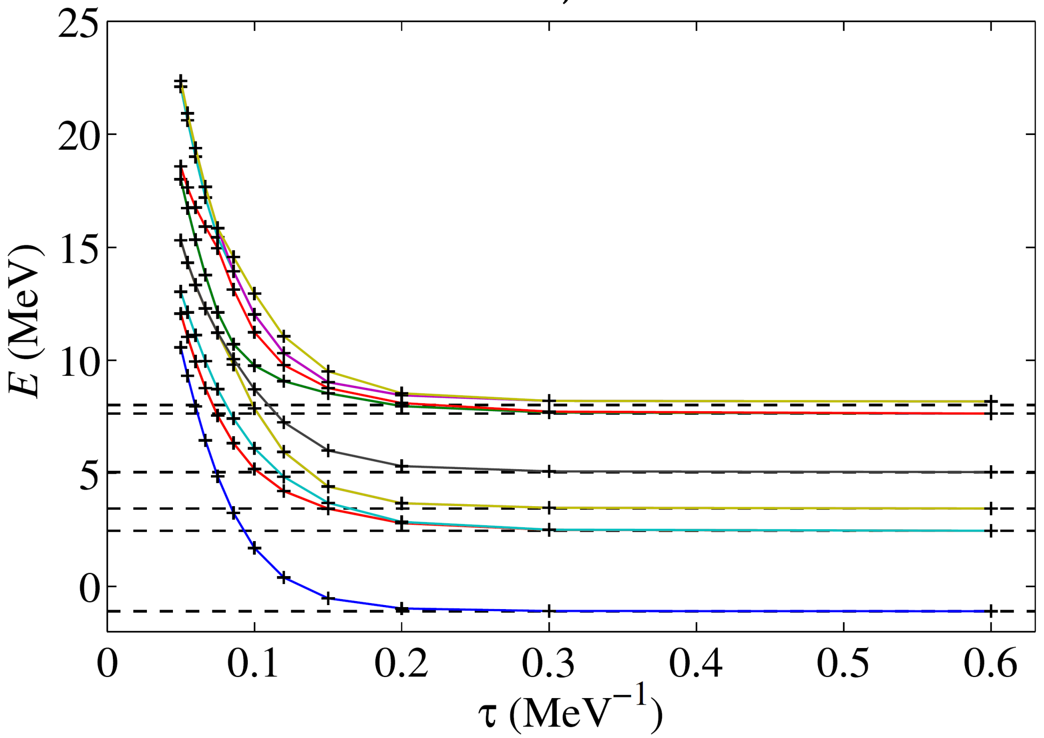
- calculation on a 7^3 lattice, lattice spacing $a = 1.93$ fm

Pine, Lee, Rupak, EPJA 49 (2013) 151

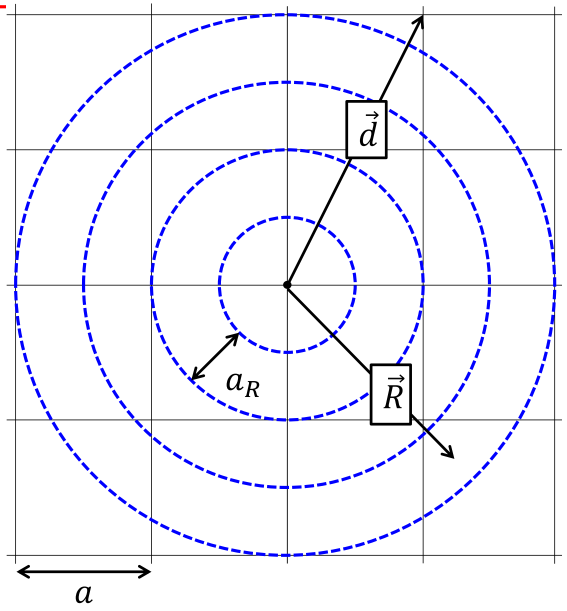
exact Lanzcos: black dashed lines

adiabatic Hamiltonian: solid colored lines

lattice size is 7^3 , $a = 1.93$ fm



The POWER of the RADIAL HAMILTONIAN



- Consider fermion-dimer scattering on large lattices:

$$|\vec{d}\,\rangle = \sum_{\vec{n}} |\vec{n} + \vec{d}\,\rangle_1 \otimes |\vec{n}\rangle_2$$

[note renaming of $\vec{R} \to \vec{d}$]

- radial projection: $|d\rangle^{\ell,\ell_z} = \sum_{\vec{d}'} \mathrm{Y}_{\ell,\ell_z}(\hat{d}\,')\delta_{d,|\vec{d}\,'|}\,|\vec{d}\,'\rangle$

- Increase efficiency: group lattice points into radial rings of width a_R

- define R as radial distance to the midpoint of the corresponding ring

- initial cluster states now are: $|R\rangle^{\ell,\ell_z} = \sum_{|d-R|<a_R/2} |d\rangle^{\ell,\ell_z}$

- Completeness: $\mathbb{1} = \sum_{R,R'} |R\rangle^{\ell,\ell_z}\ [N_0^{-1}]^{\ell,\ell_z}_{R,R'}\ {}^{\ell,\ell_z}\langle R'|$

- Norm matrix: $[N_0]^{\ell,\ell_z}_{R,R'} = {}^{\ell,\ell_z}\langle R|R'\rangle^{\ell,\ell_z}$

The POWER of the RADIAL HAMILTONIAN II

- Reduction of computational costs:

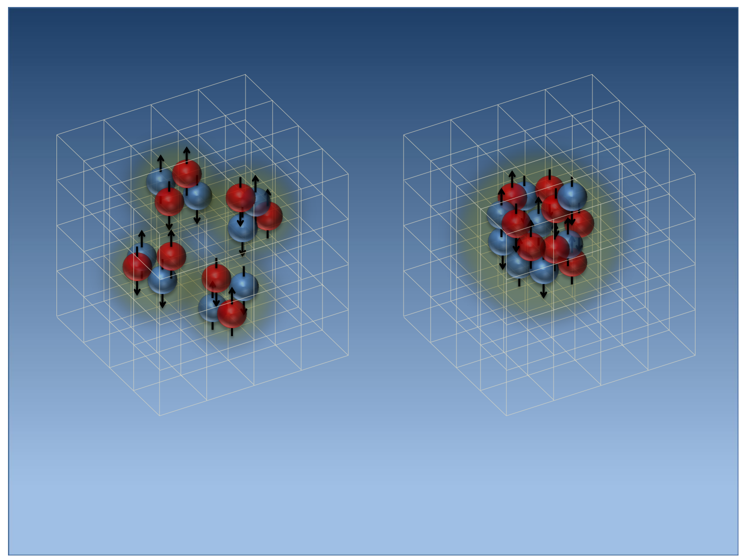
L	$[M_{L_t}]_{\vec{d},\vec{d}'}$	$[M_{L_t}]^{0,0}_{d,d'}$	$[M_{L_t}]^{0,0}_{R,R'}$ $a_R = 0.125$ l.u.	$[M_{L_t}]^{0,0}_{R,R'}$ $a_R = 0.250$ l.u.
10	$10^3 \times 10^3$	22×22	21×21	14×14
20	$20^3 \times 20^3$	85×85	58×58	34×34
30	$30^3 \times 30^3$	189×189	97×97	54×54
40	$40^3 \times 40^3$	335×335	137×137	74×74
50	$50^3 \times 50^3$	522×522	177×177	94×94
60	$60^3 \times 60^3$	752×752	217×217	114×114

$[M_{L_t}]_{\vec{d},\vec{d}'}$ = initial cluster state on the cubic lattice

$[M_{L_t}]^{0,0}_{d,d'}$ = projecting onto ang. mom. $\ell = 0, \ell_z = 0$

$[M_{L_t}]^{0,0}_{R,R'}$ = ang. mom. proj. + grouping in rings of width a_R

Assorted results



NLEFT

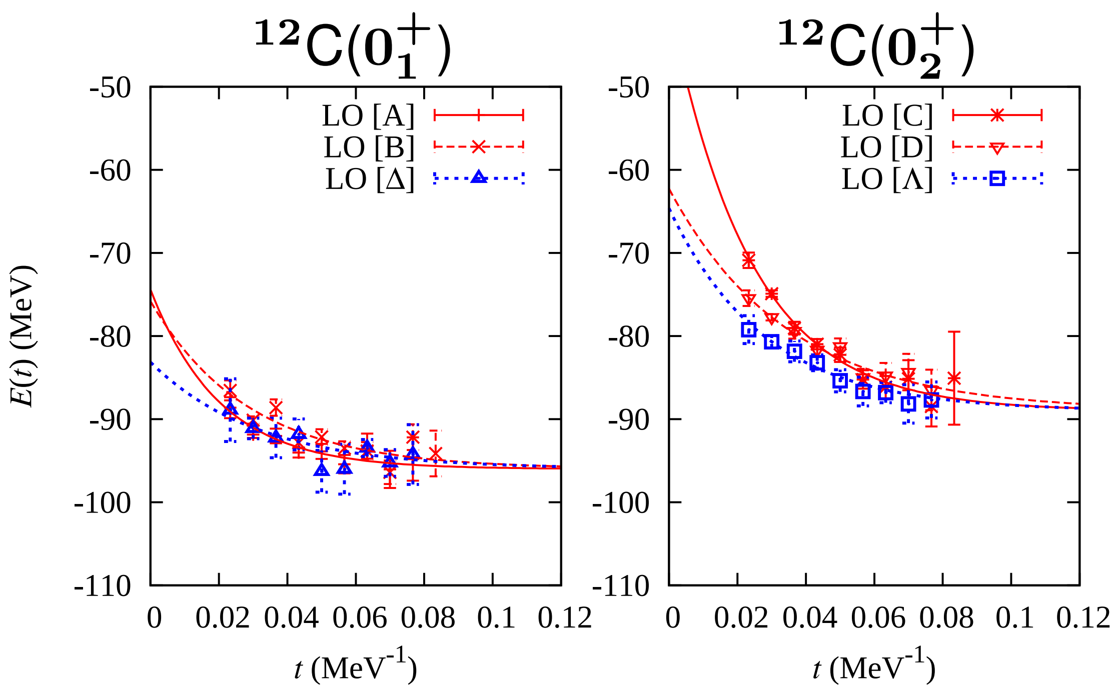
Elhatisari, Epelbaum, Krebs, Lähde, Lee, Luu, Lu, UGM, Rupak + post-docs + students

NNLO: FIXING PARAMETERS & FIRST RESULTS

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

- most simulations with coarse lattices, only recently finer lattice
- some groundstate energies and differences [NNLO, 12+2 LECs] → next slide

	E [MeV]	NLEFT	Exp.
old algorithm	^{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
new algorithm	^{16}O	−131(1)	−127.6
	^{20}Ne	−166(1)	−160.6
	^{24}Mg	−198(2)	−198.3
	^{28}Si	−234(3)	−236.5



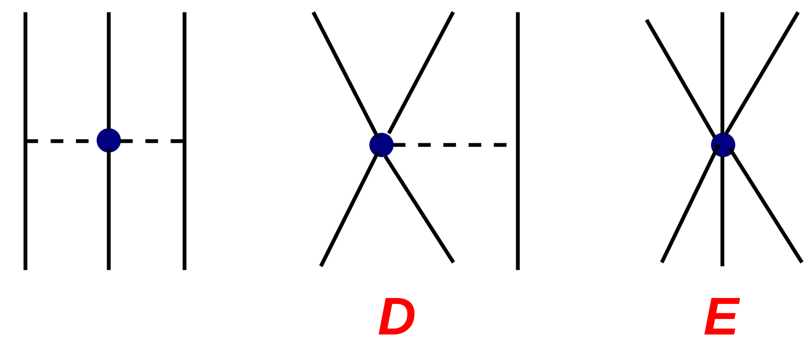
- promising results ⇒ uncertainties down to the 1% level
- excited states more difficult ⇒ projection MC method + triangulation

PARAMETERS AT NNLO

- 12 2N LECs: $C_{S,T}$, b, $C_{1\ldots7}$, $C_{pp,nn}$ from S- and P-waves, ε_1 and a_{pp}, a_{nn}

  $\hookrightarrow$ already shown before

- 3N forces at NNLO:
  - three topologies
  - two parameters *D* and *E*

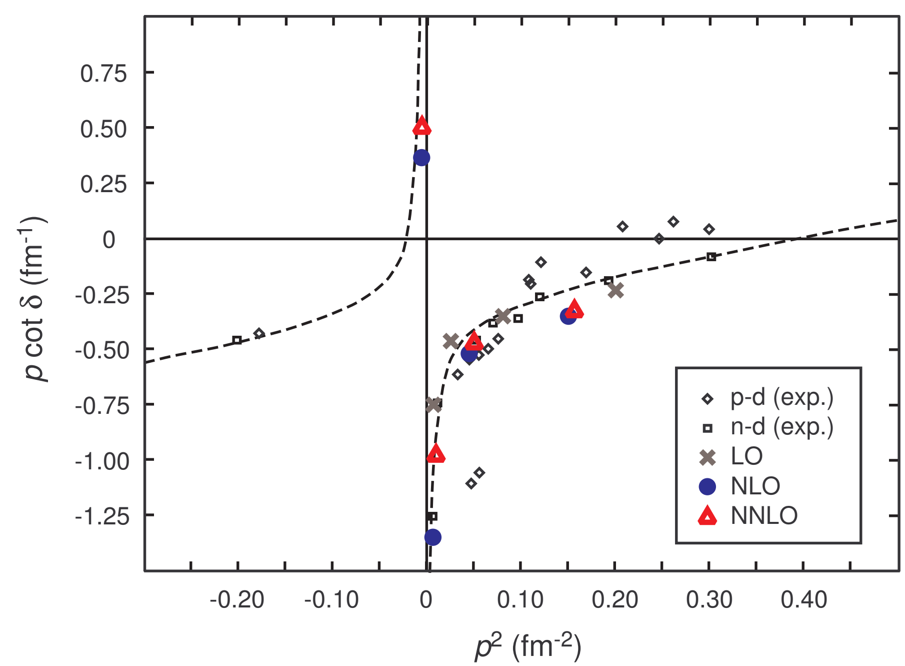


- determine *D* and *E* from fit to the E(^{3}H) and $a_{nd}^{(2)}$

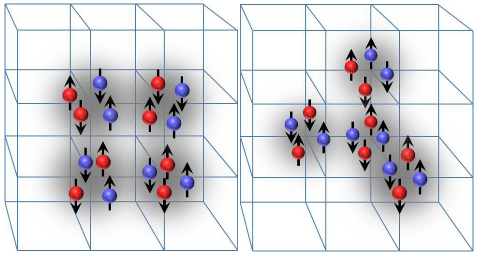
$\Rightarrow$ make predictions

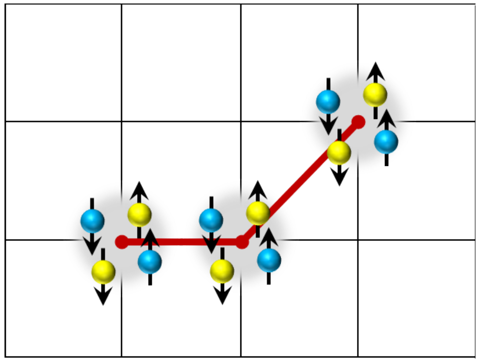
- *D* can also be determined in pion production experiments or from electroweak processes

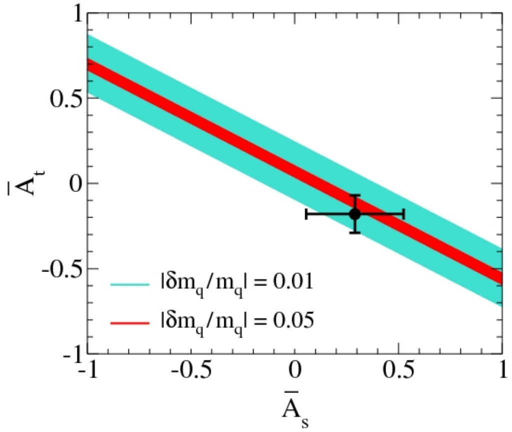
  $\rightarrow$ **power of EFT**



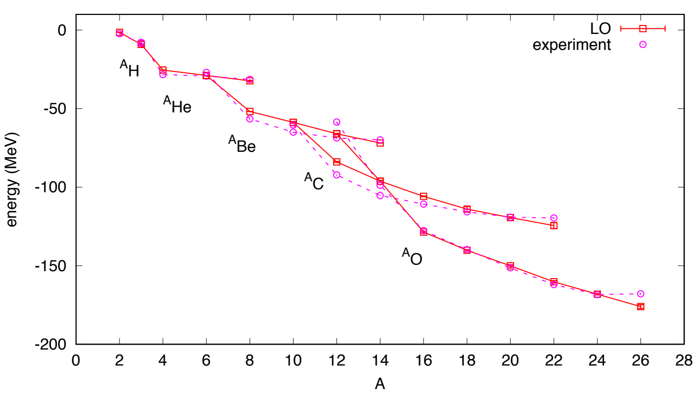
RESULTS from LATTICE NUCLEAR EFT

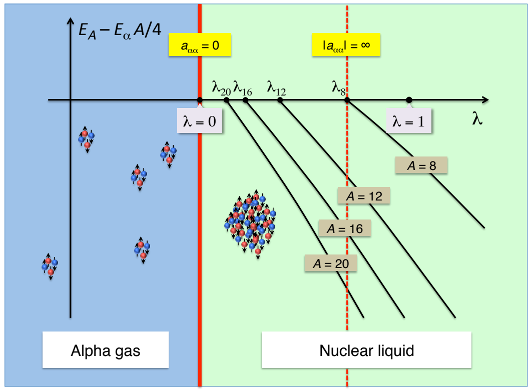


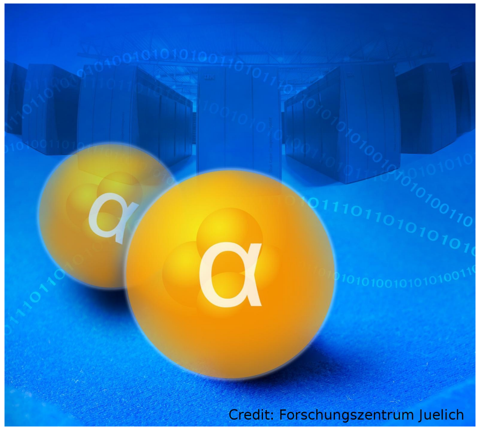




- ☐ Lattice EFT calculations for A=3,4,6,12 nuclei, PRL 104 (2010) 142501
- ☐ *Ab initio* calculation of the Hoyle state, PRL 106 (2011) 192501
- ☐ Structure and rotations of the Hoyle state, PRL 109 (2012) 142501
- ☐ Validity of Carbon-Based Life as a Function of the Light Quark Mass
  PRL 110 (2013) 142501
- ☐ *Ab initio* calculation of the Spectrum and Structure of ^{16}O,
  PRL 112 (2014) 142501
- ☐ *Ab initio* alpha-alpha scattering, Nature 528 (2015) 111
- ☐ Nuclear Binding Near a Quantum Phase Transition, PRL 117 (2016) 132501
- ☐ *Ab initio* calculations of the isotopic dependence of nuclear clustering,
  PRL 119 (2017) 222505





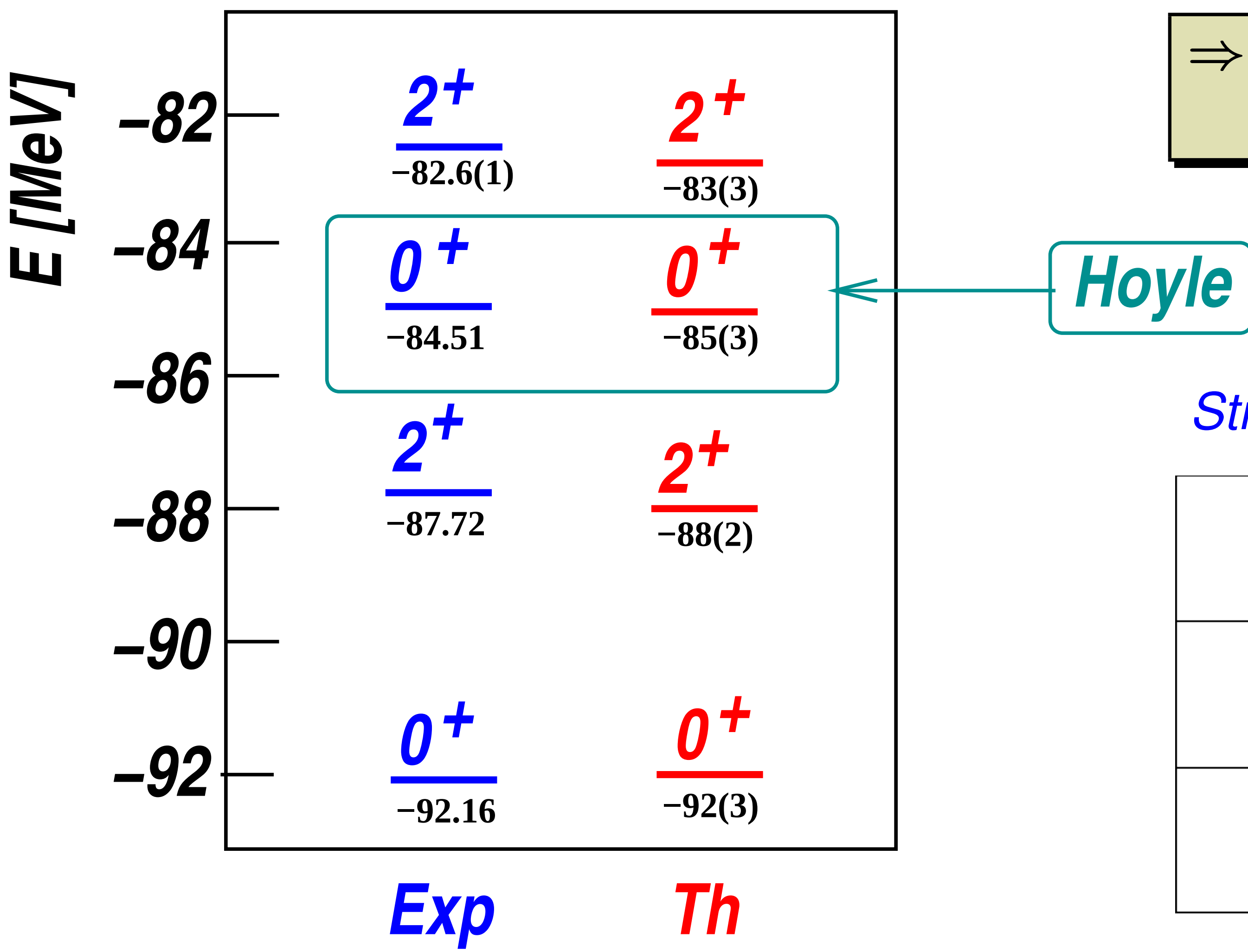


BREAKTHROUGH: SPECTRUM of CARBON-12

Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. 106 (2011) 192501

Epelbaum, Krebs, Lähde, Lee, UGM, Phys. Rev. Lett. 109 (2012) 252501

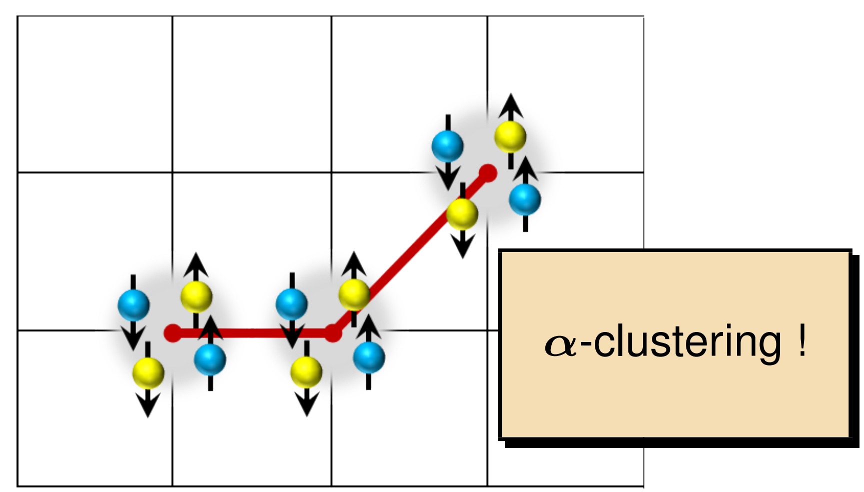
- After $8 \cdot 10^6$ hrs JUGENE/JUQUEEN (and “some” human work)



⇒ First ab initio calculation of the Hoyle state ✓

→ lesson for young people

Structure of the Hoyle state:



A SHORT HISTORY of the HOYLE STATE

- Heavy element generation in massive stars: triple-α process

Bethe 1938, Öpik 1952, Salpeter 1952, Hoyle 1954, ...

$$
\begin{aligned}
&{}^4\text{He} + {}^4\text{He} \rightleftharpoons {}^8\text{Be} \\
&{}^8\text{Be} + {}^4\text{He} \rightleftharpoons {}^{12}\text{C}^* \rightarrow {}^{12}\text{C} + \gamma \\
&{}^{12}\text{C} + {}^4\text{He} \rightleftharpoons {}^{16}\text{O} + \gamma
\end{aligned}
$$

- Hoyle's contribution: calculation of the relative abundances of ^{4}He, ^{12}C and ^{16}O
  $\Rightarrow$ need a resonance close to the ^{8}Be + ^{4}He threshold at $E_R \simeq 0.37$ MeV
  $\Rightarrow$ this corresponds to a $J^P = 0^+$ excited state 7.7 MeV above the g.s.

- a corresponding state was experimentally confirmed at Caltech at
  $E - E(\text{g.s.}) = 7.653 \pm 0.008$ MeV — Dunbar et al. 1953, Cook et al. 1957

- still on-going experimental activity, e.g. EM transitions at SDALINAC

M. Chernykh et al., Phys. Rev. Lett. 98 (2007) 032501

- side remark: relevance to the anthropic principle?

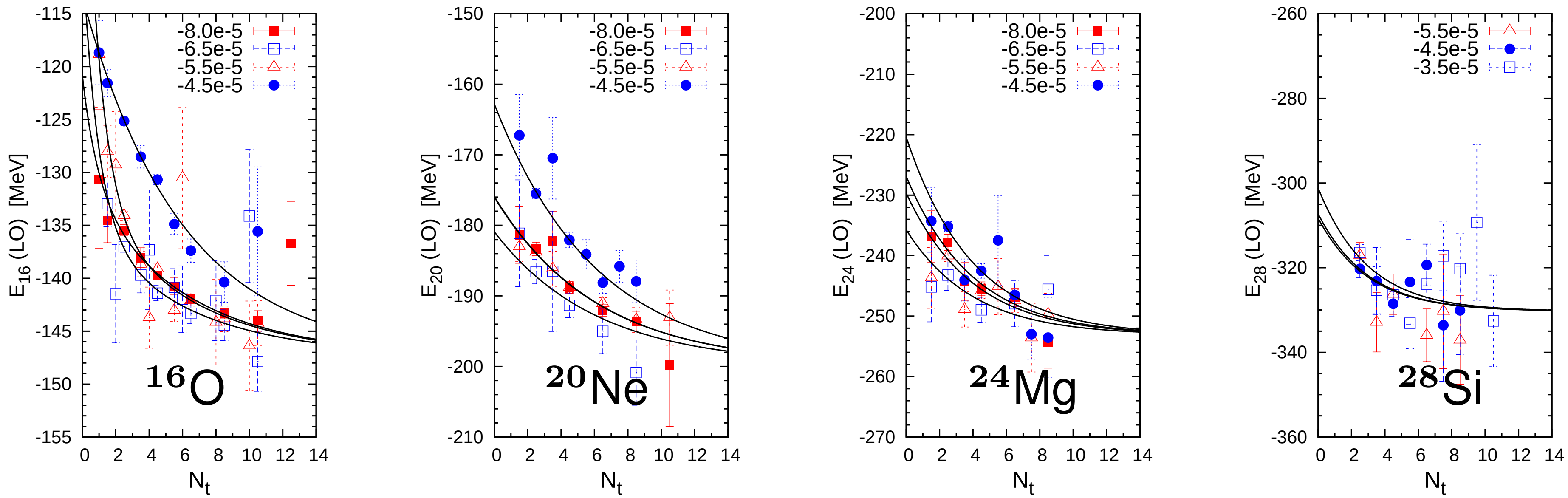
H. Kragh, An anthropic myth: Fred Hoyle's carbon-12 resonance level,
Arch. Hist. Exact Sci. 64 (2010) 721

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



$$E = -131.3(5) \qquad E = -165.9(9) \qquad E = -232(2) \qquad E = -308(3)$$

$$[-127.62] \qquad [-160.64] \qquad [-198.26] \qquad [-236.54]$$

REMOVING the OVERBINDING

Lähde, Epelbaum, Krebs, Lee, UGM, Rupak, Phys. Lett. B 732 (2014) 110

- Overbinding is due to four α clusters in close proximity

  $\Rightarrow$ remove this by an effective 4N operator [present/on-going: N3LO]

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

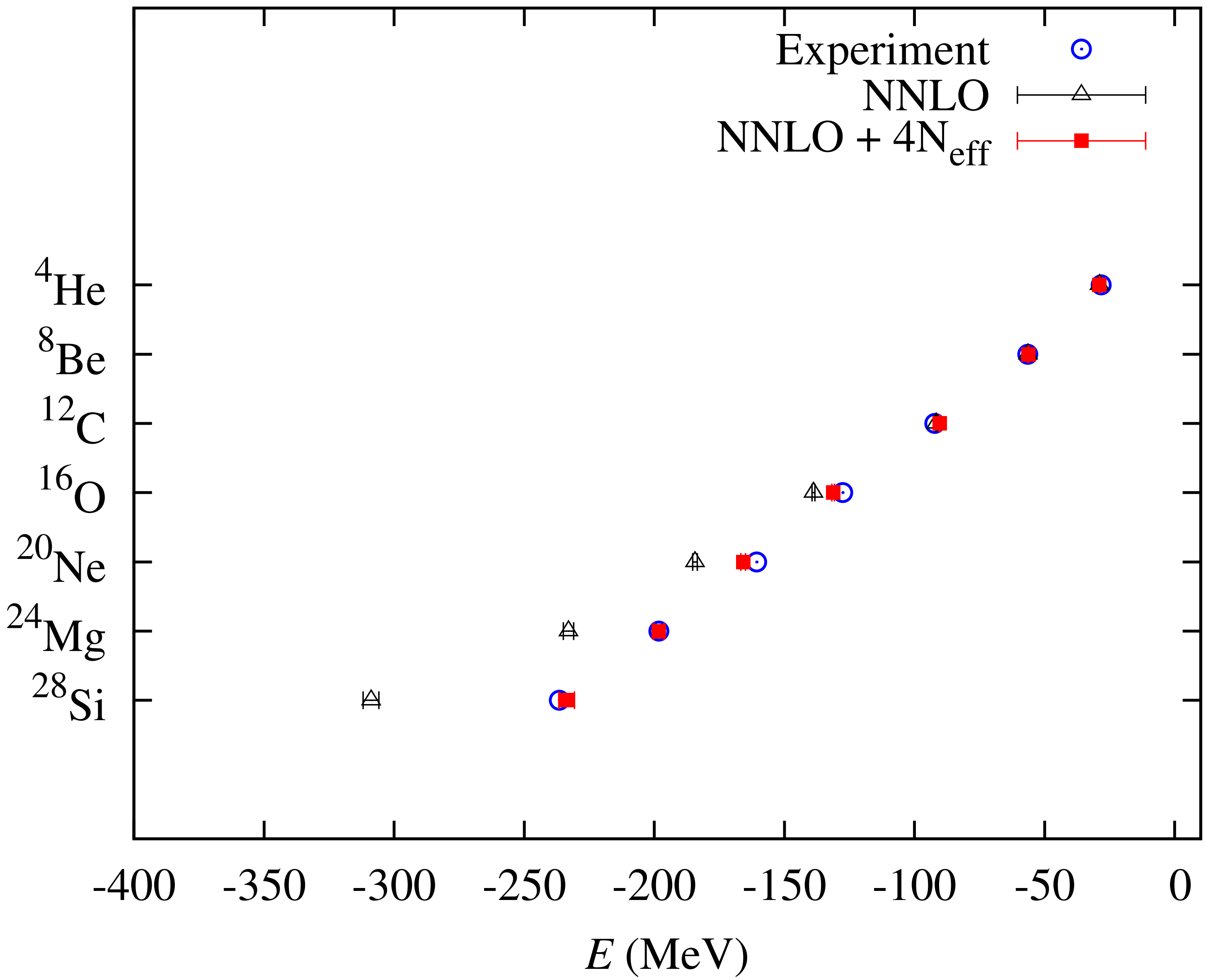
- fix the coefficient $D^{(4\mathrm{N_{eff}})}$ from the BE of ^{24}Mg

  $\Rightarrow$ 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

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

GROUND STATE ENERGIES



STRUCTURE of ^{16}O

- Mysterious nucleus, despite modern ab initio calculations

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

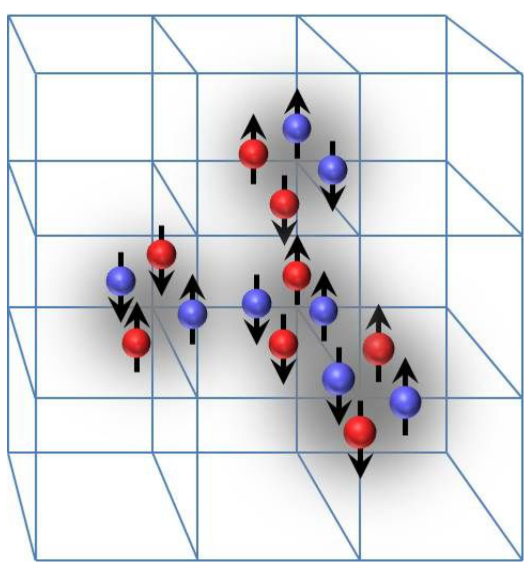
- Alpha-cluster models since decades, some experimental evidence

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

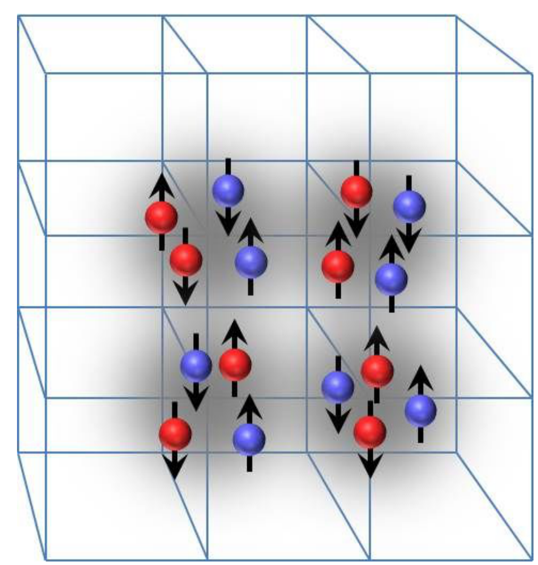
- Spectrum very close to tetrahedral symmetry group — Bijker & Iachello (2014)

- Relevant configurations in lattice simulations:

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

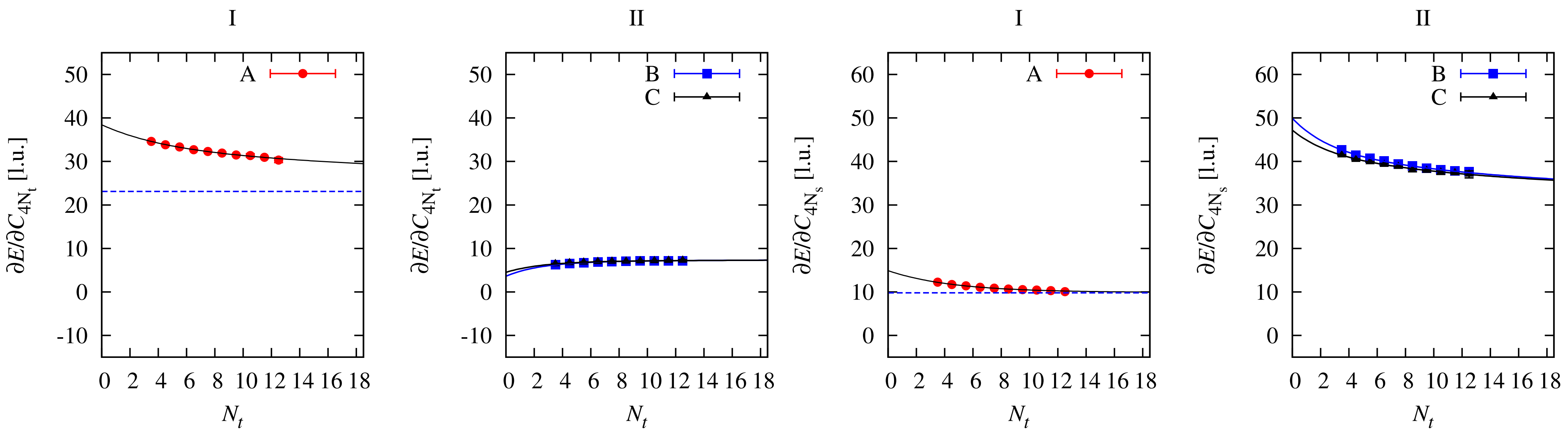
- measure the 4N density, where each of the nucleons is placed at adjacent points

$\Rightarrow$ $\mathbf{0_1^+}$ 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 rescaling 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)

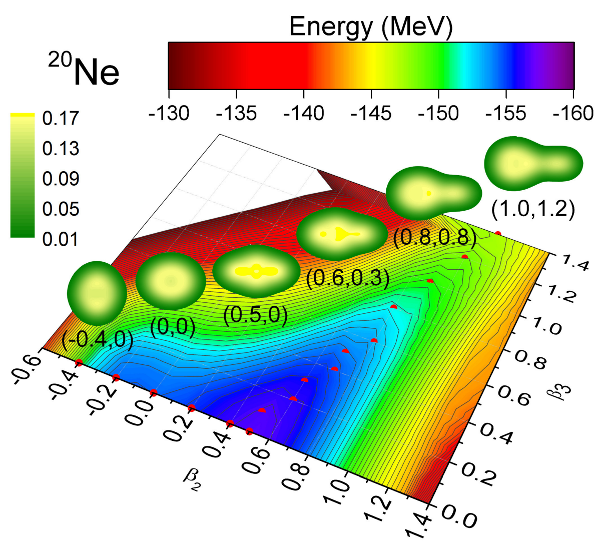
$\Rightarrow$ gives credit to the interpretation of the 2_1^+ as rotational excitation

CLUSTERING in NUCLEI

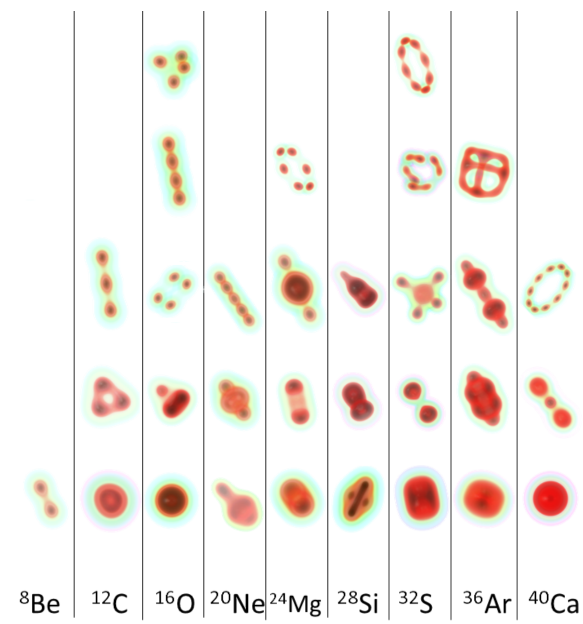
- Introduced theoretically by Wheeler already in 1937:

> John Archibald Wheeler, "Molecular Viewpoints in Nuclear Structure," Physical Review **52** (1937) 1083

- many works since then... Ikeda, Horiuchi, Freer, Ring, Schuck, Röpke, Khan, Zhou, Iachello, . . .



Zhou, Yao, Li, Ring, Meng (2015)



Ebran, Khan, Niksic, Vretenar (2014)

α-clusters

$\Rightarrow$ can we understand this phenomenon from *ab initio* calculations?

for a recent review, see Freer et al. Rev. Mod. Phys. **90** (2018) 035004

RESULTS on NUCLEAR CLUSTERING

- Already a number of intriguing results on clustering [N2LO, coarse lattice]:

  Ab initio calculation of the spectrum and structure of ^{12}C (esp. the Hoyle state)

  Ab initio calculation of the spectrum and structure of ^{16}O

  Ground state energies of α-type nuclei up to ^{28}Si within 1%

  Ab initio calculation of α-α scattering

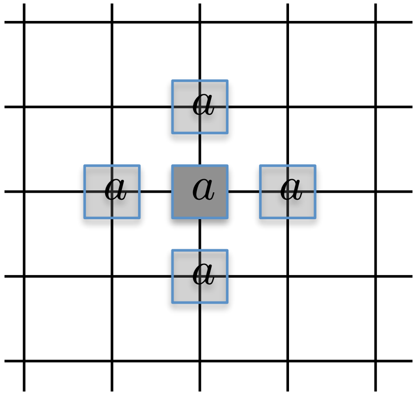
  Quantum phase transition from Bose gas of α's to nuclear liquid for α-type nuclei

- However: when adding extra neutrons/protons, the precision quickly deteriorates due to sign oscillations

- New LO action with smeared SU(4) local+non-local symmetric contact interactions & smeared one-pion exchange

$$a_{\rm NL}(\mathbf{n}) = a(\mathbf{n}) + s_{\rm NL} \sum_{\langle \mathbf{n}'\,\mathbf{n}\rangle} a(\mathbf{n}')$$

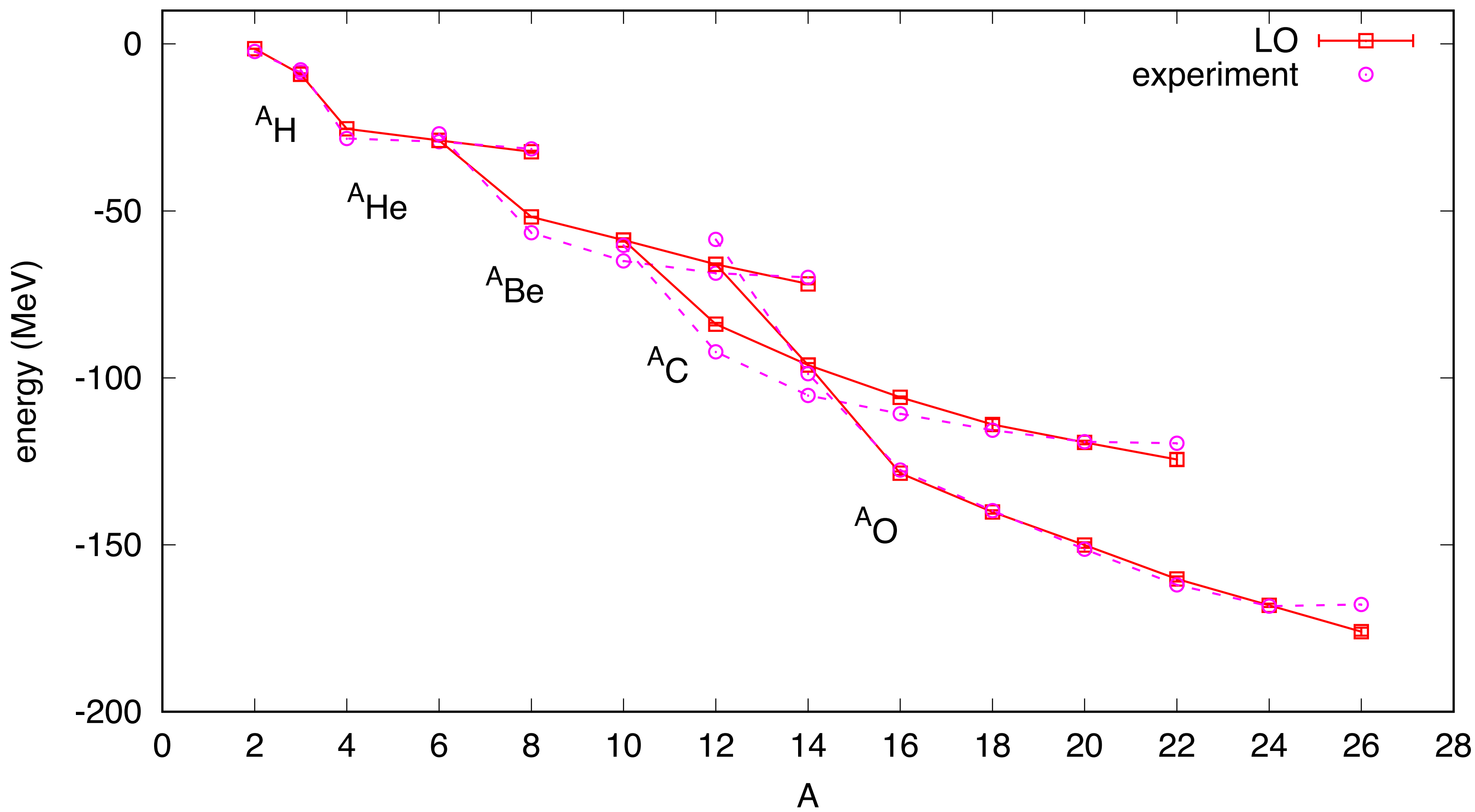
$$a^\dagger_{\rm NL}(\mathbf{n}) = a^\dagger(\mathbf{n}) + s_{\rm NL} \sum_{\langle \mathbf{n}'\,\mathbf{n}\rangle} a^\dagger(\mathbf{n}')$$



GROUND STATE ENERGIES

- Fit parameters to average NN S-wave scattering length and effective range and α-α S-wave scattering length

$\rightarrow$ predict g.s. energies of H, He, Be, C and O isotopes $\rightarrow$ quite accurate (LO)



PROBING NUCLEAR CLUSTERING

- Local densities on the lattice: $\rho(\mathbf{n})\,,\quad \rho_p(\mathbf{n})\,,\quad \rho_n(\mathbf{n})$

- Probe of alpha clusters: $\rho_4 = \sum_{\mathbf{n}} :\rho^4(\mathbf{n})/4!:$

- Another probe for $Z = N =$ even nuclei: $\rho_3 = \sum_{\mathbf{n}} :\rho^3(\mathbf{n})/3!:$

- ρ_4 couples to the center of the α-cluster while ρ_3 gets contributions from a wider portion of the alpha-particle wave function

- Both ρ_3 and ρ_4 depend on the regulator, a, but not on the nucleus

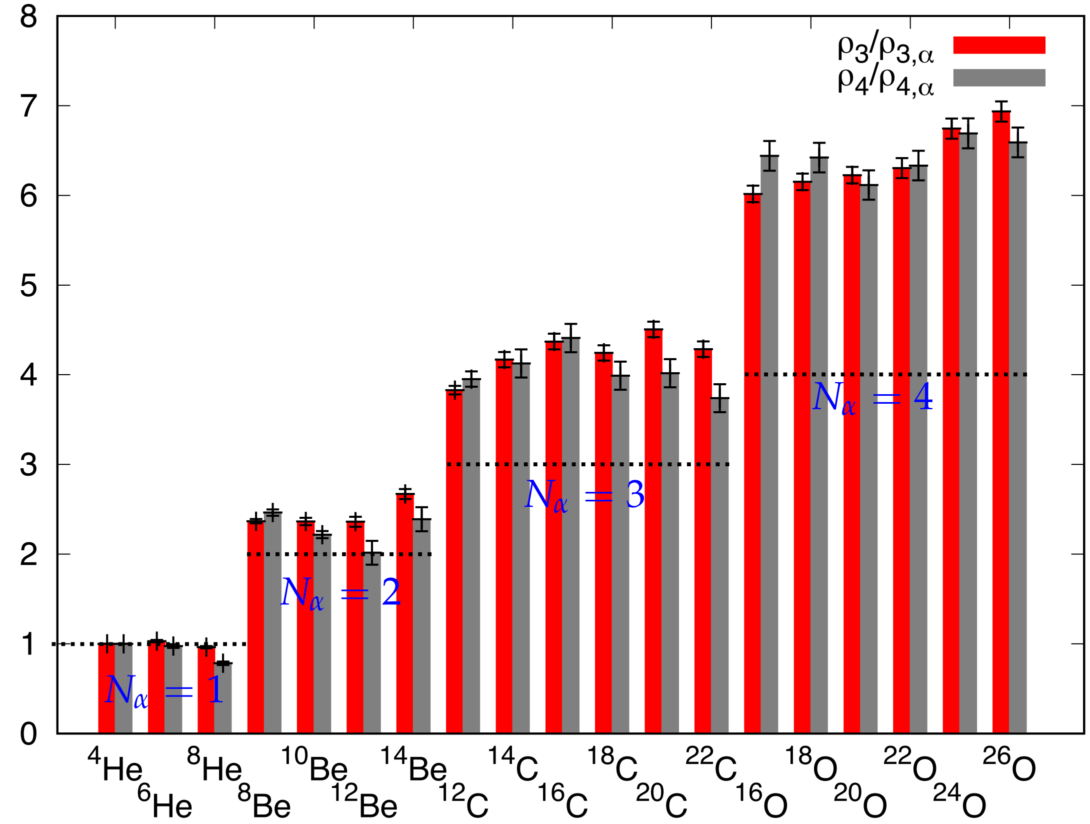
- The ratios $\rho_3/\rho_{3,\alpha}$ and $\rho_4/\rho_{4,\alpha}$ free of short-distance ambiguities and model-independent

- $\rho_3/\rho_{3,\alpha}$ measures the effective number of alpha-cluster N_α

$\Rightarrow$ Any deviation from $N_\alpha =$ integer measures the entanglement of the α-clusters in a given nucleus

PROBING NUCLEAR CLUSTERING

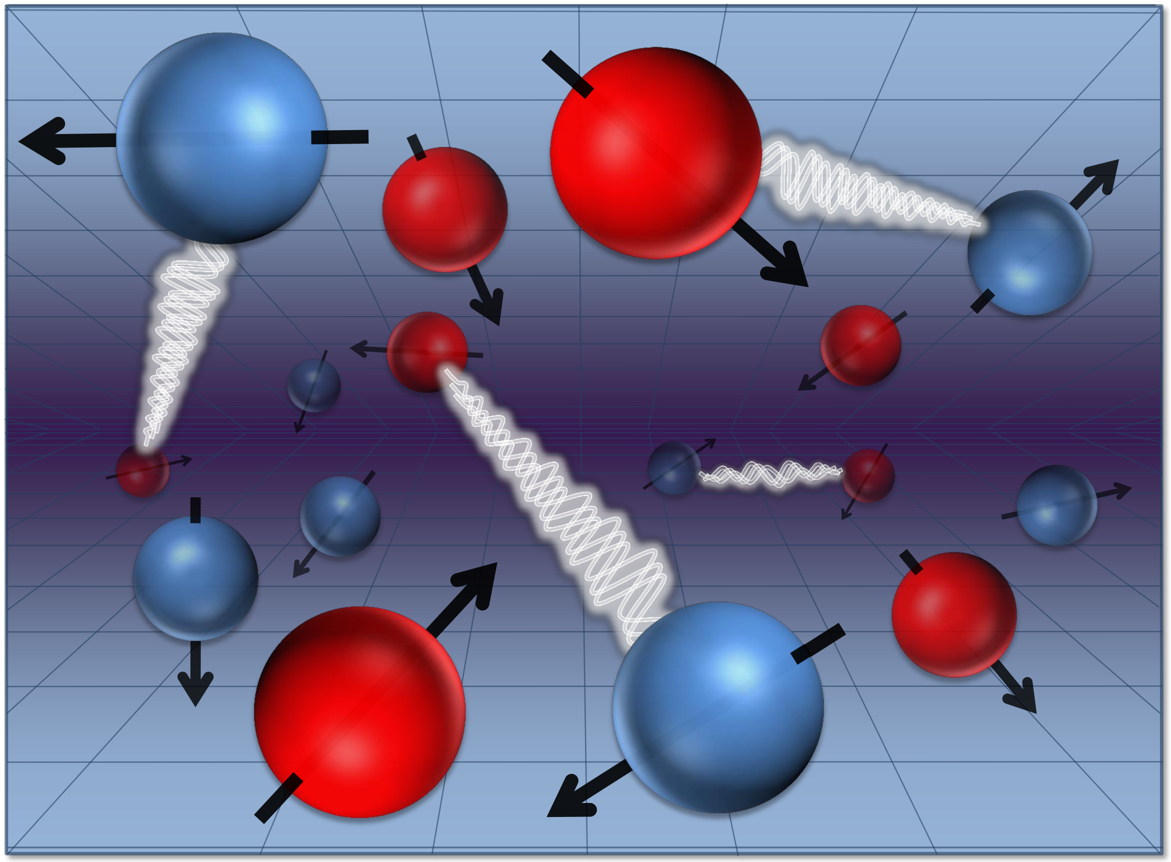
- ρ_3-entanglement of the α-clusters: $$\frac{\Delta_\alpha^{\rho_3}}{N_\alpha} = \frac{\rho_3/\rho_{3,\alpha}}{N_\alpha} - 1$$



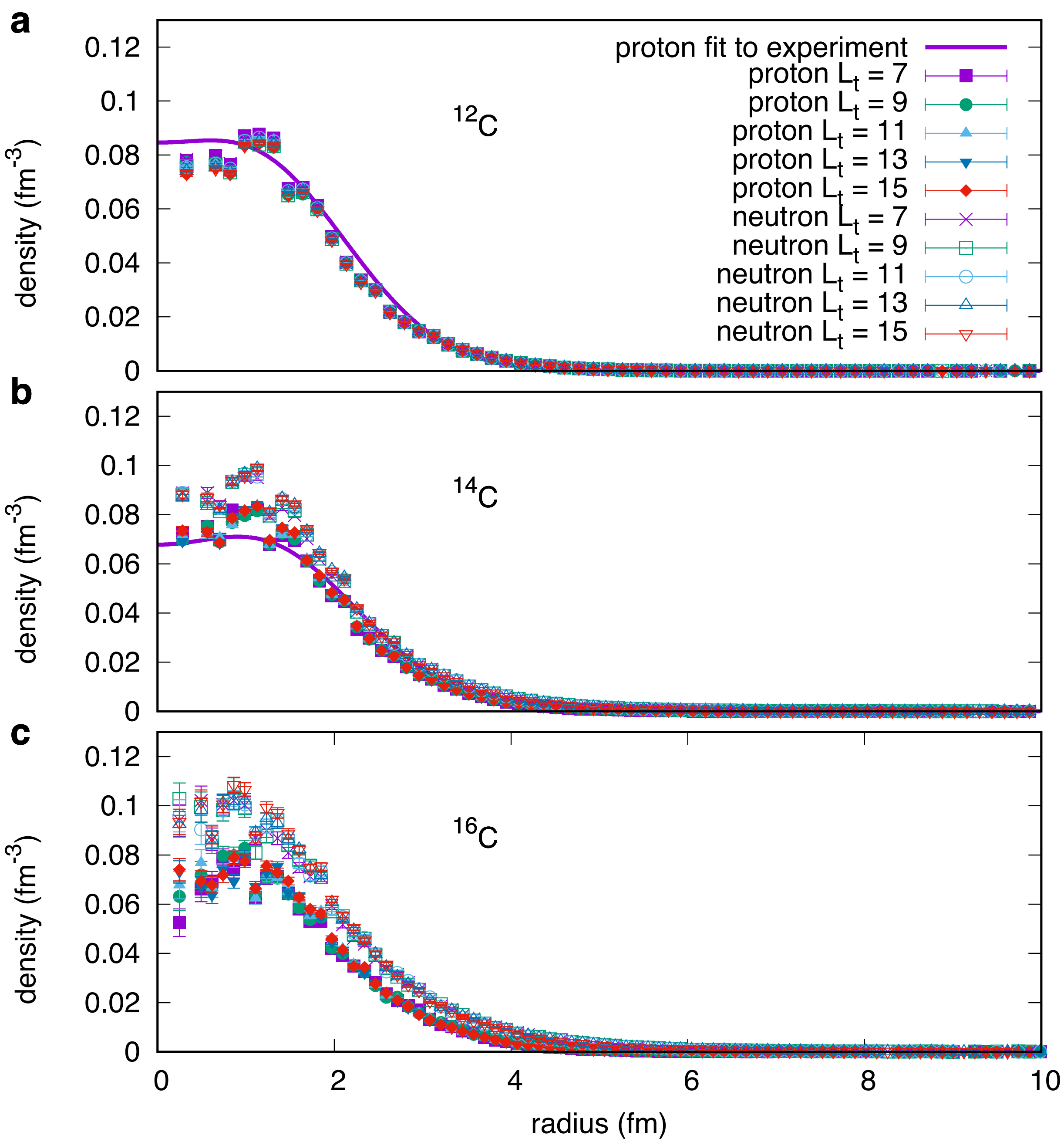
Nucleus	^{4,6,8}He	^{8,10,12,14}Be	^{12,14,16,18,20,22}C	^{16,18,20,22,24,26}O
$\Delta_\alpha^{\rho_3}/N_\alpha$	0.00 - 0.03	0.20 - 0.35	0.25 - 0.50	0.50 - 0.75

PROBING NUCLEAR CLUSTERING

- The transition from cluster-like states in light systems to nuclear liquid-like states in heavier systems should not be viewed as a simple suppression of multi-nucleon short-distance correlations, but rather as an increasing *entanglement* of the nucleons involved in the multi-nucleon correlations.



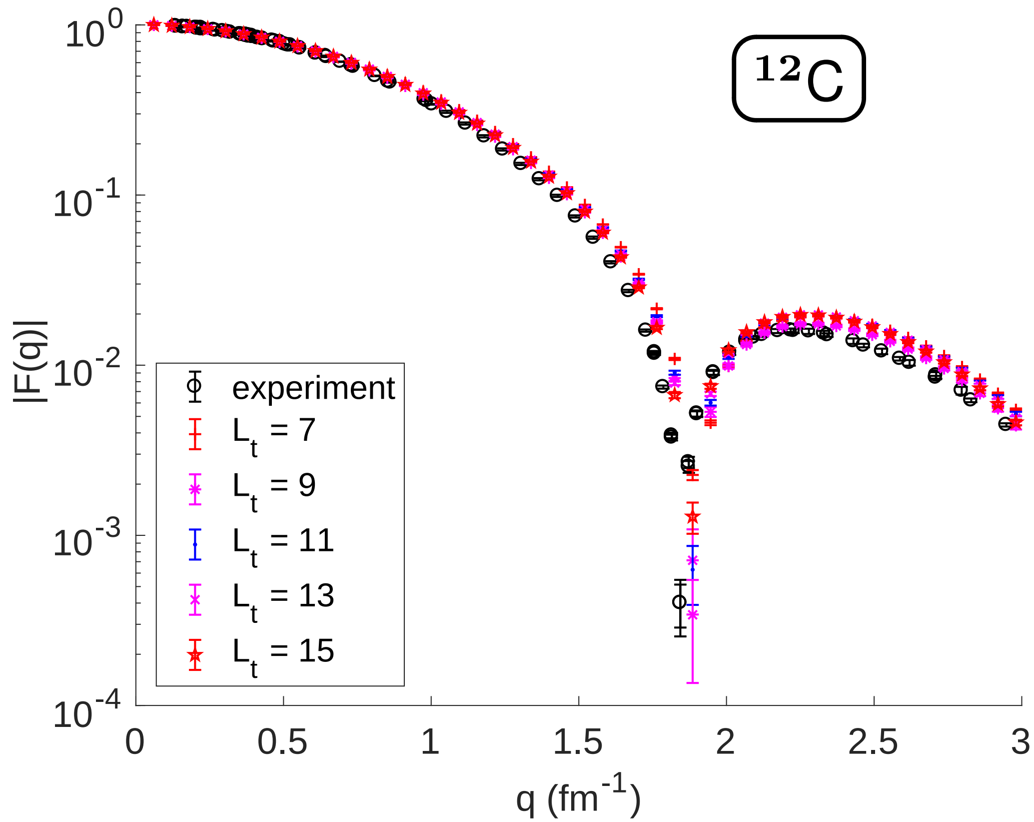
PROTON and NEUTRON DENSITIES in CARBON



- Pinhole algorithm at work!
- open symbols: neutron
- closed symbols: proton
- proton size accounted for
- asymptotic properties of the distributions from the volume dependence of N-body bound states
  König, Lee, Phys. Lett. B779 (2018) 9
- consistent with data
- fit to data from
  Kline et al., Nucl. Phys. A209 (1973) 381

FORM FACTORS

- Fit charge distributions by a Wood-Saxon shape
  ↪ get the form factor from the Fourier-transform (FT)
  ↪ uncertainties from a direct FT of the lattice data



⇒ detailed structure studies become possible

Anthropic considerations

UGM, Sci. Bull. **60** (2015) no.1, 43-54

THE ANTHROPIC PRINCIPLE

- so **many** parameters in the Standard Model, the landscape of string theory, . . .

$\Rightarrow$ The anthropic principle:

"The observed values of all physical and cosmological quantities are not equally probable but they take on values restricted by the requirement that there exist sites where carbon-based life can evolve and by the requirements that the Universe be old enough for it to have already done so."

Carter 1974, Barrow & Tippler 1988, . . .

$\Rightarrow$ can this be tested? / have physical consequences?

- Ex. 1: "Anthropic bound on the cosmological constant" Weinberg (1987) [849 cites]
- Ex. 2: "The anthropic string theory landscape" Susskind (2003) [998 cites]

A PRIME EXAMPLE for the ANTHROPIC PRINCIPLE

- Hoyle (1953):

Prediction of an excited level in carbon-12 to allow for a sufficient production of heavy elements (^{12}C, ^{16}O,...) in stars

- was later heralded as a prime example for the AP:

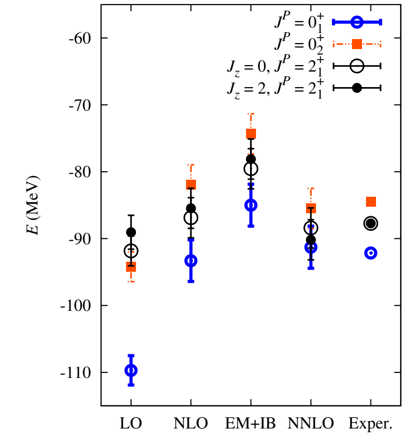
"As far as we know, this is the only genuine anthropic principle prediction"
Carr & Rees 1989

"In 1953 Hoyle made an anthropic prediction on an excited state – 'level of life' – for carbon production in stars"
Linde 2007

"A prototype example of this kind of anthropic reasoning was provided by Fred Hoyle's observation of the triple alpha process..."
Carter 2006

The RELEVANT QUESTION

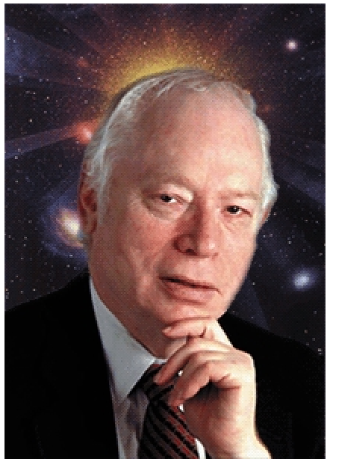
Date: Sat, 25 Dec 2010 20:03:42 -0600
From: Steven Weinberg ⟨weinberg@zippy.ph.utexas.edu⟩
To: Ulf-G. Meissner ⟨meissner@hiskp.uni-bonn.de⟩
Subject: Re: Hoyle state in 12C



Dear Professor Meissner,

Thanks for the colorful graph. It makes a nice Christmas card. But I have a detailed question. Suppose you calculate not only the energy of the Hoyle state in C12, but also of the ground states of He4 and Be8. How sensitive is the result that the energy of the Hoyle state is near the sum of the rest energies of He4 and Be8 to the parameters of the theory? I ask because I suspect that for a pretty broad range of parameters, the Hoyle state can be well represented as a nearly bound state of Be8 and He4.

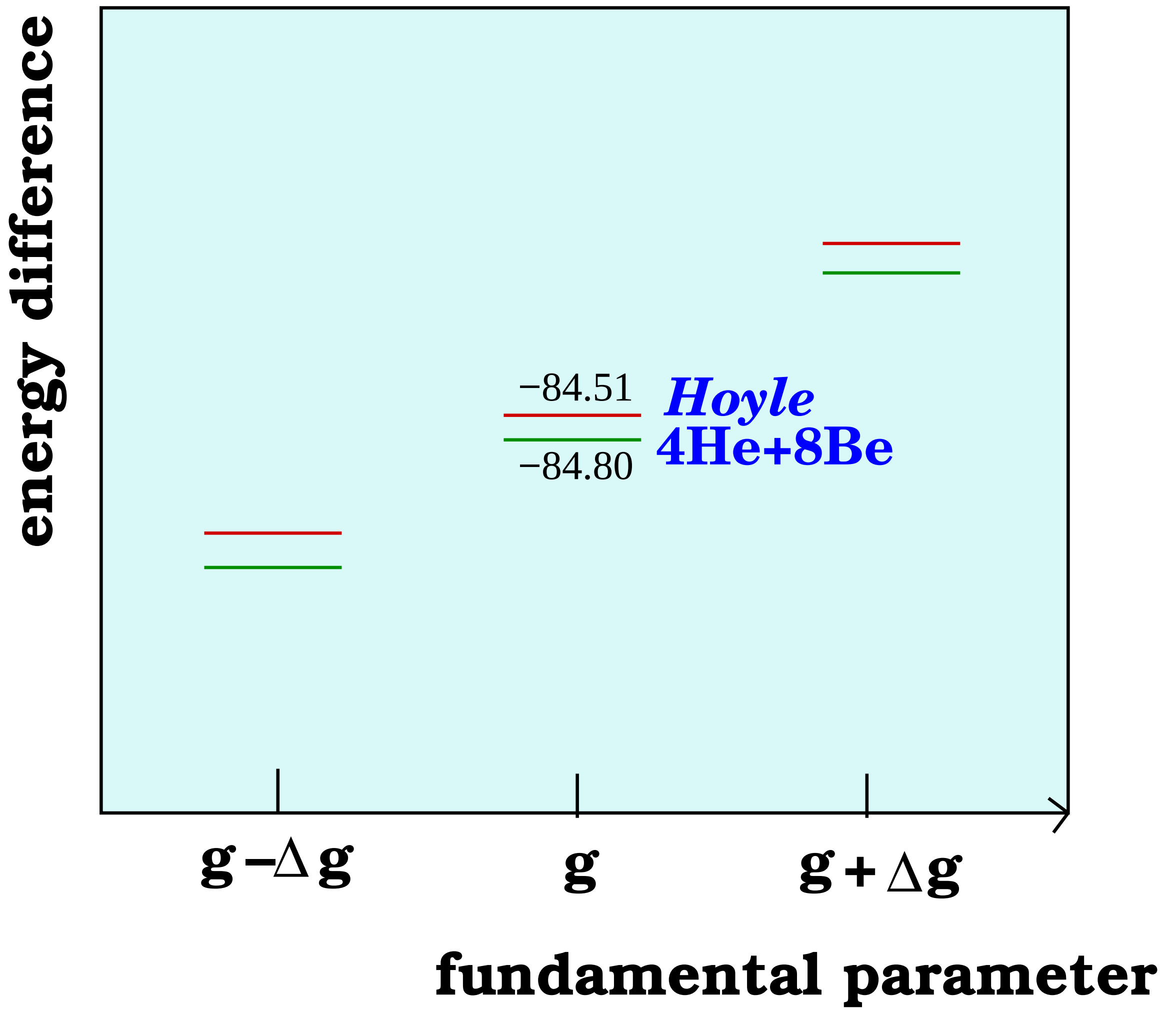
All best,
Steve Weinberg



- How does the Hoyle state move relative to the ^{4}He+^{8}Be threshold, if we change the fundamental parameters of QCD+QED?
- not possible in nature, *but on a high-performance computer!*

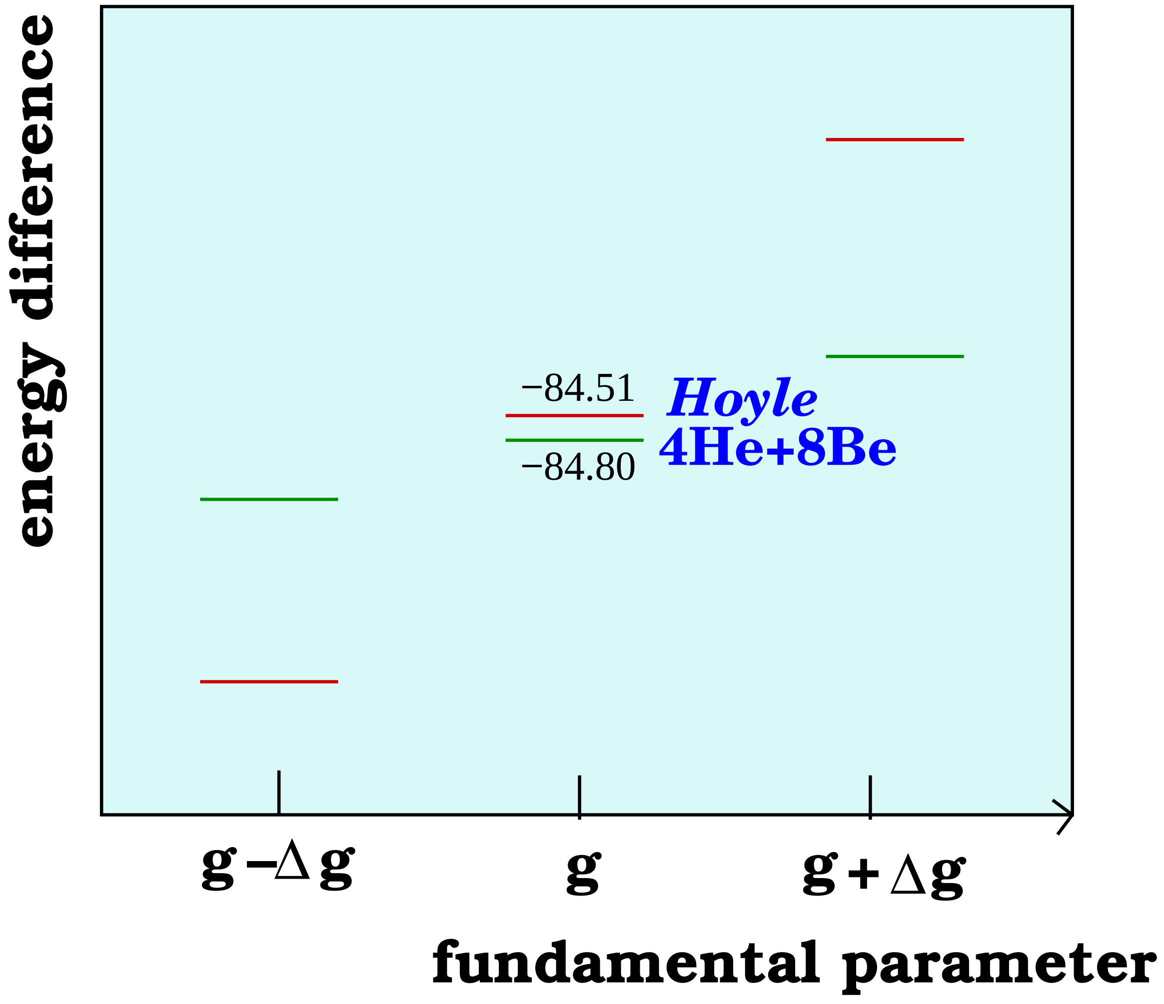
The NON-ANTHROPIC SCENARIO

- Weinberg's assumption: The Hoyle state stays close to the 4He+8Be threshold



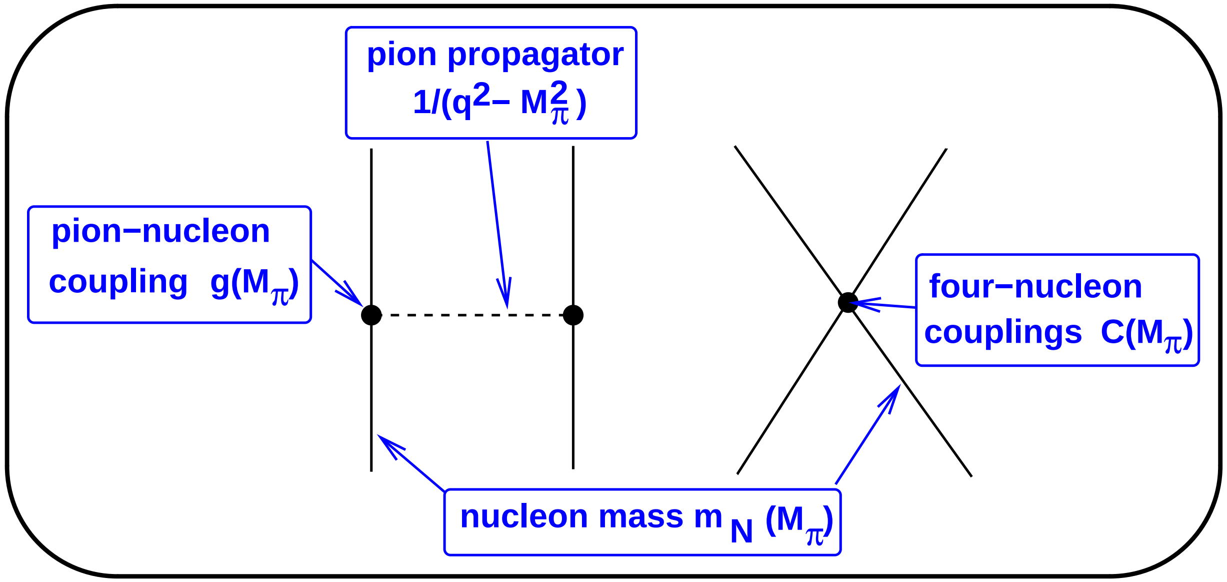
The ANTHROPIC SCENARIO

- The AP strikes back: The Hoyle state moves away from the 4He+8Be threshold



NUCLEAR FORCES for VARYING QUARK MASSES

- Nuclear forces: Pion-exchange contributions & short-distance multi-N operators
- graphical representation of the quark mass dependence of the LO potential

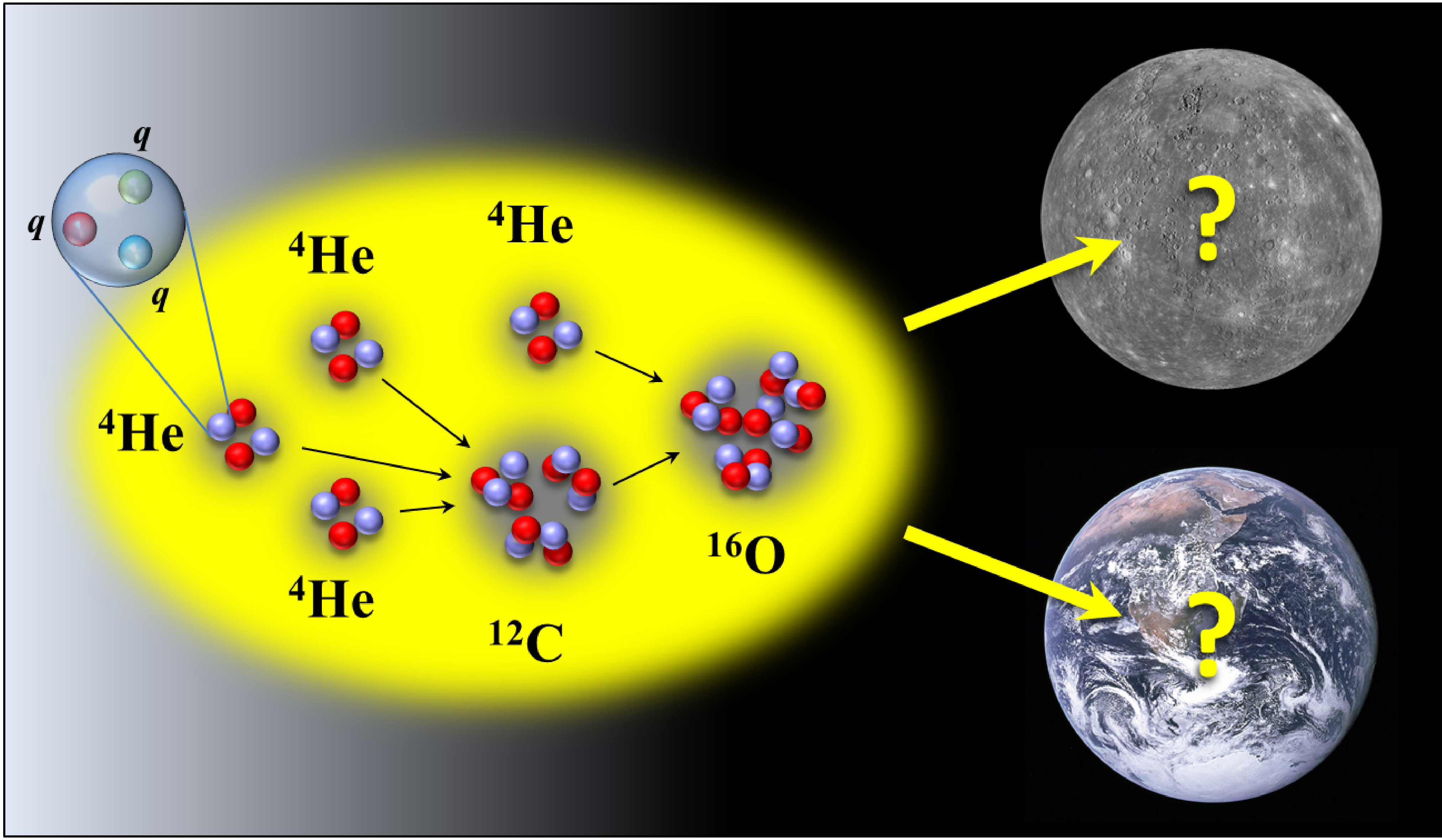


- always use the Gell-Mann–Oakes–Renner relation: $M^2_{\pi^\pm} \sim (m_u + m_d)$
- fulfilled in QCD to better than 94% Colangelo, Gasser, Leutwyler 2001

$\Rightarrow$ Quark mass dependence of hadron properties from lattice QCD,
contact interaction require modeling $\to$ challenge to lattice QCD

FINE-TUNING of FUNDAMENTAL PARAMETERS

Fig. courtesy Dean Lee



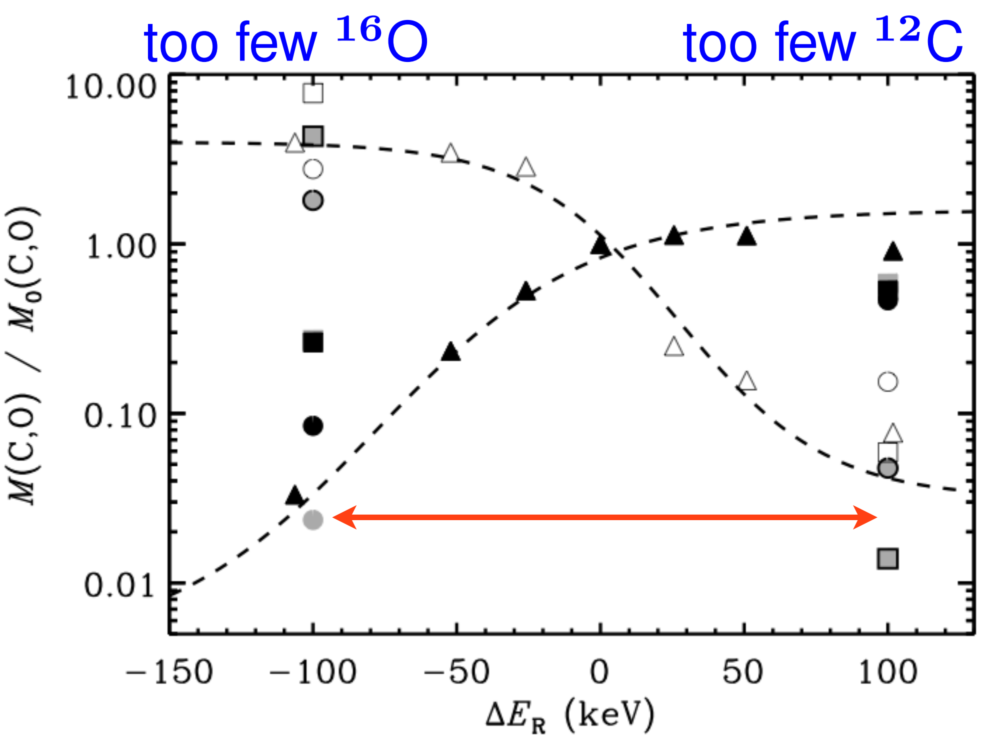
EARLIER STUDIES of the ANTHROPIC PRINCIPLE

- 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?

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



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]

RECENT STELLAR SIMULATIONS

Adams, Huang, Grohs, Astropart. Phys. **105** (2019) 13

- Stellar evolution calculations for massive stars in the range $M_* = 15 - 40 M_\odot$

  ↪ study yields of ^{12}C and ^{16}O consistent with present abundances

- 2 scenarios: low metallicity ($\mathcal{Z} = 10^{-4}$) and solar metallicty ($\mathcal{Z} = 0.02$)

  ↪ main effect of $\mathcal{Z}$: relative importance of p-p chain versus CNO cycle

- Results:

$$^{12}\text{C}(\mathcal{Z} = 10^{-4}): \quad -300 \text{ keV} \leq \Delta E_{h+b} \leq 500 \text{ keV}$$

$$^{16}\text{O}(\mathcal{Z} = 10^{-4}): \quad -300 \text{ keV} \leq \Delta E_{h+b} \leq 300 \text{ keV}$$

$$^{12}\text{C}(\mathcal{Z} = 0.02): \quad -300 \text{ keV} \leq \Delta E_{h+b} \leq 160 \text{ keV}$$

$$^{16}\text{O}(\mathcal{Z} = 0.02): \quad -150 \text{ keV} \leq \Delta E_{h+b} \leq 200 \text{ keV}$$

- asymmetric and less fine-tuned than before

- for stars with low metallicity, ^{16}O production is more limiting

FINE-TUNING: MONTE-CARLO ANALYSIS

Epelbaum, Krebs, Lähde, Lee, UGM, Phys. Rev. Lett. **110** (2013) 112502

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

^{4}He + ^{4}He ↔ ^{8}Be ⇝ $$\boxed{\Delta E_b \equiv E_8 - 2E_4}$$

^{4}He + ^{8}Be → ^{12}C* ⇝ $$\boxed{\Delta E_h \equiv E_{12}^* - E_8 - E_4}$$

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

$$\boxed{E_i = E_i\left(M_\pi^{\rm OPE}, m_N(M_\pi), \tilde{g}_{\pi N}(M_\pi), C_0(M_\pi), C_I(M_\pi)\right)}$$

$$\tilde{g}_{\pi N} \equiv g_A/(2F_\pi)$$

- QED in the same manner → calculate $\partial\Delta E/\partial\alpha_{\rm EM}$

PION MASS VARIATIONS

- consider pion mass changes as *small perturbations*

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

with

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

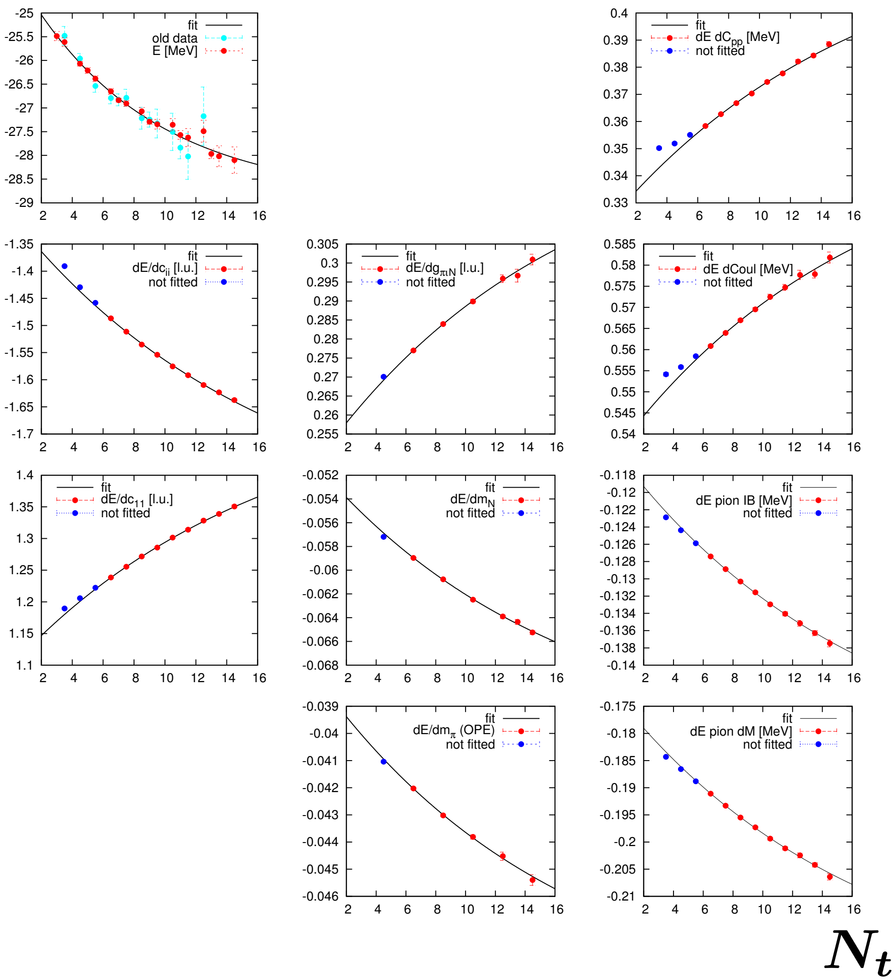
⇒ problem reduces to the calculation of the various derivatives using AFQMC and the determination of the x_i

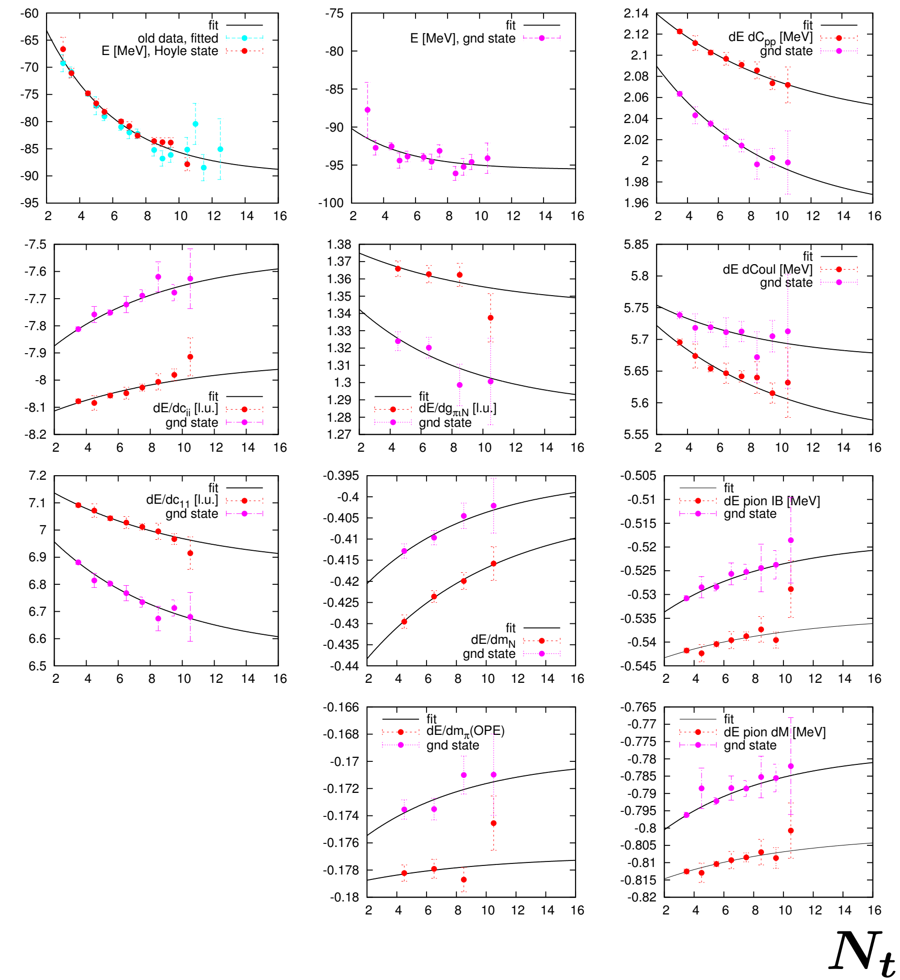
- x_1 and x_2 can be obtained from LQCD plus CHPT
- x_3 and x_4 can be obtained from two-body scattering and its M_π-dependence

AFQMC RESUTS for the DERIVATIVES

- ^{4}He
- ^{12}C$(0_1^+, 0_2^+)$

$$E(N_t) = E(\infty) + \text{const}\,\exp(-N_t/\tau)$$





DETERMINATION of the x_i

- x_1 from the quark mass expansion of the nucleon mass:

Hoferichter, Ruiz de Elvira, Kubis, UGM, Phys. Rev. Lett. **115** (2015) 092301; J. Phys. **G45** (2018) 024001

$$x_1 = 2\frac{\sigma_{\pi N}}{M_\pi} = 0.84(7)$$

- x_2 from the quark mass expansion of the pion decay constant and the nucleon axial-vector constant:

Chang et al., Nature **558** (2018) 91

$$x_2 = \frac{1}{2F_\pi}\left.\frac{\partial g_A}{\partial M_\pi}\right|_{M_\pi^{\rm phys}} - \frac{g_A}{2F_\pi^2}\left.\frac{\partial F_\pi}{\partial M_\pi}\right|_{M_\pi^{\rm phys}} = 0.078(2)\ \text{l.u.}$$

- x_3 and x_4 can be mapped onto:

$$\bar{A}_s = \left.\frac{\partial a_s^{-1}}{\partial M_\pi}\right|_{M_\pi^{\rm phys}}, \quad \bar{A}_t = \left.\frac{\partial a_t^{-1}}{\partial M_\pi}\right|_{M_\pi^{\rm phys}}$$

- these are most difficult to determine $\to$ recent progress

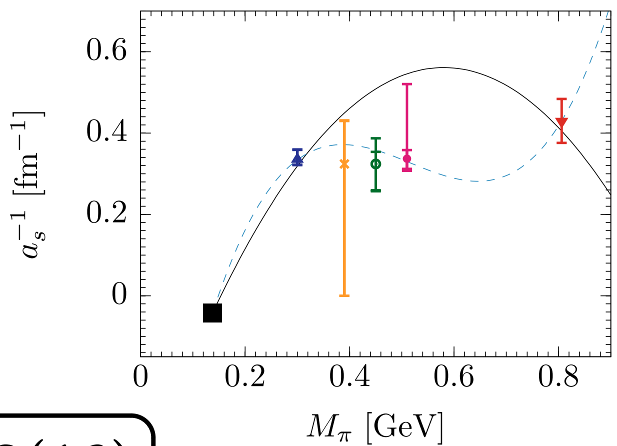
UPDATE on $\bar{A}_{s,t}$

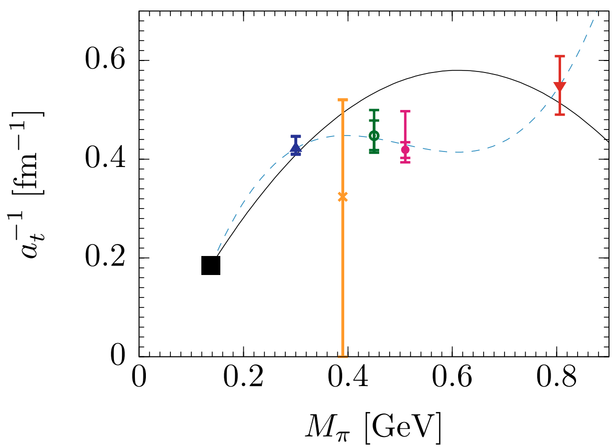
Lähde, UGM, Epelbaum, arXiv:1906.00607 [nucl-th]

- Combine LQCD results with Low-Energy Theorems   next slides

Baru et al., Phys Rev. C **92** (2015) 014001, Phys Rev. C **94** (2016) 014001

- LQCD results from NPLQCD and Yamazaki et al.
- quadratic and cubic interpolations





$$\bar{A}_s = 0.54(24)\ ,\quad \bar{A}_t = 0.33(16)$$

- note the postive sign of $\bar{A}_t$

- Original estimate (resonance saturation): $$\bar{A}_s = 0.29^{+0.25}_{-0.23}\ ,\quad \bar{A}_t = -0.18(10)$$

Berengut et al., Phys. Rev. **D87** (2013) 085018

- LO Lorentz-invariant chiral EFT: $$\bar{A}_s = 0.50(23)\ ,\quad \bar{A}_t = -0.12(08)$$

Behrendt et al., Eur. Phys. J. **A52** (2016) 296

LOW-ENERGY THEOREMS for NN SCATTERING

Cohen, Hansen (1999), Baru et al (2015,2016)

- Basic idea: consider non-relativistic scattering for particles with mass m and interacting by a non-singular potential of finite range

$$S = \mathrm{e}^{2i\delta(k)} = 1 - i\left(\frac{km}{8\pi^2}\right)T(k), \quad T(k) = -\frac{16\pi^2}{m}\frac{1}{F(k) - ik}$$

- Central object: **the effective range function**: $F(k) = k\cot(\delta(k))$

- Effective range expansion (ERE): $F(k) = -\frac{1}{a} + \frac{1}{2}r\,k^2 + v_2\,k^4 + v_3\,k^6 + v_4\,k^8 + \ldots$

- Generalization: consider a potential made of a long-range & a short-range piece

$$V = V_L + V_S\ , \quad r_L \sim M_L^{-1}\ , \quad r_S \sim M_S^{-1} \ll M_L^{-1}$$

- Idea: Keep the long-range physics explicitely $\to$ **modified ERE** (determined by V_S)

$$F^M(k^2) \equiv \lim_{r\to 0}\left[\frac{d}{dr}\frac{f^L(k,r)}{f^L(k)}\right] + \frac{k}{|f^L(k)|}\cot\left[\delta(k) - \delta^L(k)\right], \quad \underbrace{f_L(k) \equiv f_L(k,r)\big|_{r=0}}_{\text{Jost function, solves SEq}}$$

- $F^M(k^2)$ is a meromorphic fct in a larger region set by r_S^{-1}, modified ERE:

$$F^M(k) = -\frac{1}{a^M} + \frac{1}{2} r^M k^2 + v_2^M k^4 + v_3^M k^6 + v_4^M k^8 + \ldots$$

- Meaning of the LETs: calculate the phase shift in terms of the known long-range part:

$$k \cot \delta(k) = \frac{|f^L(k)| \left(F^M(k^2) - R^L(k^2)\right) k \cot \delta^L(k) - k^2}{|f^L(k)| \left(F^M(k^2) - R^L(k^2)\right) + k \cot \delta^L(k)}$$

- At leading order, the MERE is given by $F^M_{\rm l.o.}(k^2) \simeq -1/a^M \to$ a single piece of information on a^M or, equivalently a, lets one predict **all** coefficients in the ERE:

$$r = \frac{f_1(aM_L)}{M_L}\,, \quad v_2 = \frac{f_2(aM_L)}{M_L^3}\,, \quad v_3 = \frac{f_3(aM_L)}{M_L^5}\,, \ldots$$

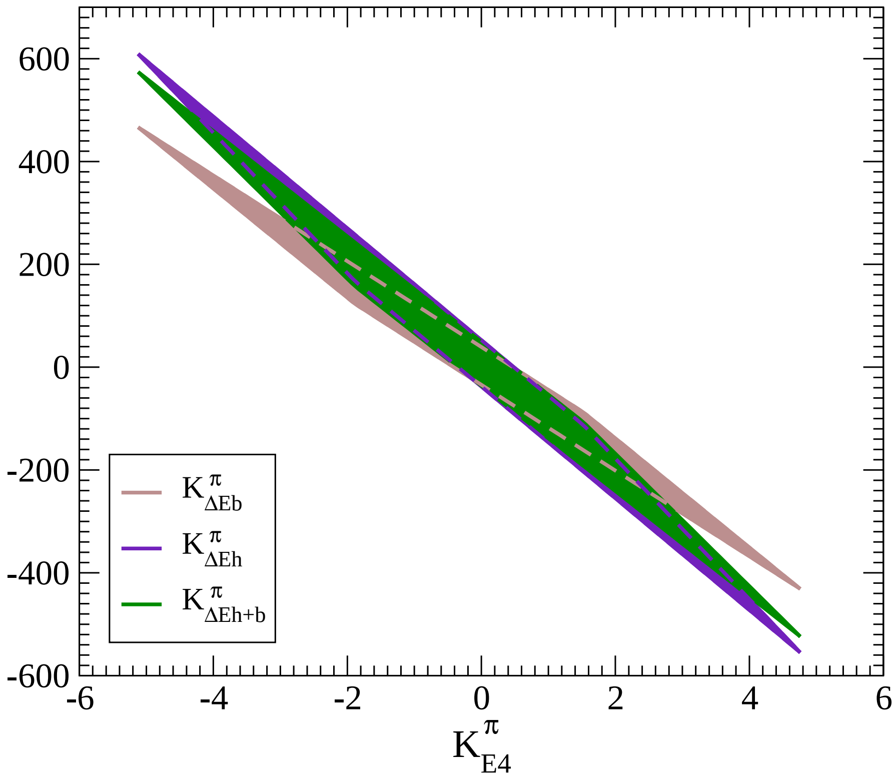
- with known polynomials $f_1, f_2, \ldots$. These LETs are accurate up to corrections from the second term in the MERE

- Using a^M and r^M (or a and r) as input $\to$ refined predictions/LETs

CORRELATIONS

- map $C_{0,I}(M_\pi)$ onto $\bar{A}_{s,t} \equiv \partial a_{s,t}^{-1}/\partial M_\pi\big|_{M_\pi^{\rm phys}}$ [singlet/triplet scatt. length]

- vary the derivatives $\bar{A}_{s,t} \equiv \partial a_{s,t}^{-1}/\partial M_\pi\big|_{M_\pi^{\rm phys}}$ within $-1,\ldots,+1$:



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

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

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

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

- all fine-tunings in the triple-alpha process are *correlated*, as speculated

Weinberg (2000)

THE END-OF-THE-WORLD PLOTS

- Combine results to generate exclusion plots

- Sensitivity on $\mathcal{Z}$

$\hookrightarrow$ low $\mathcal{Z}$ $\to$ less fine-tuning

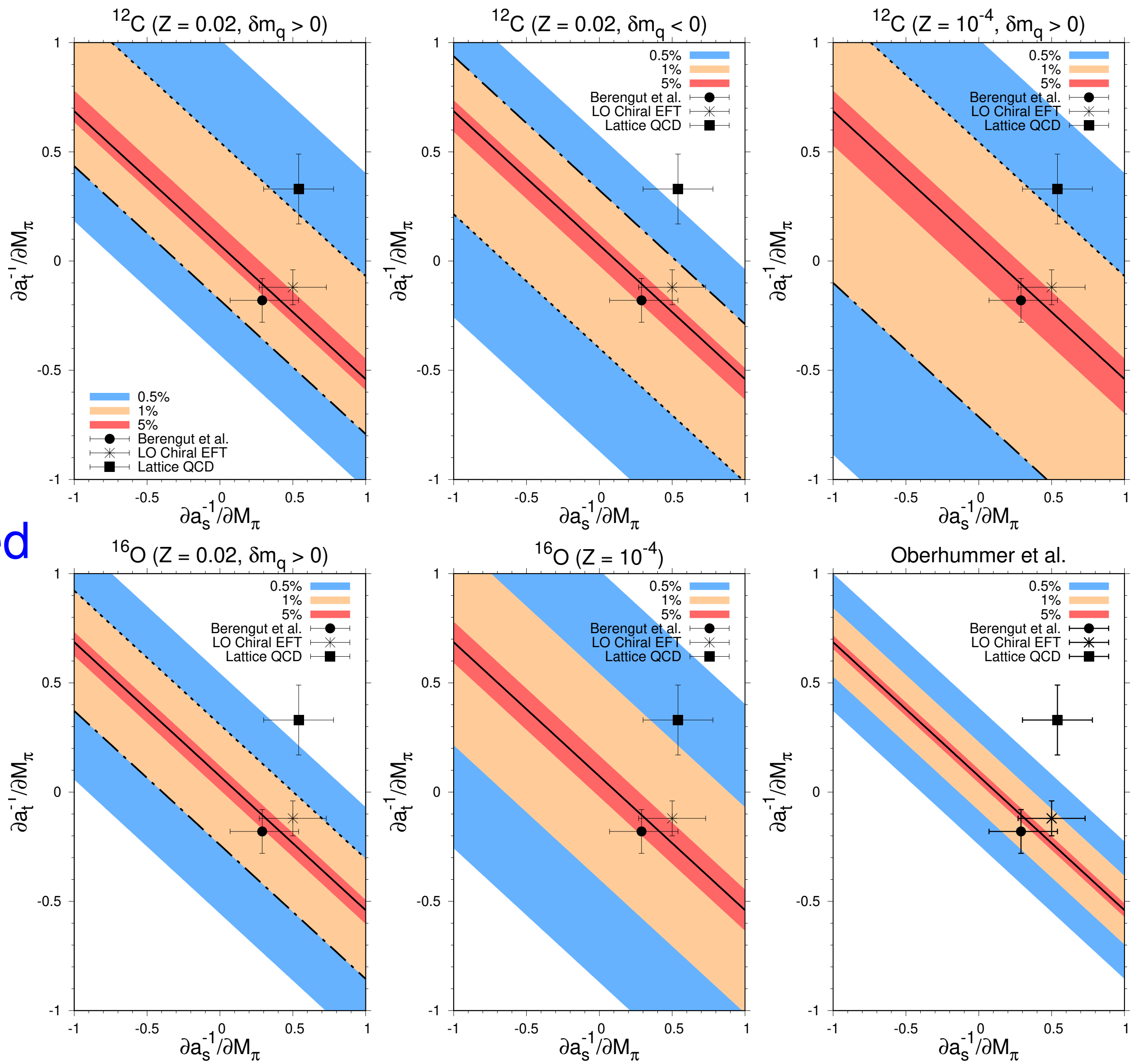
- LQCD constraints on $\bar{A}_{s,t}$

$\hookrightarrow$ no fine-tuning-scenario excluded

- other determinations of $\bar{A}_{s,t}$ allow for larger variations in m_q

- need better LQCD calc's of the NN system!

- tolerance for variations in $\alpha_{\rm EM}$ increased from 2.5% to 7.5%



[NB: black diagonal line = no fine-tuning]

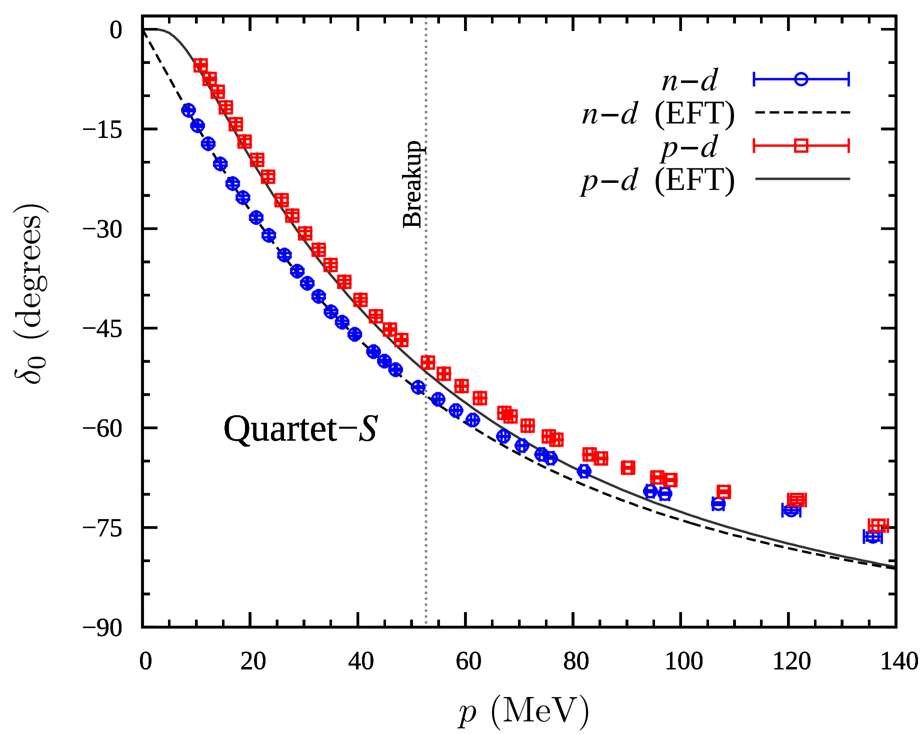
Scattering on a lattice: Results

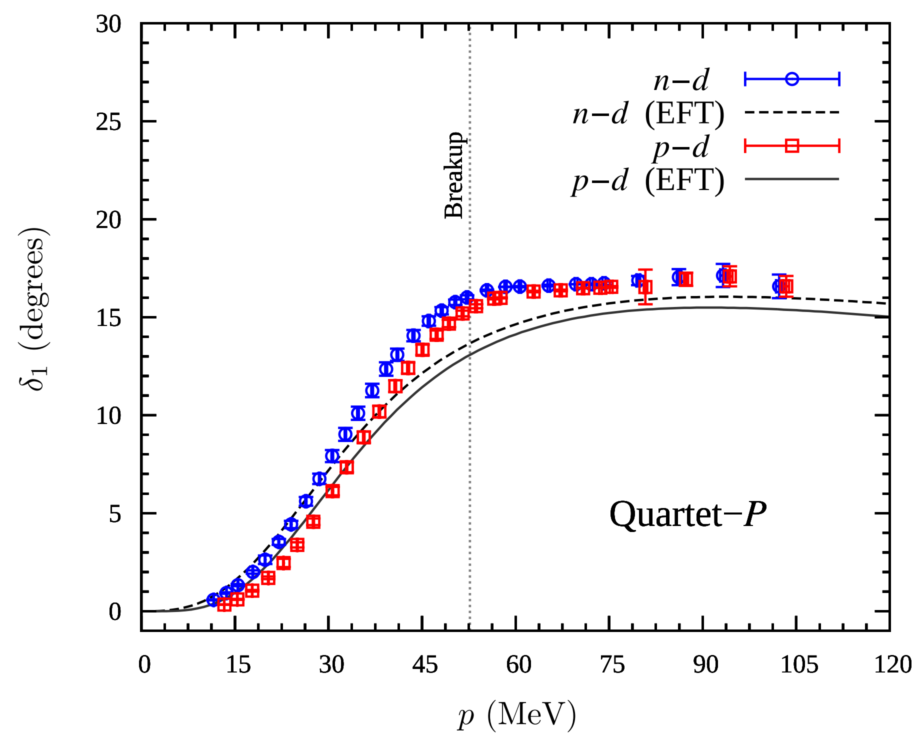
NUCLEON–DEUTERON SCATTERING

Elhatisari, Lee, UGM, Rupak, Eur. Phys. J. A **52** (2016) 174

- Use improved methods (cluster states projected onto spherical harmonics, etc.) & algorithmic improvements
- Precision calculation of proton-deuteron and neutron-deuteron scattering

Pionless EFT: König, Hammer, Gabbiani, Bedaque, Rupak, Griesshammer, van Kolck, 1998-2011





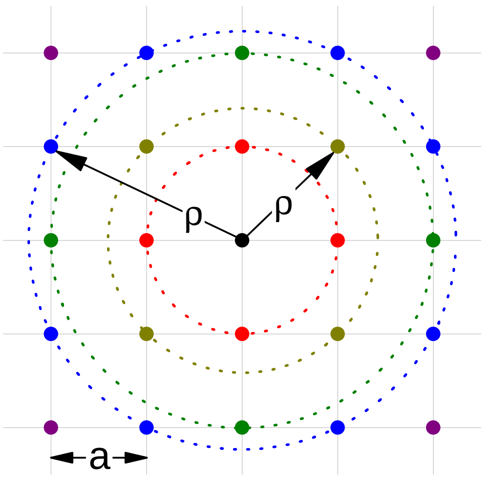
- Note: the quartet channel has no 3NF

ALPHA–ALPHA SCATTERING

Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, UGM, Nature **528** (2015) 111

- same lattice action as for the Hoyle state in ^{12}C and the structure of ^{16}O
- 9 NN + 2 3N LECs, coarse lattice $a = 1.97$ fm, $N = 8$
- new algorithm for Monte Carlo updates and alpha clusters
- adiabatic projection method to construct a two-alpha Hamiltonian
- spherical wall method to extract the phase shifts using radial Hamiltonian

$$|R\rangle^{\ell,\ell_z} = \sum_{\vec{R}'} Y_{\ell,\ell_z}(\vec{R}')\, \delta_{R,|\vec{R}'|}\, |\vec{R}'\rangle$$



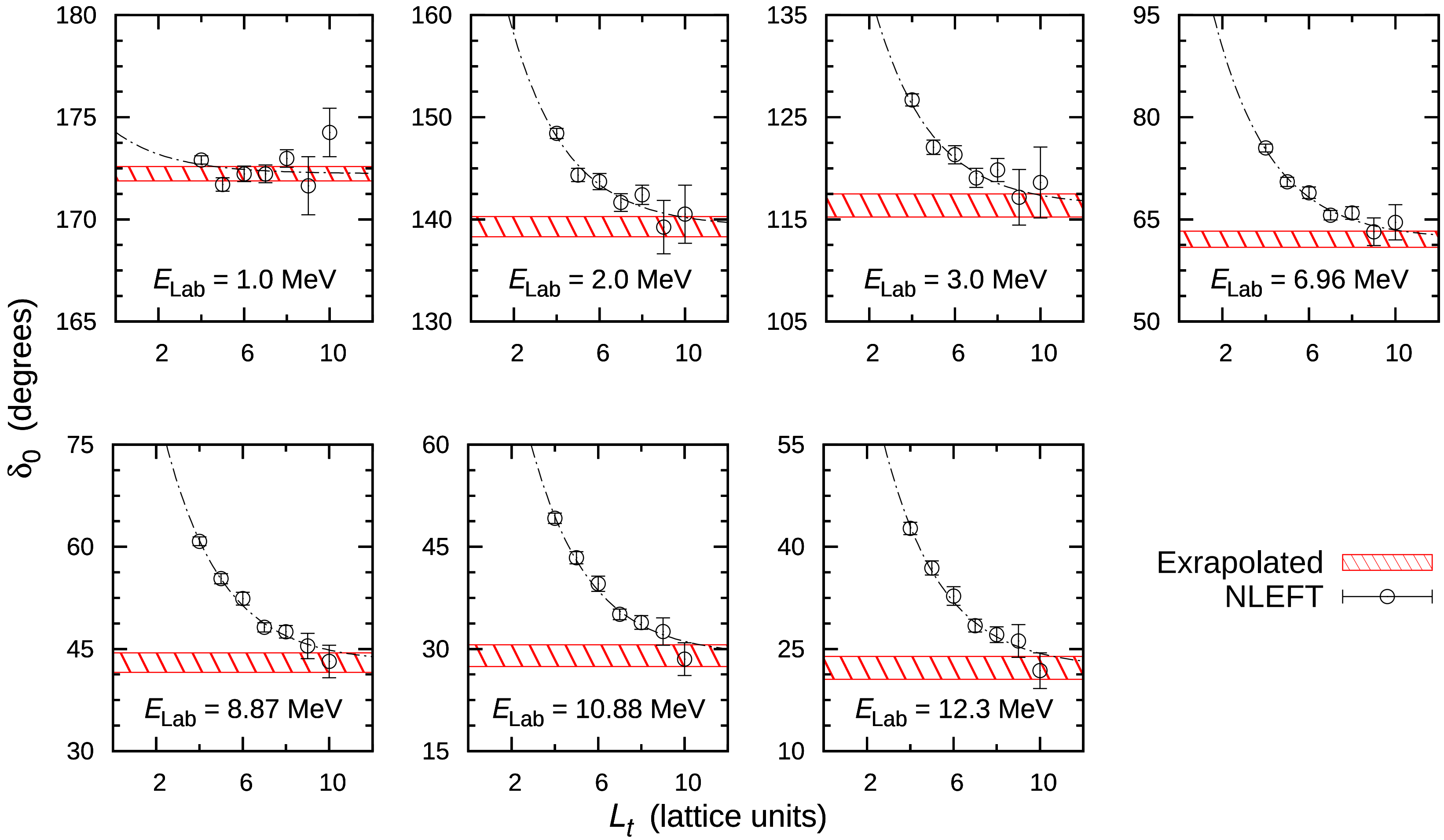
$\rightarrow$ precise extraction of phase shifts & mixing angles

$\rightarrow$ inclusion of long-range Coulomb effects (important!)

- Uncertainty analysis tbd w/ better action

LATTICE DATA I

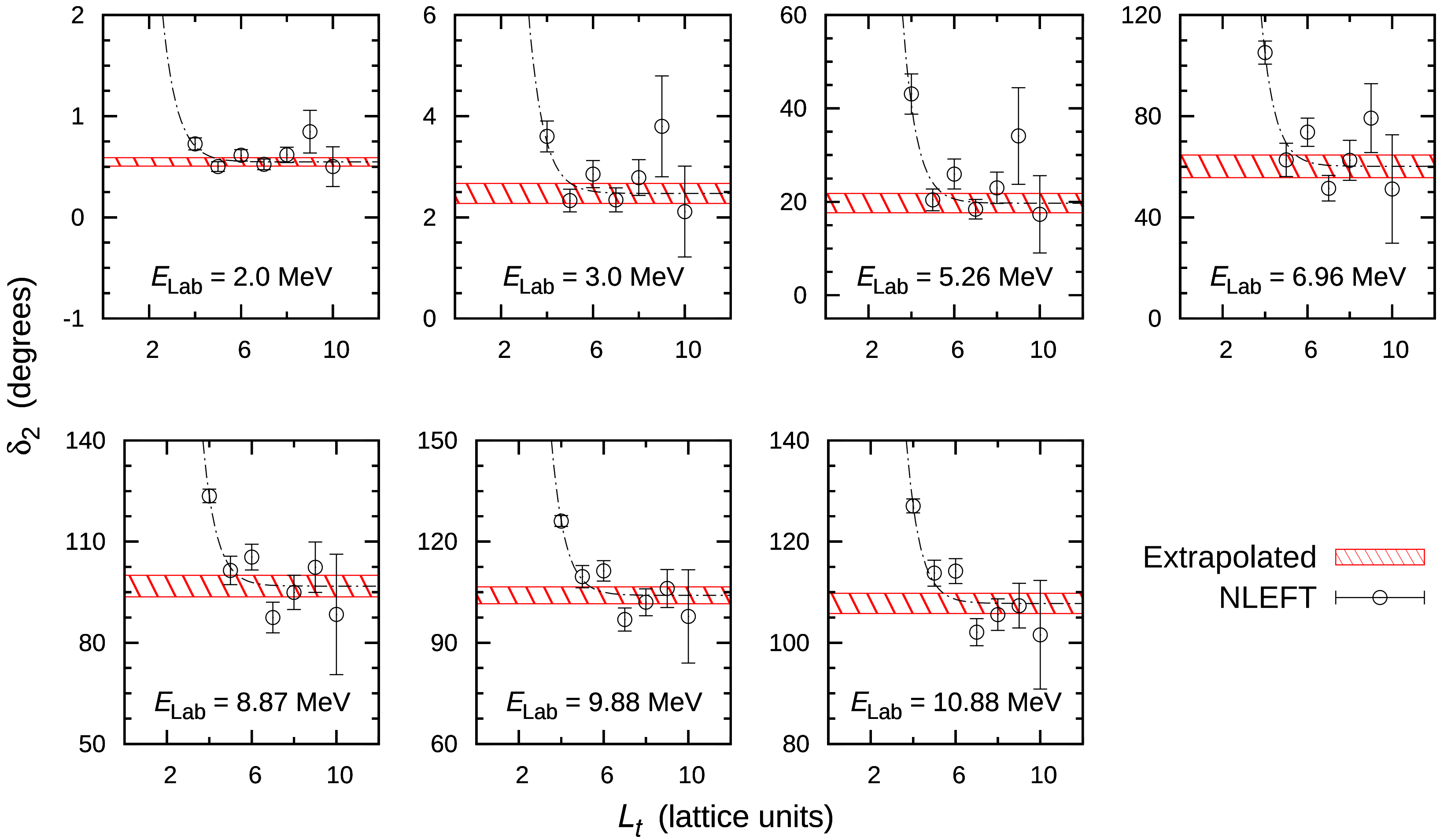
- Show data for the S-wave:



$$\delta_0(L_t, E) = \delta_0(E) + \underbrace{c_0(E)}_{\text{fit parameter}} \exp[-\underbrace{\Delta E_0}_{\text{exc. state cont.}} L_t a_t]$$

LATTICE DATA II

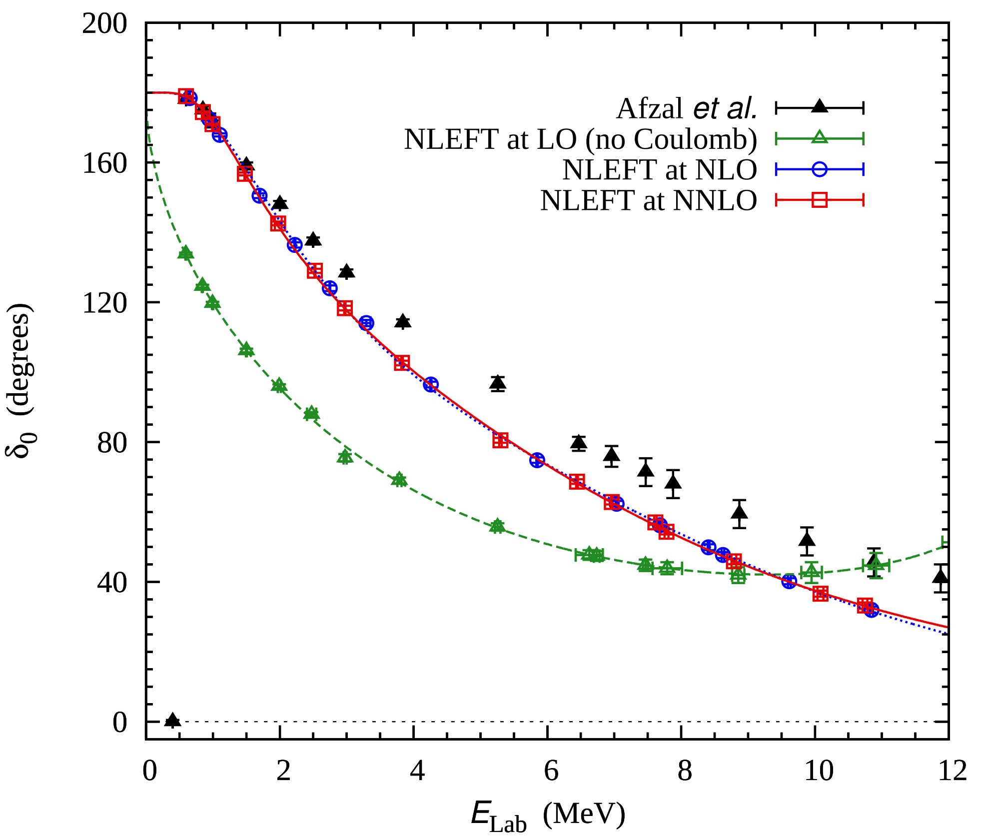
- Show data for the D-wave:

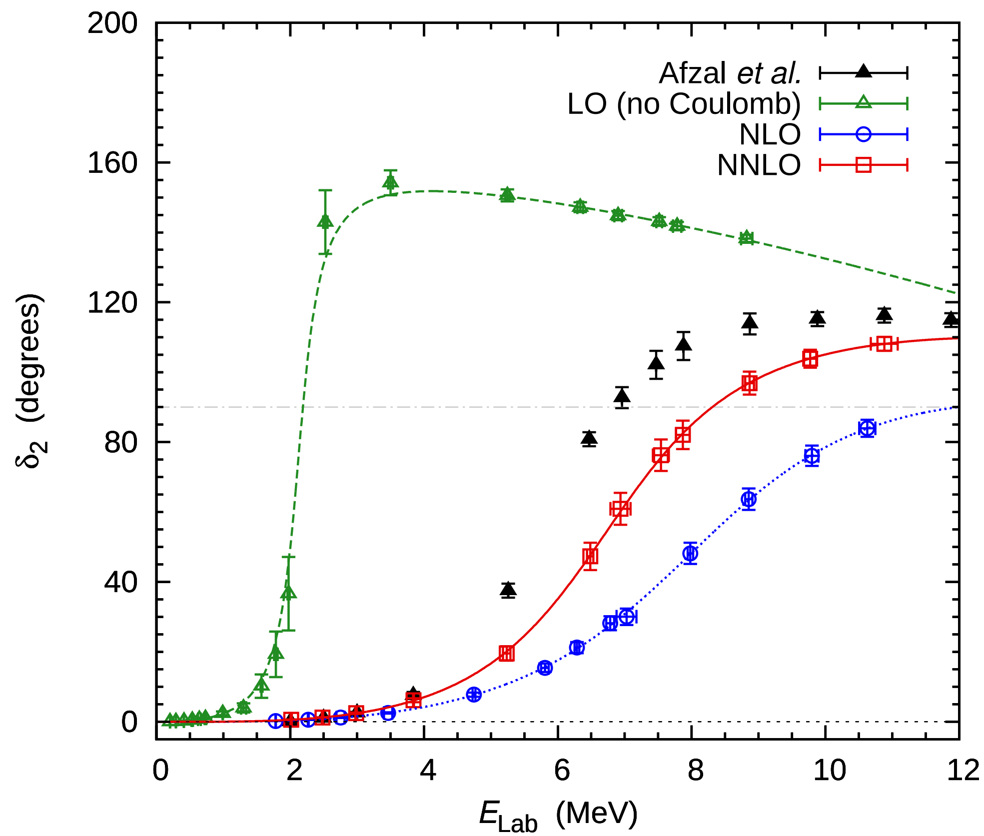


$$\delta_2(L_t, E) = \delta_2(E) + \underbrace{c_2(E)}_{\text{fit parameter}} \exp[-\underbrace{\Delta E_2}_{\text{exc. state cont.}} L_t a_t]$$

PHASE SHIFTS

- S-wave and D-wave phase shifts (LO has no Coulomb)





$E_R^{\rm NNLO} = -0.11(1)$ MeV [$+0.09$ MeV]

$E_R^{\rm NNLO} = 3.27(12)$ MeV [$2.92(18)$ MeV]

$\Gamma_R^{\rm NNLO} = 2.09(16)$ MeV [$1.35(50)$ MeV]

Data: Afzal et al., Rev. Mod. Phys. **41** (1969) 247

Nuclear binding near a quantum phase transition

Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, UGM, Epelbaum, Krebs, Lähde, Lee, Rupak,
Phys. Rev. Lett. **117** (2016) 132501 [arXiv:1602.04539]

Editors' suggestion, featured in Physics viewpoint: D.J. Dean, Physics 9 (2016) 106

GENERAL CONSIDERATIONS

- *Ab initio* chiral EFT is an excellent theoretical framework

- not guaranteed to work well with increasing A

$\rightarrow$ possible sources of problems:

higher-body forces, higher orders, cutoff dependence, ...

- very many ways of formulating chiral EFT at any given order (smearing etc.)

$\rightarrow$ use not only NN scattering and light nuclei BEs
but also light nucleus-nucleus scattering data
to pin down the pertinent interactions

$\rightarrow$ troublesome corrections might be small

$\rightarrow$ investigate these issues using two seemingly equivalent interactions
[not a precision study!]

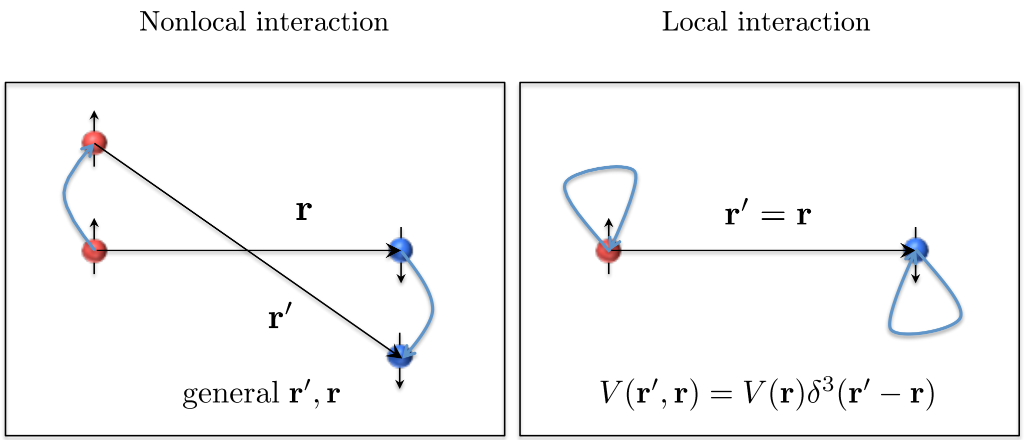
LOCAL and NON–LOCAL INTERACTIONS

- General potential: $V(\vec{r}, \vec{r}\,')$

- Two types of interactions:

  local: $\vec{r} = \vec{r}\,'$

  non-local: $\vec{r} \neq \vec{r}\,'$

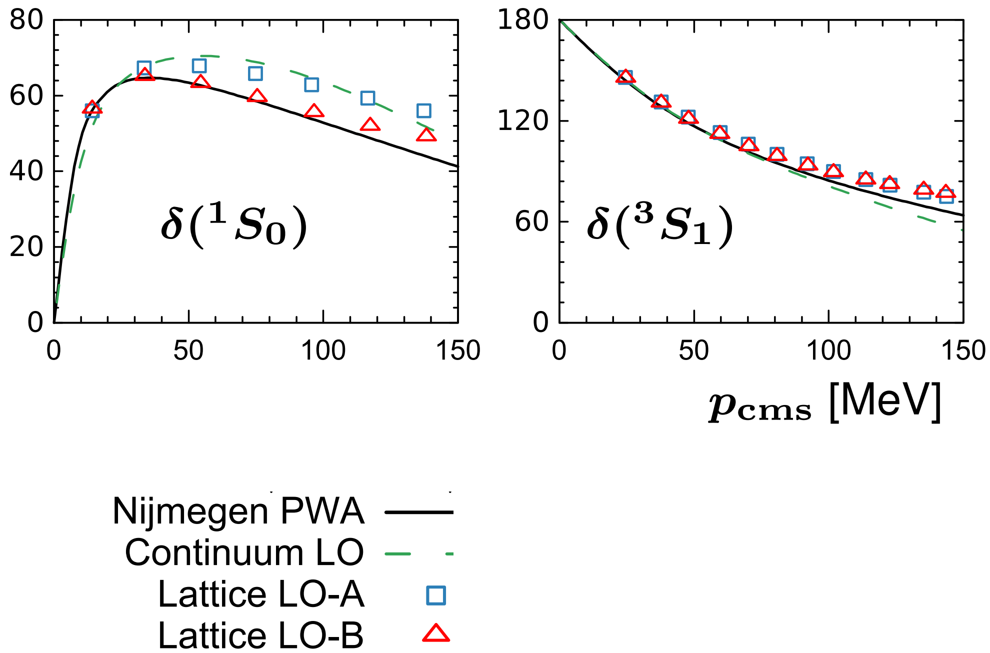


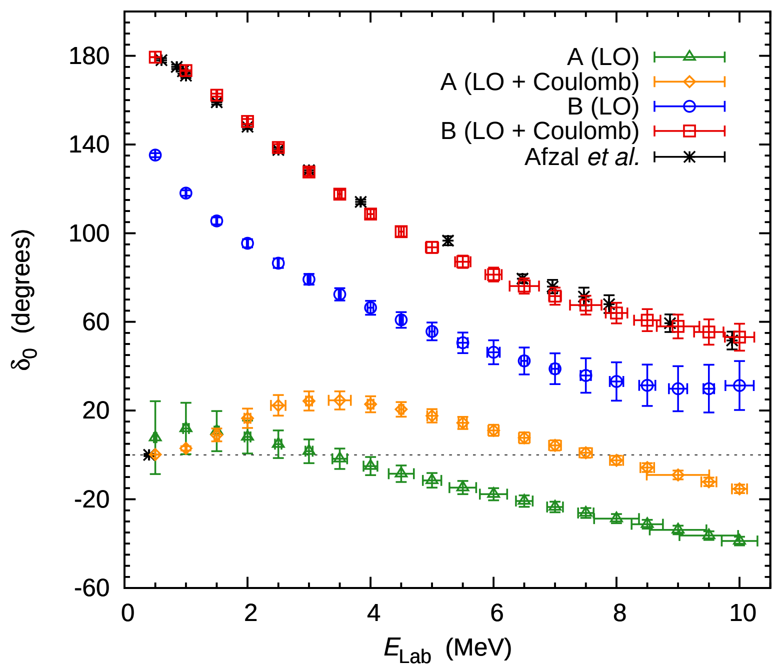
- Taylor two very different interactions:

Interaction A at LO (+ Coulomb)	Interaction B at LO (+ Coulomb)
Non-local short-range interactions	Non-local short-range interactions
+ One-pion exchange interaction	+ Local short-range interactions
(+ Coulomb interaction)	+ One-pion exchange interaction
	(+ Coulomb interaction)
$\rightarrow$ tuned to NN phase shifts	$\rightarrow$ tuned to NN + α-α phase shifts

NN and ALPHA–ALPHA PHASE SHIFTS

- Both interactions very similar for NN but **not** for α-α phase shifts:



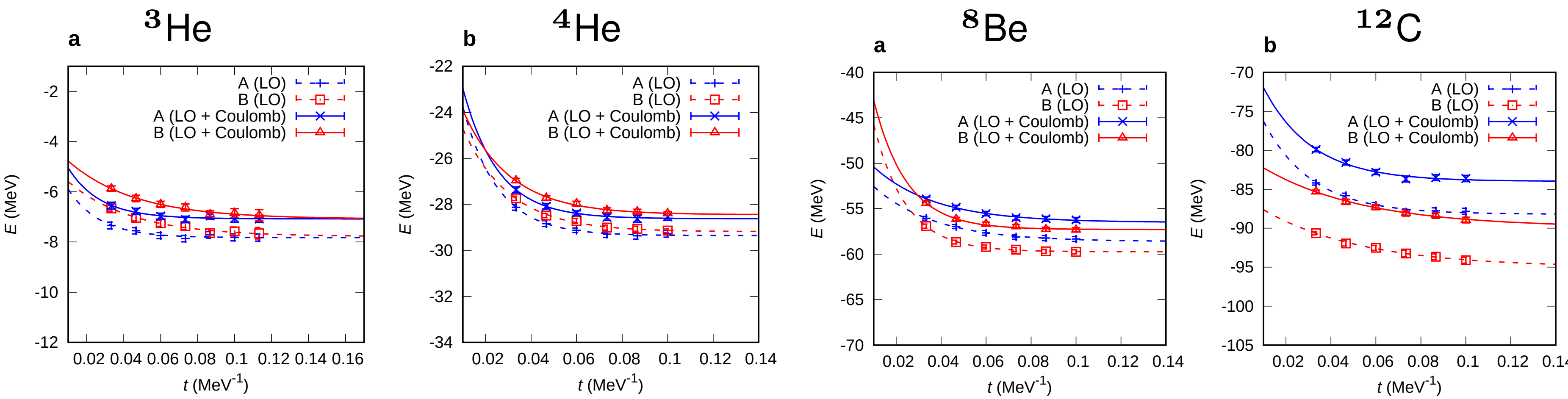


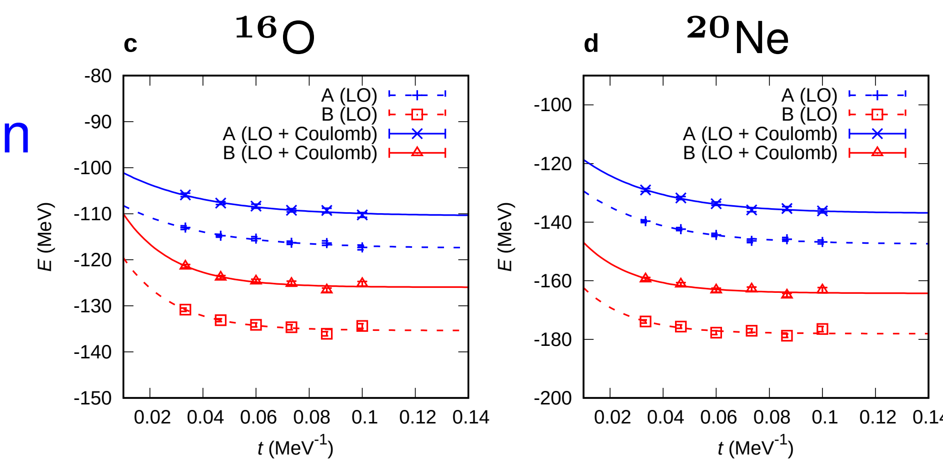
$\longrightarrow$ Interaction A fails, interaction B fitted

$\hookrightarrow$ consequences for nuclei?

GROUND STATE ENERGIES I

- Ground state energies for alpha-type nuclei plus ^{3}He:





- small errors, excellent thermalization

$\Rightarrow$ Both interactions significantly reduce the Monte Carlo sign oscillations (original motivation)

GROUND STATE ENERGIES I

- Ground state energies for alpha-type nuclei (in MeV):

	A (LO)	A (LO+C.)	B (LO)	B (LO+C.)	Exp.
^{4}He	$-29.4(4)$	$-28.6(4)$	$-29.2(1)$	$-28.5(1)$	-28.3
^{8}Be	$-58.6(1)$	$-56.5(1)$	$-59.7(6)$	$-57.3(7)$	-56.6
^{12}C	$-88.2(3)$	$-84.0(3)$	$-95.0(5)$	$-89.9(5)$	-92.2
^{16}O	$-117.5(6)$	$-110.5(6)$	$-135.4(7)$	$-126.0(7)$	-127.6
^{20}Ne	$-148(1)$	$-137(1)$	$-178(1)$	$-164(1)$	-160.6

- B (LO+Coulomb) quite close to experiment (within 2% or better)

- A (LO) describes a Bose condensate of particles:

$$E(^8\mathrm{Be})/E(^4\mathrm{He}) = 1.997(6) \quad E(^{12}\mathrm{C})/E(^4\mathrm{He}) = 3.00(1)$$

$$E(^{16}\mathrm{O})/E(^4\mathrm{He}) = 4.00(2) \quad E(^{20}\mathrm{Ne})/E(^4\mathrm{He}) = 5.03(3)$$

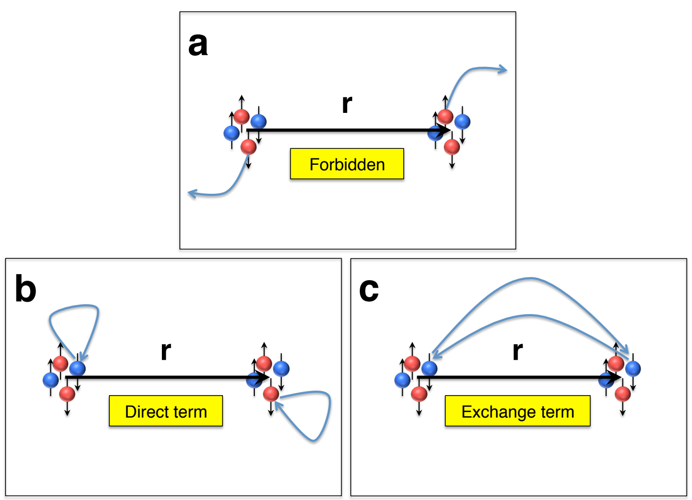
FIRST INSIGHT

- Interaction B was tuned to the nucleon-nucleon phase shifts, the deuteron binding energy, and the S-wave α-α phase shift

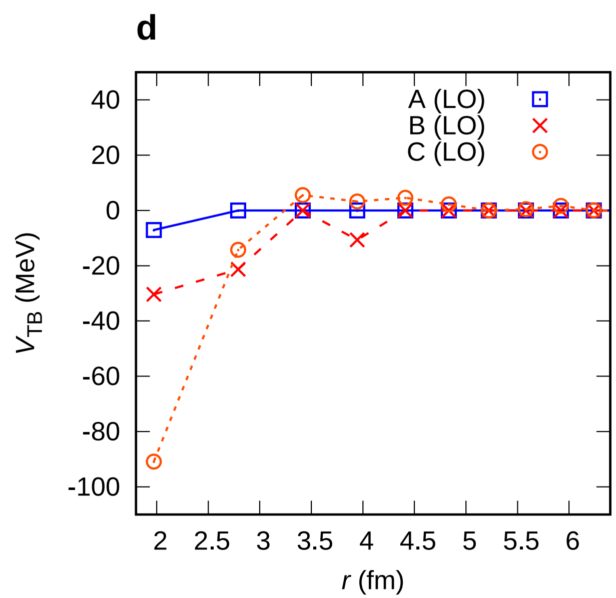
- Interaction A starts from interaction B, but *all* local short-distance interactions are switched off, then the LECs of the non-local terms are refitted to describe the nucleon-nucleon phase shifts and the deuteron binding energy

$\rightarrow$ The alpha-alpha interaction is sensitive to the degree of locality of the NN int.

$\rightarrow$ Qualitative understanding: tight-binding approximation (eff. α-α int.)



$\Longrightarrow$



CONSEQUENCES for NUCLEI and NUCLEAR MATTER

- Define a one-parameter family of interactions that interpolates between the interactions A and B:

$$\boxed{V_\lambda = (1-\lambda)\,V_A + \lambda\,V_B}$$

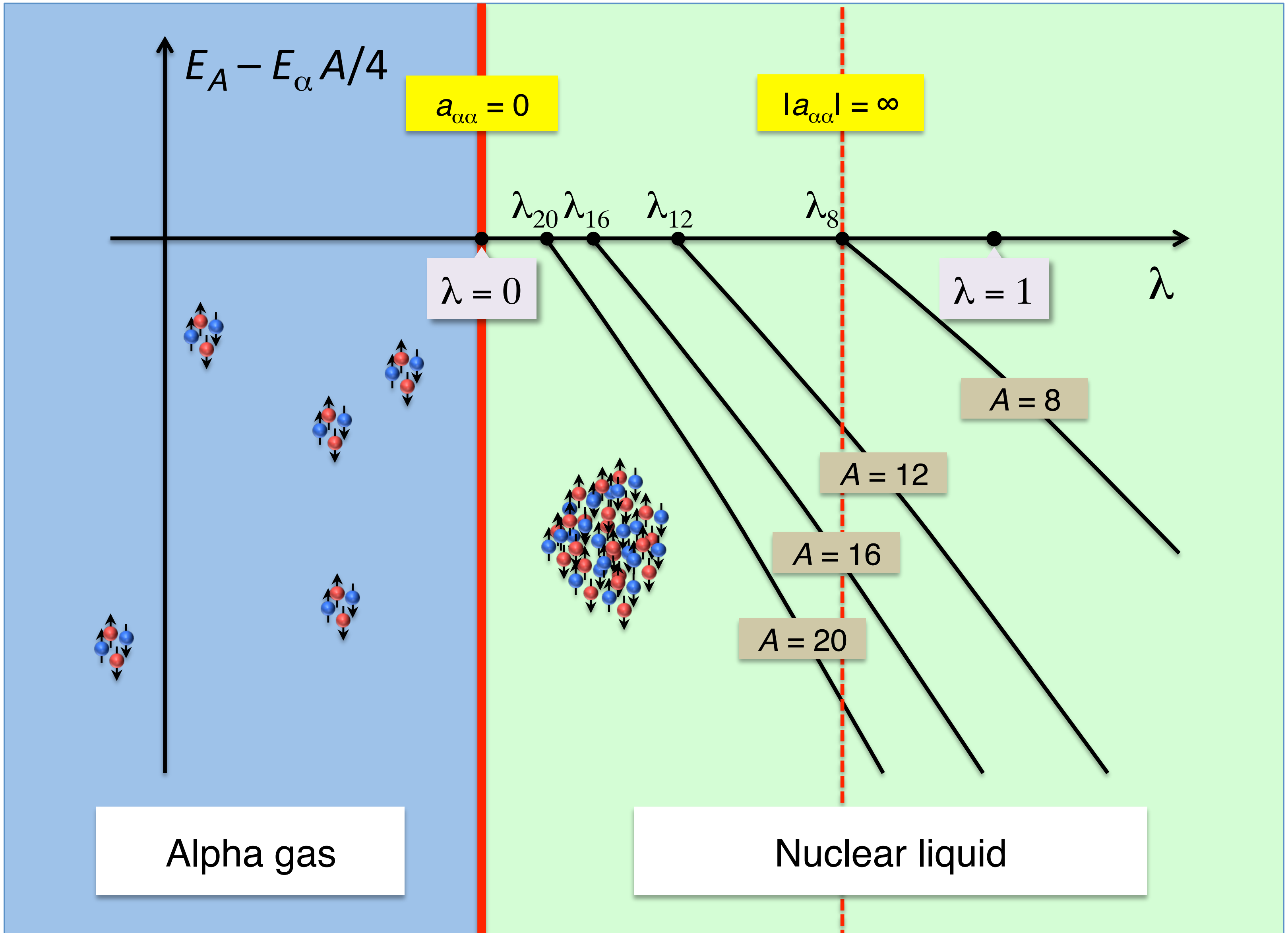
- To discuss the many-body limit, we turn off the Coulomb interaction and explore the zero-temperature phase diagram

- As a function of λ, there is a quantum phase transition at the point where the alpha-alpha scattering length vanishes

Stoof, Phys. Rev. A **49** (1994) 3824

- The transition is a first-order transition from a Bose-condensed gas of alpha particles to a nuclear liquid

ZERO–TEMPERATURE PHASE DIAGRAM



$$\lambda_8 = 0.7(1)$$
$$\lambda_{12} = 0.3(1)$$
$$\lambda_{16} = 0.2(1)$$
$$\lambda_{20} = 0.2(1)$$
$$\lambda_\infty = 0.0(1)$$

FURTHER CONSEQUENCES

- By adjusting the parameter λ in *ab initio* calculations, one can move the of any α-cluster state up and down to alpha separation thresholds.

$\longrightarrow$ This can be used as a new window to view the structure of these exotic nuclear states

- In particular, one can tune the α-α scattering length to infinity!

$\longrightarrow$ In the absence of Coulomb interactions, one can thus make contact to **universal Efimov physics**:

for a review, see Braaten, Hammer, Phys. Rept. **428** (2006) 259

Hoyle state of ^{12}C $\xrightarrow{\lambda}$ Universal Efimov trimer

Second 0^+ of ^{16}O $\xrightarrow{\lambda}$ Universal Efimov tetramer

Open ends / On-going developments

STRANGENESS NUCLEAR PHYSICS

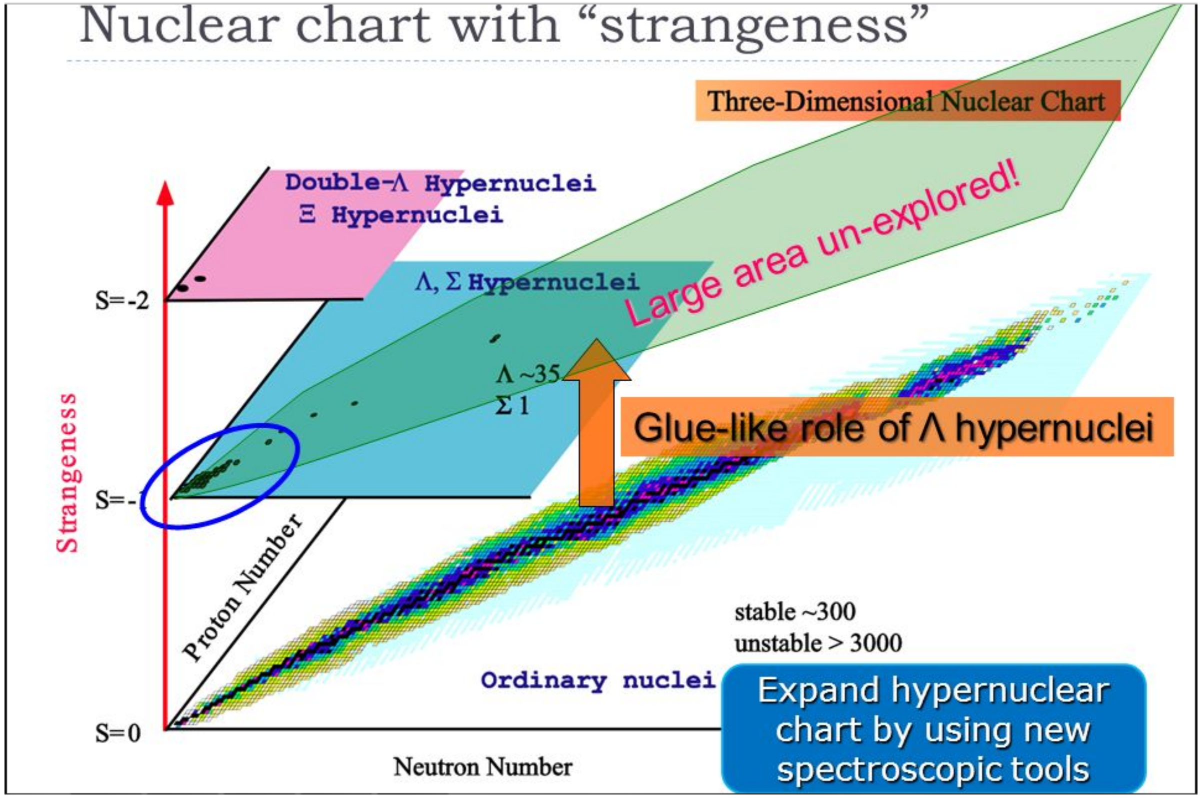
- Substitute one (or two) nucleon(s) by a hyperon (Λ, Σ)

- A few known **hypernuclei**

- Also: very few hyperon-nucleon scattering data

$\Rightarrow$ important role of hypernuclear spectra

$\Rightarrow$ lattice can make an impact!



- Step 1: Crash course on YN/YY scattering in chiral EFT

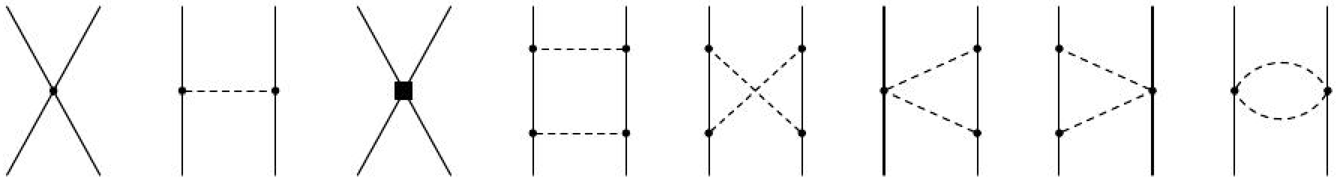
- Step 2: Impurity Lattice Monte Carlo (ILMC) algorithm

BARYON-BARYON INTERACTIONS in CHIRAL EFT

LO: Polinder, Haidenbauer, UGM, Nucl. Phys. A **779** (2006) 244

NLO: Haidenbauer, Petschauer, Kaiser, UGM, Nogga, Weise, Nucl. Phys. A **915** (2013) 24

- Goldstone boson octet
  interacts with the
  the ground-state baryon octet
  and via contact interactions (just like NN)



$$M = \begin{pmatrix} \frac{\pi^0}{\sqrt{2}} + \frac{\eta}{\sqrt{6}} & \pi^+ & K^+ \\ \pi^- & -\frac{\pi^0}{\sqrt{2}} + \frac{\eta}{\sqrt{6}} & K^0 \\ K^- & \bar{K}^0 & -\frac{2\eta}{\sqrt{6}} \end{pmatrix} \quad B = \begin{pmatrix} \frac{\Sigma^0}{\sqrt{2}} + \frac{\Lambda}{\sqrt{6}} & \Sigma^+ & p \\ \Sigma^- & -\frac{\Sigma^0}{\sqrt{2}} + \frac{\Lambda}{\sqrt{6}} & n \\ -\Xi^- & \Xi^0 & -\frac{2\Lambda}{\sqrt{6}} \end{pmatrix}$$

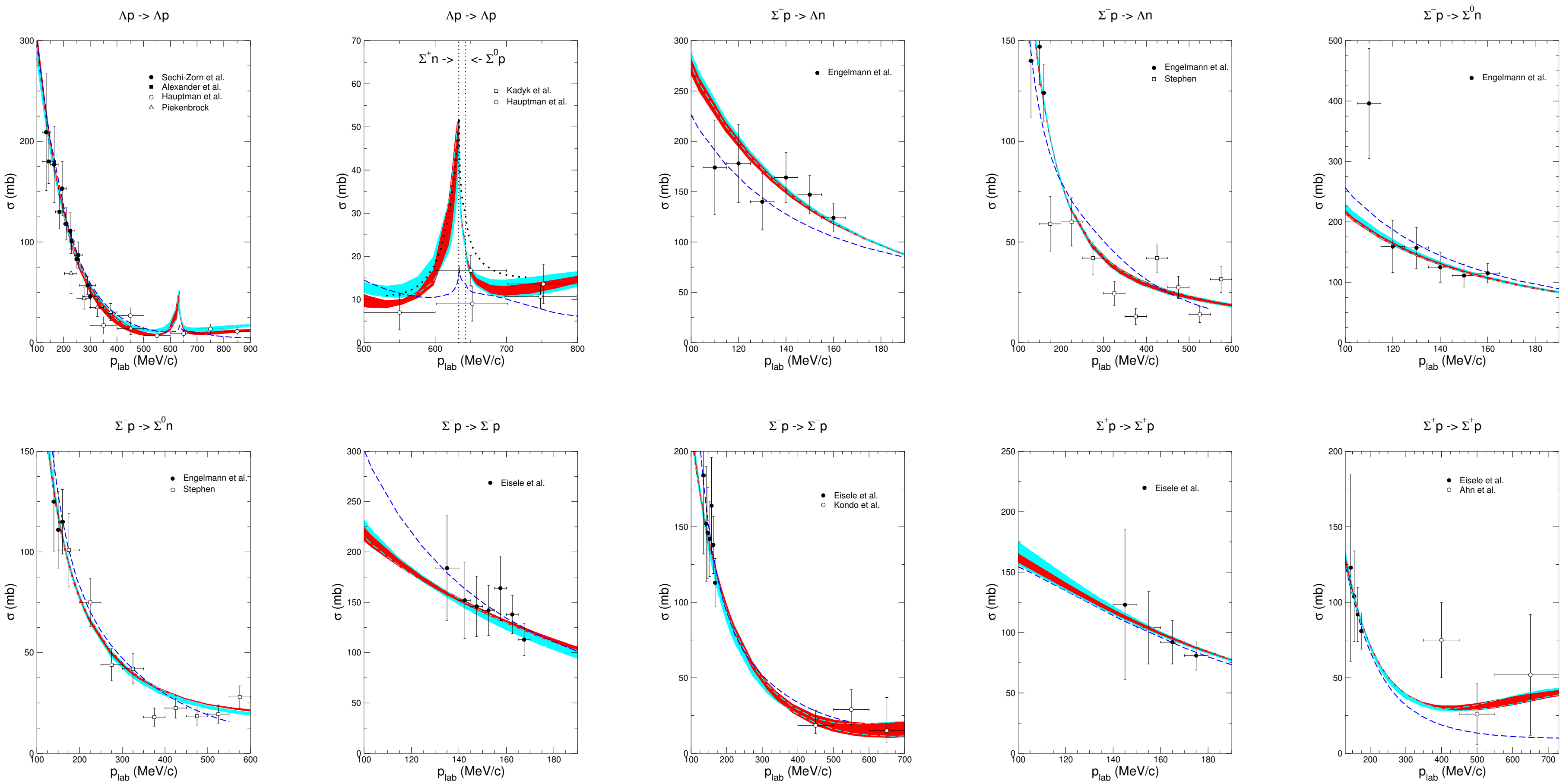
- Use SU(3) symmetry to relate MBB couplings and the various contact term LECs

- Need SU(3) breaking for a combined description of NN and YN interactions

- Exercise: how many LECs contribute to YN scattering at LO (use group th'y)?

BARYON-BARYON INTERACTIONS in CHIRAL EFT

- Total XS results (fit to 36 low-energy data points, only cut-off variations)



NLO13

NLO19

J'04

closed symbols: fit
open symbols: prediction

Jülich '04 potential: Haidenbauer and UGM, Phys. Rev. C **72** (2005) 044005

HYPERON-NUCLEON INTERACTIONS in LIGHT NUCLEI

- Separation energies in light hyper-nuclei (all in MeV)

YN interaction	$E_\Lambda({}^3_\Lambda\mathrm{H})$	$E_\Lambda({}^4_\Lambda\mathrm{He}(0^+))$	$E_\Lambda({}^4_\Lambda\mathrm{He}(1^+))$
NLO13(500)	0.135	1.705	0.790
NLO13(550)	0.097	1.503	0.586
NLO13(600)	0.090	1.477	0.580
NLO13(650)	0.087	1.490	0.615
NLO19(500)	0.100	1.643	1.226
NLO19(550)	0.094	1.542	1.239
NLO19(600)	0.091	1.462	1.055
NLO19(650)	0.095	1.530	0.916
Jülich'04	0.046	1.704	2.312
Expt.	0.13(5)	2.39(3)	0.98(3)

- NLO13 as described before

- NLO19: make use of explicit SU(3) breaking contact terms at NLO
  $\hookrightarrow$ remedy friction between the NN and YN S-waves

Haidenbauer, UGM, Nogga, arXiv:1906.11681

LATTICE FORMULATION

- Simpler physics as there are no unnaturally large scattering lengths (as far as they are known)

- Formulation as for the NN is possible, spin-flavor matrices:

$$\begin{pmatrix} a_{0,0} \\ a_{1,0} \\ a_{0,1} \\ a_{1,1} \\ a_{0,2} \\ a_{1,2} \\ a_{0,3} \\ a_{1,3} \\ a_{0,4} \\ a_{1,4} \\ a_{0,5} \\ a_{1,5} \end{pmatrix} = \begin{pmatrix} a_{\uparrow,p} \\ a_{\downarrow,p} \\ a_{\uparrow,n} \\ a_{\downarrow,n} \\ a_{\uparrow,\Lambda} \\ a_{\downarrow,\Lambda} \\ a_{\uparrow,\Sigma^+} \\ a_{\downarrow,\Sigma^+} \\ a_{\uparrow,\Sigma^0} \\ a_{\downarrow,\Sigma^0} \\ a_{\uparrow,\Sigma^-} \\ a_{\downarrow,\Sigma^-} \end{pmatrix}$$

- LO simulations for the contact interactions
  - $\Rightarrow$ feasible, LECs fitted to threshold ratios
  - $\Rightarrow$ volume dependence of the scattering lengths consistent with the Lüscher formula

    S. Bour, diploma thesis, Bonn, 2009

- however, no follow-up due to missing SU(4) Wigner symmetry
  - $\hookrightarrow$ too little control on the sign oscillations (expectation, not a calculation)

- is there another method to deal with hyperons in nuclei?

IMPURITY MONTE CARLO

Elhatisari, Lee, Phys. Rev. C **90** (2014) 046001

- Basic idea: Consider the hyperon(s) as **impurity(ies)** in a sea of nucleons

- Benchmark calculation: a ↓-particle in a sea of ↑-particles ($m_\uparrow = m_\downarrow = m$)

- Lattice Hamiltonian ($H_0 + V$):

$$H_0 = H_0^\uparrow + H_0^\downarrow$$

$$H_0^s = \frac{1}{2m}\sum_{l=1}^{3}\sum_{\vec{n}}\left[2a_s^\dagger(\vec{n})a_s(\vec{n}) - a_s^\dagger(\vec{n})a_s(\vec{n}+\hat{l}) - a_s^\dagger(\vec{n})a_s(\vec{n}-\hat{l})\right]$$

$$V = C_0\sum_{\vec{n}}\rho_\uparrow(\vec{n})\,\rho_\downarrow(\vec{n}) \qquad (s = \uparrow, \downarrow)$$

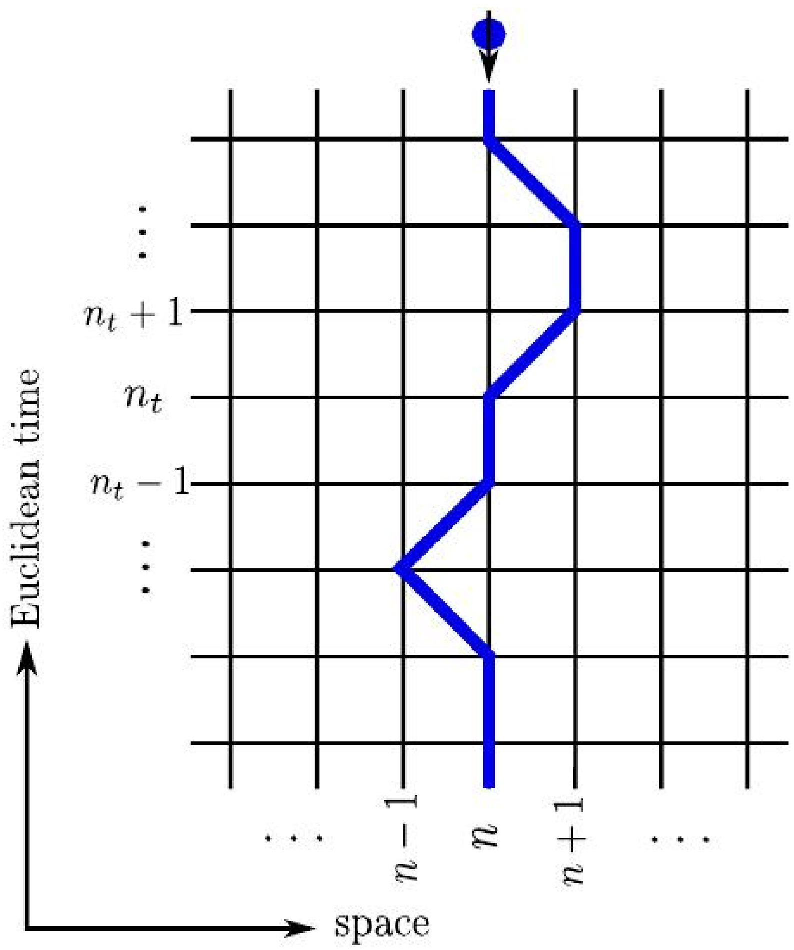
- Work in occupation number basis:

$$\left|\chi_{n_t}^\uparrow, \chi_{n_t}^\downarrow\right\rangle = \prod_{\vec{n}}\left\{\left[a_\uparrow^\dagger(\vec{n})\right]^{\chi_{n_t}^\uparrow(\vec{n})}\left[a_\downarrow^\dagger(\vec{n})\right]^{\chi_{n_t}^\downarrow(\vec{n})}\right\}, \quad \chi_{n_t}^s(\vec{n}) = 0 \text{ or } 1$$

- allows to calculate the transfer matrix: $\langle\chi_{n_t+1}^\uparrow, \chi_{n_t+1}^\downarrow|\, M\, |\chi_{n_t}^\uparrow, \chi_{n_t}^\downarrow\rangle$

IMPURITY MONTE CARLO continued

- Worldline configuration and the reduced transfer matrix (integrate out the impurity)



- impurity makes one spatial hop:

$$M_{\vec{n}''\pm\hat{l},\vec{n}''} = \left(\frac{\alpha_t}{2m}\right) : \exp\left[-\alpha_t H_0^{\uparrow}\right]$$

- impurity worldline remains stationary:

$$M_{\vec{n}'',\vec{n}''} = \left(1 - \frac{3\alpha_t}{m}\right)$$
$$\times : \exp\left[-\alpha_t H_0^{\uparrow} - \frac{\alpha_t C_0}{1-3\alpha_t/m}\rho_{\uparrow}(\vec{n}'')\right]$$

- can also be extended to the Adiabatic Projection Method

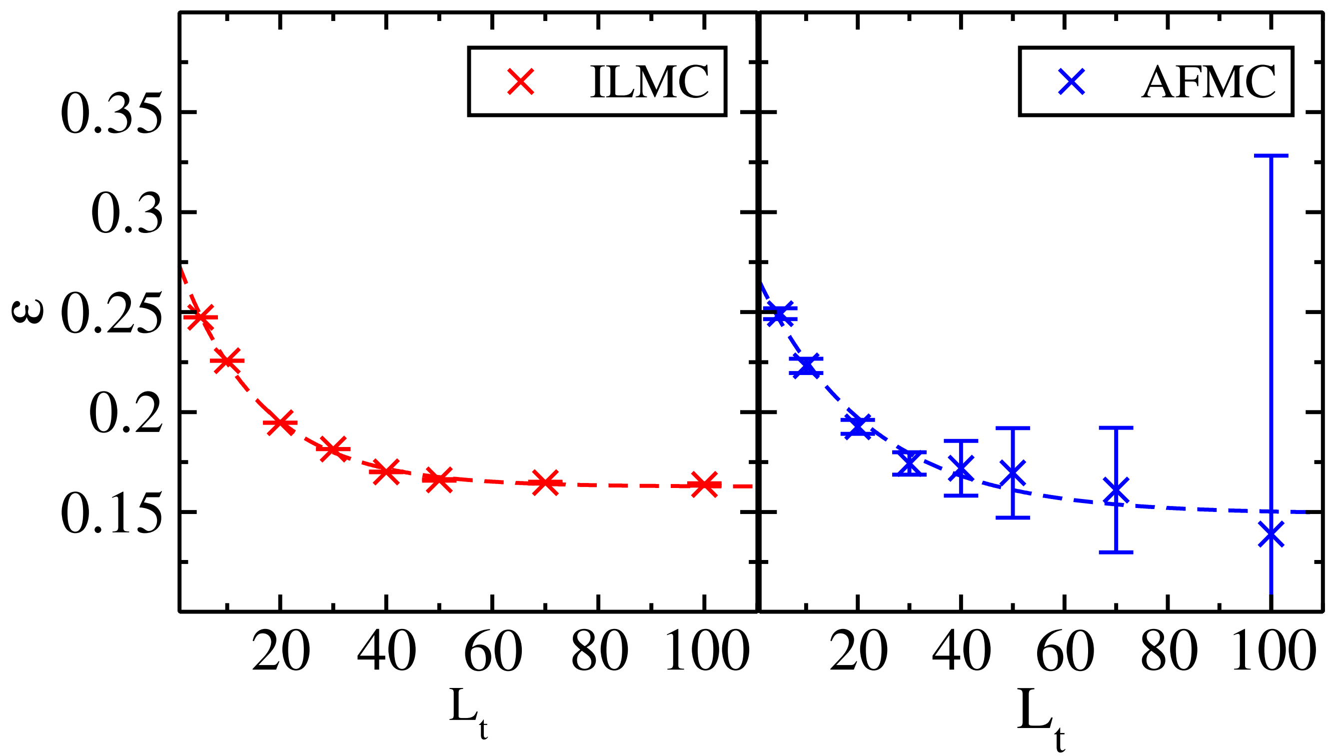
IMPURITY MONTE CARLO: BENCHAMRK CALCULATION

Bour, Lee, Hammer, UGM, Phys. Rev. Lett. **115** (2015) 185301

- $9\,|\uparrow\rangle + 1\,|\downarrow\rangle\,, L = 10^3$, zero range interaction

- caluclate the ground-state energy:

$$\epsilon = \frac{1}{a_t} \lim_{L_t \to \infty} \ln \frac{Z(L_t - 1)}{Z(L_t)}$$



- ILMC outperforms AFMC

↪ computationally simpler and faster

↪ far smaller sign oscillations

- apply the method to the polaron in two and three dimensions

WHAT is a POLARON?

- Polaron = quasiparticle to understand the electron-atom interactions

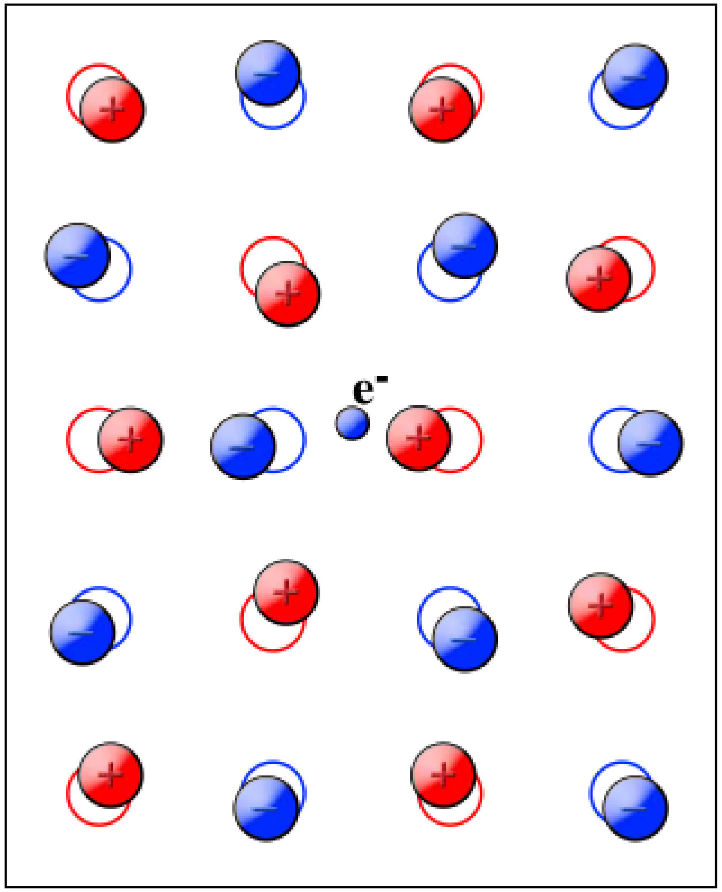
Landau, Phys. Z. Sowjetunion **3** (1933) 644

- consider an electron moving in a dielectric crystal

$\Rightarrow$ the atoms move from their equilibrium positions to effectively screen the charge of an electron (phonon cloud)

$\Rightarrow$ this lowers the electron mobility and increases the electron's effective mass

- for details, see:
  J. T. Devreese
  Encyclopedia of Applied Physics **14** (1996) 383



@Wikipedia

IMPURITY MONTE CARLO: POLARON RESULTS

Bour, Lee, Hammer, UGM, Phys. Rev. Lett. **115** (2015) 185301

- Energy of the 3D polaron (in units of the fermi energy) in the unitary limit

- linear fit in $1/N$ (particle no.):

$$\epsilon_P/\epsilon_F = -0.622(9)$$

- Diagrammatic MC:

$$\epsilon_P/\epsilon_F = -0.618$$

Prokofev, Svistunov, Phys. Rev. B **77** (2008) 020408

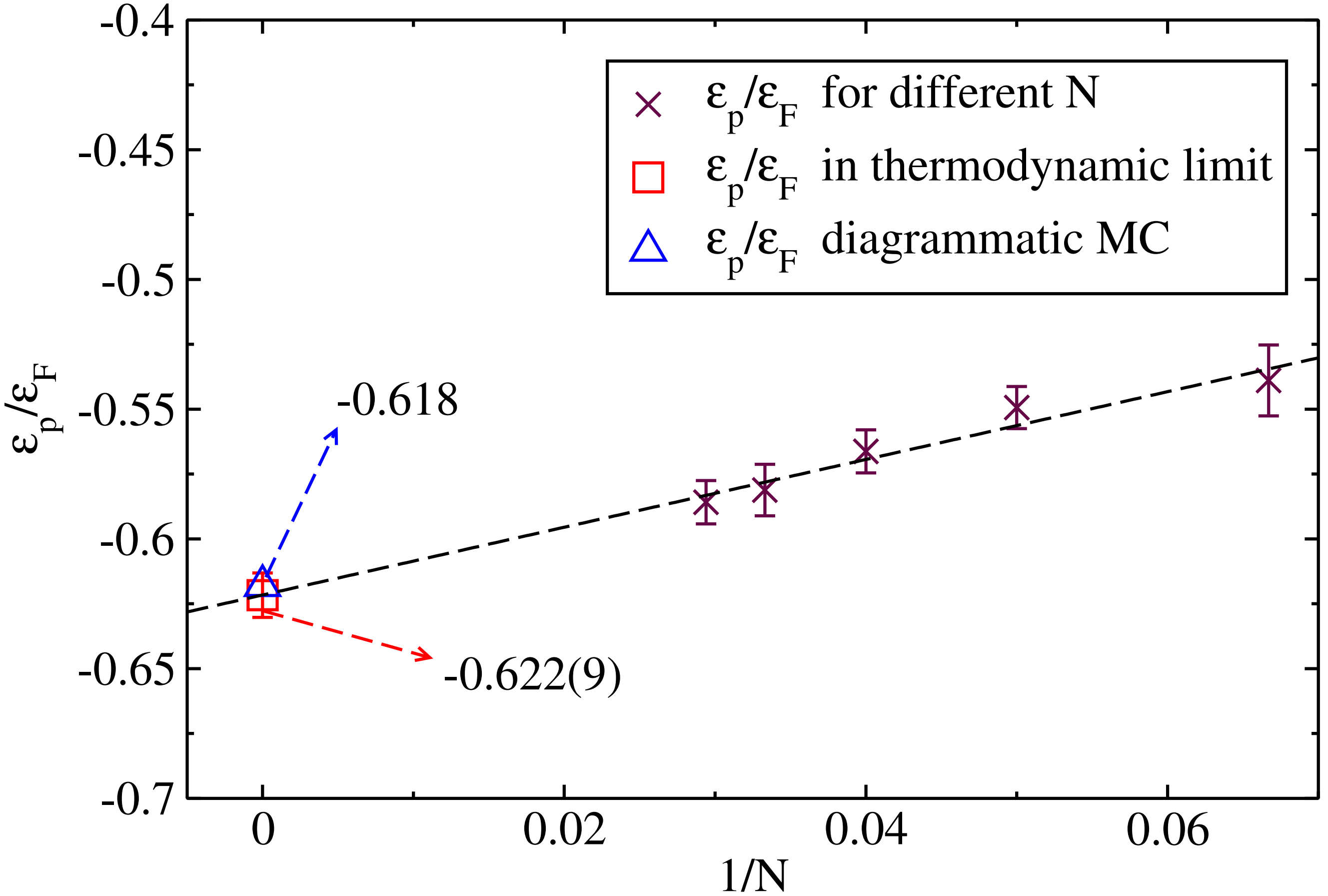
- Experiment:

$$\epsilon_P/\epsilon_F = -0.58(5)$$

$$\epsilon_P/\epsilon_F = -0.64(7)$$

Shin, Phys. Rev. A **77** (2008) 041603

Schirotzek et al., Phys. Rev. Lett. **102** (2009) 023402



IMPURITY MONTE CARLO: POLARON RESULTS

Bour, Lee, Hammer, UGM, Phys. Rev. Lett. **115** (2015) 185301

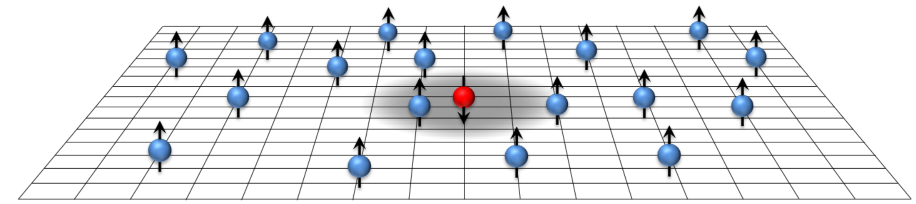


Figure courtesy Dean Lee

- Attractive polarons in 2D
  (two-body bound state develops)

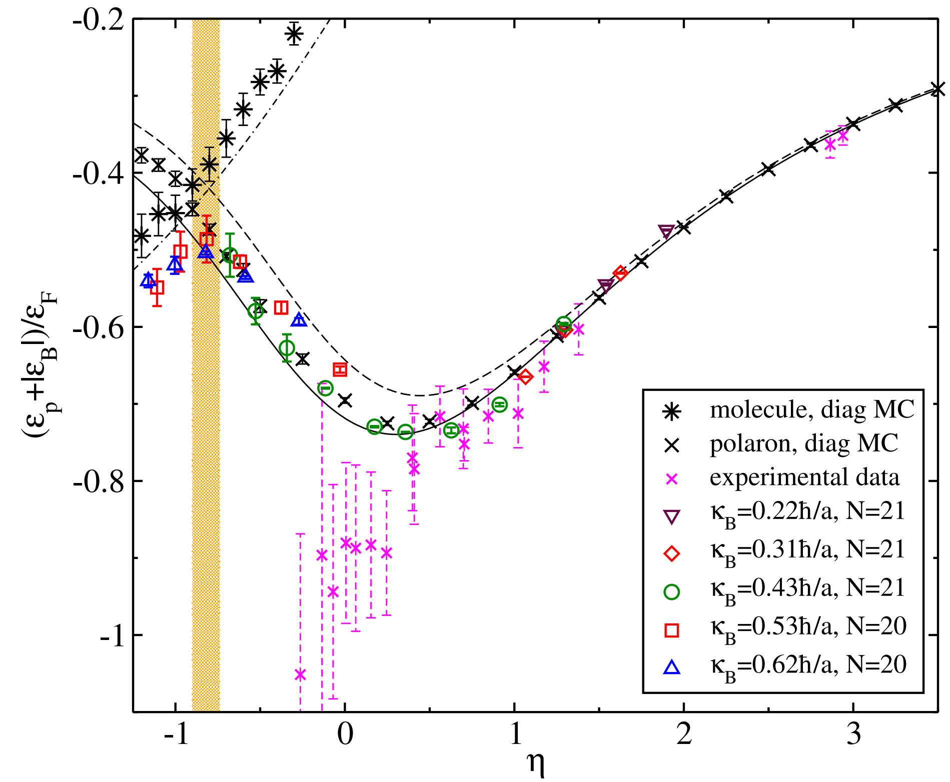
- First calculation that covers
  the whole range in η

$$\eta = \frac{1}{2}\ln(2\epsilon_F/|\epsilon_B|)$$

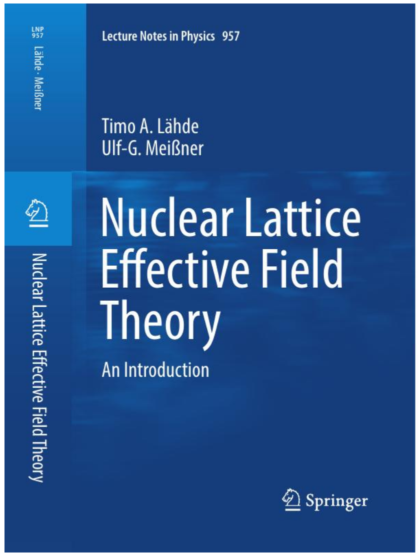
- good agreement with earlier calculations
  and experiment (where available)

- smooth crossover form the polaron
  to the molecular state (new!) by looking
  at density-density correlations

- ILMC is a **powerful** method



SUMMARY & OUTLOOK



- Chiral EFT for nuclear forces
  - → based on the symmetries of QCD
  - → systematic, precise and controlled theoretical errors
- Nuclear lattice EFT: a new quantum many-body approach
  - → based on the successful continuum chiral EFT
  - → a number of highly visible results already obtained
  - → clustering emerges naturally, α-cluster nuclei
  - → appears to be *the framework* for *ab initio* nuclear structure & reaction calc's
- Further improvements / not treated
  - → algorithms, CPU/GPU architectures, eigenvector continuation, . . .
    Frame et al., Phys. Rev. Lett. 121 (2018) 032501
  - → heavier nuclei, nuclear/neutron matter, thermodynamics, . . .

SPARES

HYBRID MONTE CARLO

Duane et al., Phys. Lett. B **195** (1986) 216

- apply hybrid MC to fields s, s_I, π_I for the calculation of the path-integral

- introduce conjugate fields p_{π_I}, p_s, p_{S_I}

$$H_{HMC} = \frac{1}{2} \sum_{I,\vec{n}} \left(p^2_{\pi_I}(\vec{n}\,) + p^2_s(\vec{n}\,) + p^2_{s_I}(\vec{n}\,) \right) + V(\pi_I, s, s_I)$$

$$V(\pi_I, s, s_I) = S_{\pi\pi} + S_{ss} - \log\{|\det\mathcal{M}|\}$$

generate new configs for $p_{\pi_I}, p_s, p_{S_I}, \pi_I, S, s_I$
by molecular dynamics trajectories

⇓

apply Metropolis accept/reject step for new config
according to the probability $\exp(-H_{HMC})$

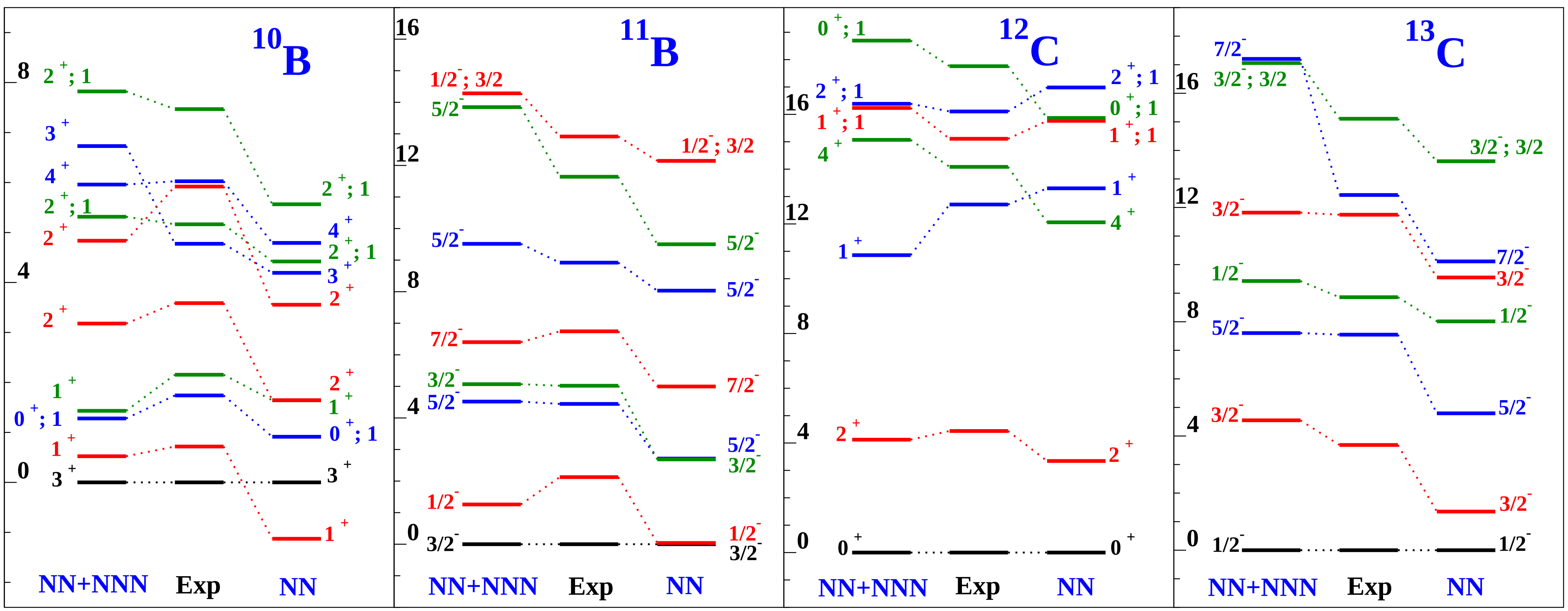
repeat steps
many times

NO-CORE-SHELL MODEL: p-SHELL NUCLEI

- No-core-shell-model calculation — Navratil *et al.*, Phys. Rev. Lett. **99**, 042501 (2007)

- NN interaction at N^3LO and NNN interaction at N^2LO

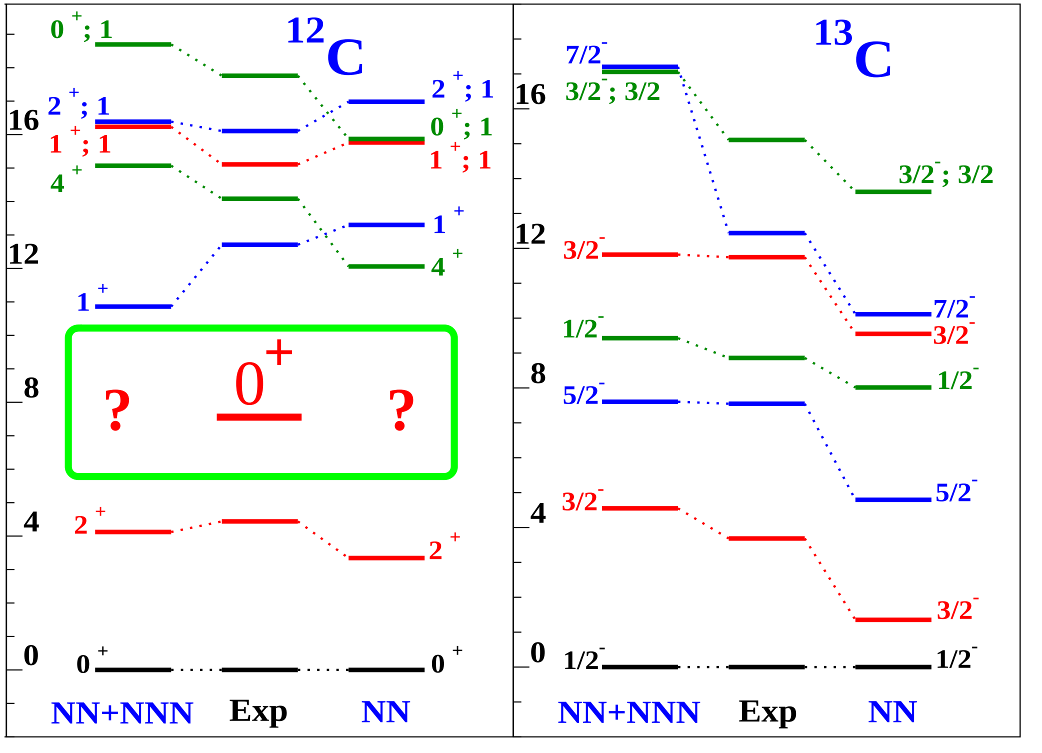
- Fix $D\&E$ from BE of ^{3}H and level structure of ^{4}He, ^{6}Li, ^{10,11}B and ^{12,13}C



MODERN MANY-BODY THEORY and the HOYLE STATE

- one of the most sophisticated many-body theories (No-Core-Shell-Model)
- excellent description of p-shell nuclei from ^{6}Li to ^{13}C

P. Navratil et al., Phys. Rev. Lett. **99** (2007) 042501 + updates



⇒ NO signal of the Hoyle state (i.g. α-cluster states)

⇒ must develop a better method

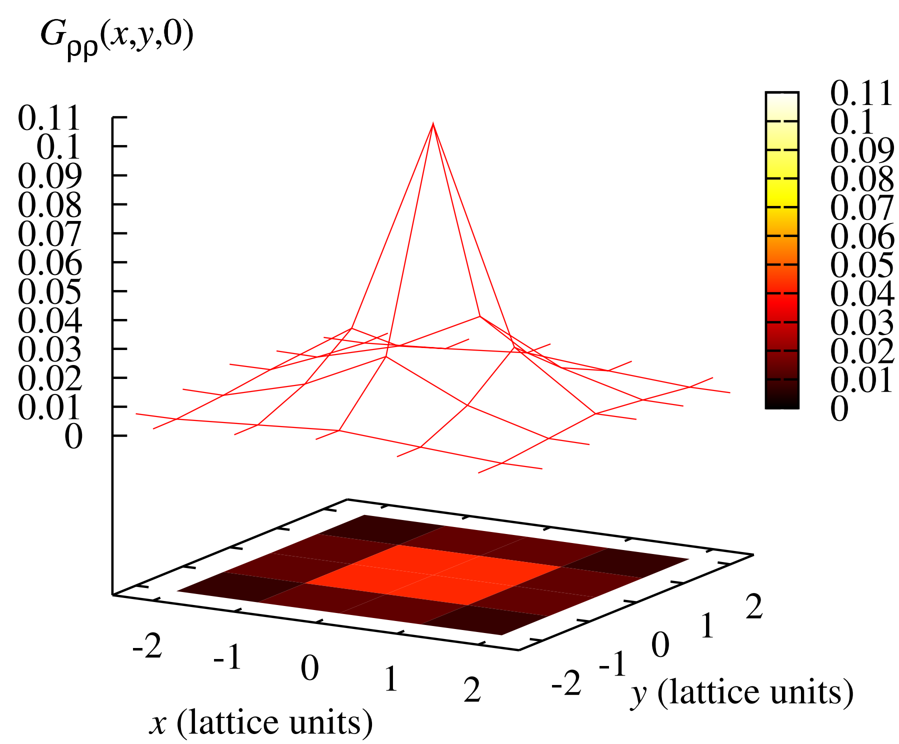
RESULTS at LEADING ORDER

Borasoy, Epelbaum, Krebs, Lee, M., Eur. Phys. J. **A31** (2007) 105

- 2 LECs fitted to B_d and $a_{np}(^1S_0)$
- Promising results for $A = 2, 3, 4$

  $\rightarrow$ b fitted from the average effective range

	Simulation	Experiment
r_d [fm]	1.989(1)	1.9671(6)
Q_d [fm^2]	0.278(1)	0.2859(3)
B_t [fm]	$-8.9(2)$	-8.482
r_t [fm]	2.27(7)	1.755(9)
B_α [fm]	$-21.5(9)$	-28.296
r_α [fm]	1.50(14)	1.673(1)



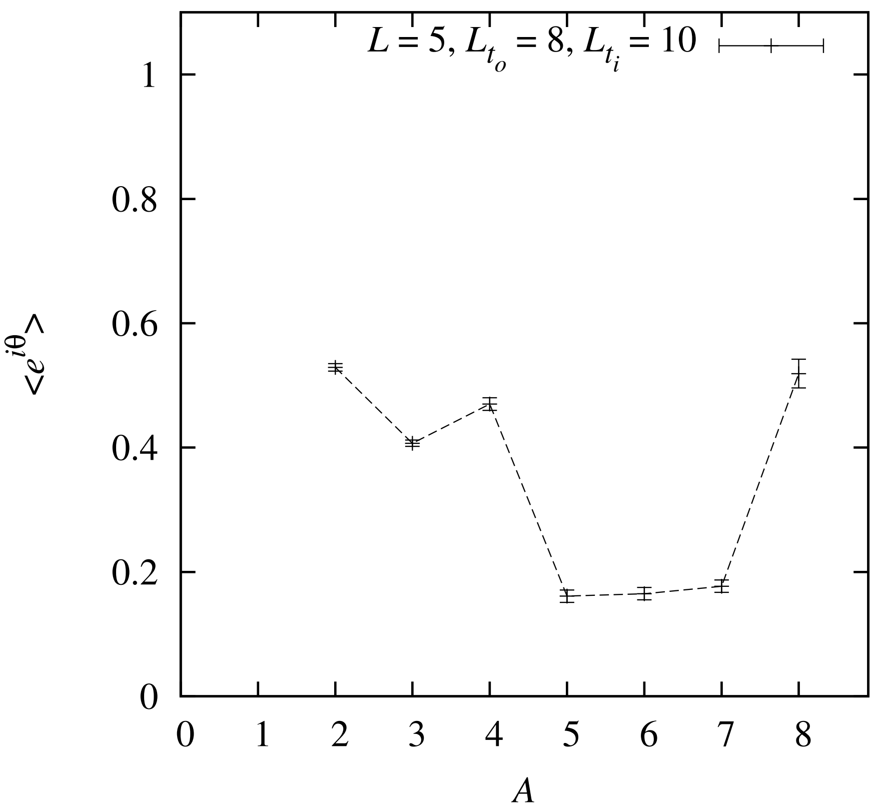
- *CPU time scales linear with A ($A \leq 10$)*

Nucleon density correlation in ^{3}H in the x-y plane

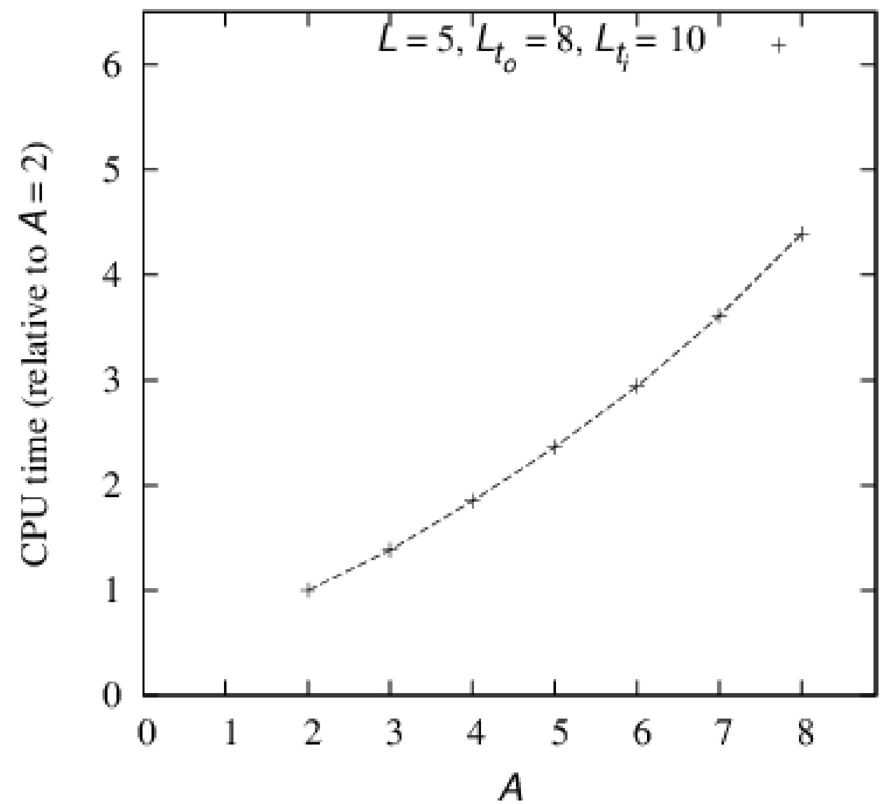
RESULTS at LEADING ORDER

Borasoy, Epelbaum, Krebs, Lee, M., Eur. Phys. J. **A31** (2007) 105

- Phase



- CPU time



$\rightarrow$ much improved by now

Neutron-proton scattering at NNLO for varying lattice spacings

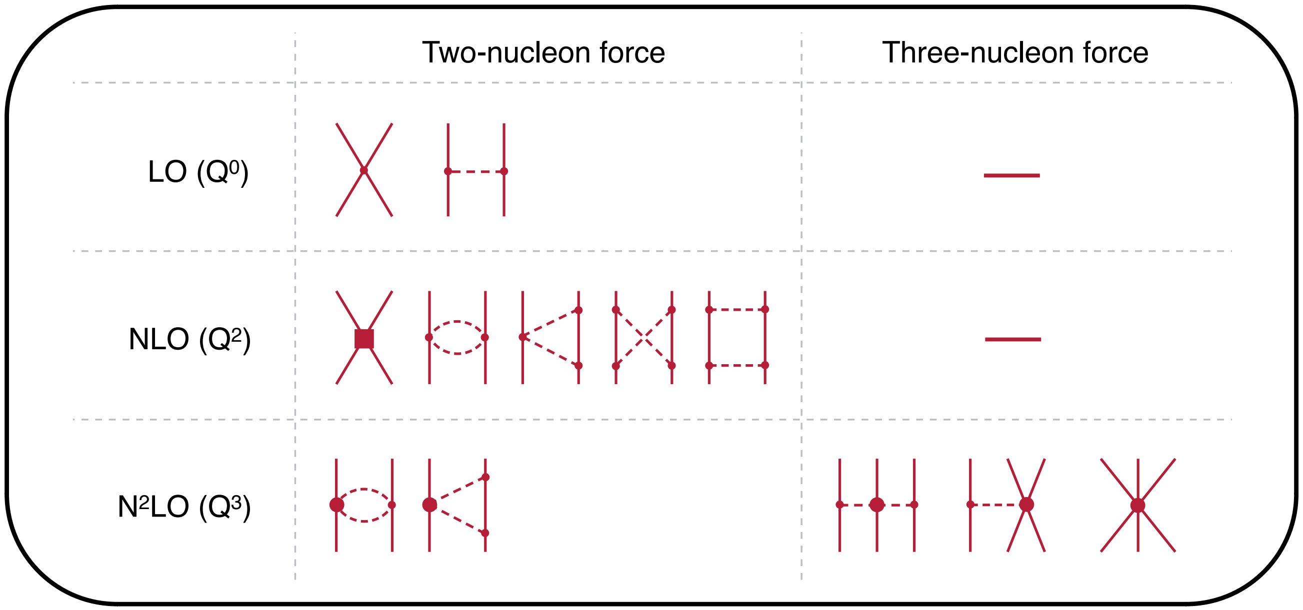
Alarcón, Du, Klein, Lähde, Lee, Li, Luu, UGM

Eur. Phys. J. **A** (2017) in print [arXiv:1702.05319]

NUCLEAR FORCES at NNLO

for details, see: Epelbaum, Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773

- Potential at next-to-next-to-leading order $[Q = \{p/\Lambda, M_\pi/\Lambda\}]$:



- NN potential to NNLO [all πN and $\pi\pi N$ LECs fixed from πN scattering]:

$$
\begin{aligned}
V_{\rm NN} &= V_{\rm LO}^{(0)} + V_{\rm NLO}^{(2)} + V_{\rm NNLO}^{(3)} \\
&= V_{\rm LO}^{\rm cont} + V_{\rm LO}^{\rm OPE} + V_{\rm NLO}^{\rm cont} + V_{\rm NLO}^{\rm TPE} + V_{\rm NNLO}^{\rm TPE}
\end{aligned}
$$

NUCLEAR FORCES at NNLO continued

- Analytic expressions [2+7 LECs]:

$$V_{\rm LO}^{\rm cont} = C_S + C_T\,(\vec\sigma_1\cdot\vec\sigma_2)$$

$$V_{\rm LO}^{\rm OPE} = -\frac{g_A^2}{4F_\pi^2}\,\tau_1\cdot\tau_2\,\frac{(\vec\sigma_1\cdot\vec q)\,(\vec\sigma_2\cdot\vec q)}{q^{\,2}+M_\pi^2}$$

$\vec q$ = t-channel mom. transfer

$$V_{\rm NLO}^{\rm cont} = C_1 q^2 + C_2 k^2 + \left(C_3 q^2 + C_4 k^2\right)(\vec\sigma_1\cdot\vec\sigma_2) + iC_5\tfrac{1}{2}\,(\vec\sigma_1+\vec\sigma_2)\cdot(\vec q\times\vec k)$$
$$+\, C_6\,(\vec\sigma_1\cdot\vec q)\,(\vec\sigma_2\cdot\vec q) + C_7(\vec\sigma_1\cdot\vec k)(\vec\sigma_2\cdot\vec k)$$

$\vec k$ = u-channel mom. transfer

$$V_{\rm NLO}^{\rm TPE} = -\frac{\tau_1\cdot\tau_2}{384\pi^2F_\pi^4}L(q)\Big[4M_\pi^2\left(5g_A^4-4g_A^2-1\right)+q^2\left(23g_A^4-10g_A^2-1\right)$$
$$+\,\frac{48g_A^4M_\pi^4}{4M_\pi^2+q^2}\Big] - \frac{3g_A^4}{64\pi^2F_\pi^4}L(q)\left[(\vec q\cdot\vec\sigma_1)\,(\vec q\cdot\vec\sigma_2)-q^2\,(\vec\sigma_1\cdot\vec\sigma_2)\right]$$

- Loop function: $L(q) = \frac{1}{2q}\sqrt{4M_\pi^2+q^2}\,\ln\frac{\sqrt{4M_\pi^2+q^2}+q}{\sqrt{4M_\pi^2+q^2}-q}$

$$\to 1+\frac{1}{3}\frac{q^2}{4M_\pi^2}+\cdots \text{ for } q \ll \Lambda$$

$\to$ for coarse lattices $a \simeq 2$ fm, the TPE at N(N)LO can be absorbed in the LECs C_i

$\to$ no longer true as a decreases, need to account for the TPE explicitly

A FEW DETAILS ON THE FITS

- Fits in large & fixed volumes, vary a from 1 to 2 fm:

a^{-1} [MeV]	a [fm]	L	La [fm]
100	1.97	32	63.14
120	1.64	38	62.48
150	1.32	48	63.14
200	0.98	64	63.14

- OPE and TPE LECs completely fixed ($g_A \sim g_{\pi NN}$ and $c_{1,2,3,4}$ from RS analysis)

Hoferichter, Ruiz de Elvira, Kubis, UGM, Phys. Rev. Lett. **115** (2015) 092301

- Smeared LO S-wave contact interactions: $f(\vec{q}) \equiv f_0^{-1} \exp\left(-b_s \frac{\vec{q}^{\,4}}{4}\right)$

- Partial-wave projection of the contact interactions

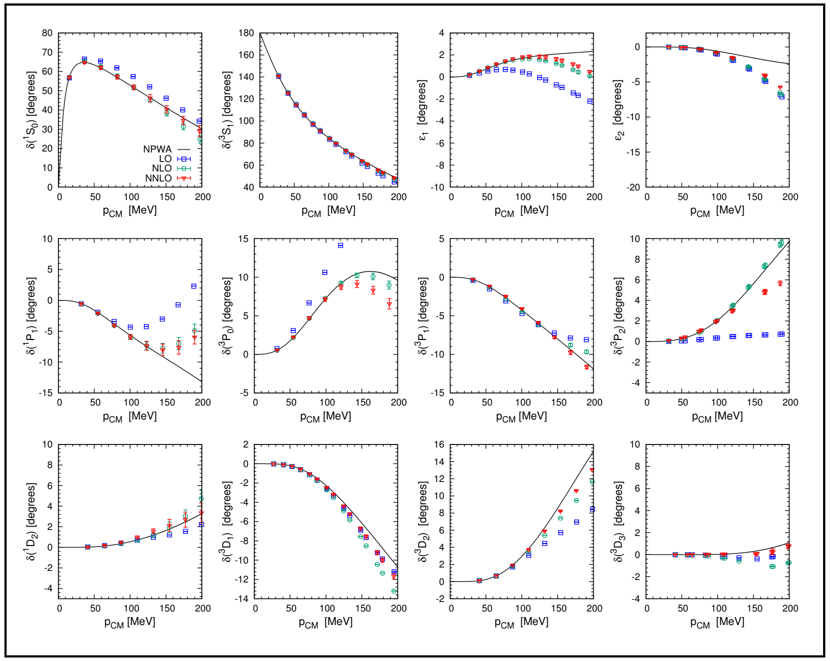
$\to$ fit b_s and two S-wave LECs C_i at LO up to $p_{\rm cm} = 100$ MeV

$\to$ w/ b_s fixed, fit two/seven S/P-wave LECs C_i at NLO/NNLO up to $p_{\rm cm} = 150$ MeV

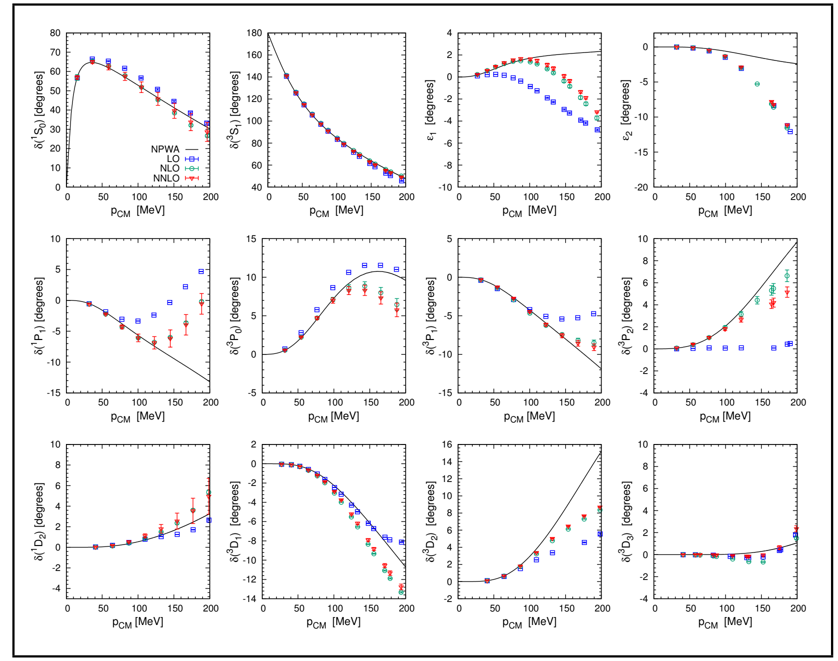
$\to$ treat NLO and NNLO corrections perturbatively and non-perturbatively

RESULTS for VARIOUS LATTICE SPACINGS - nonpert.

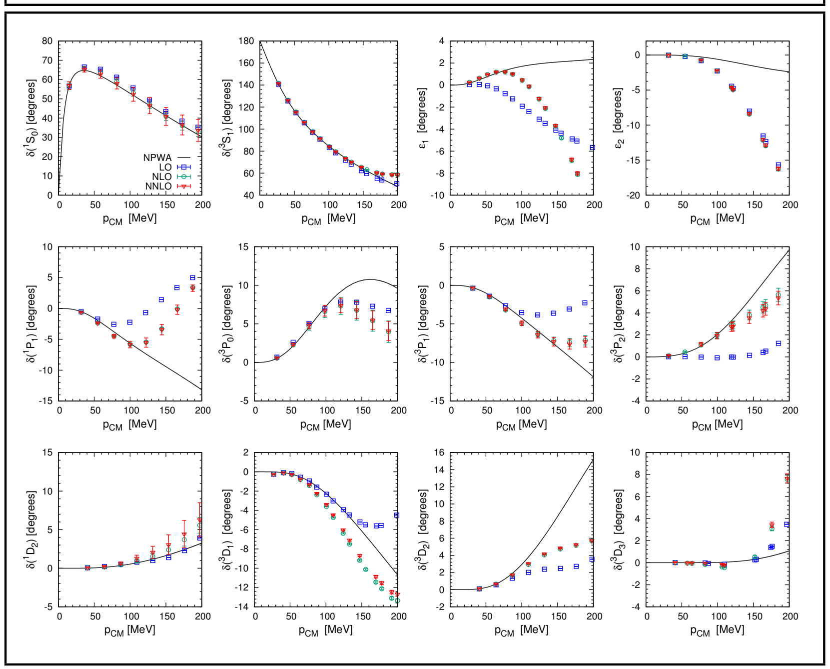
$a = 0.98$ fm



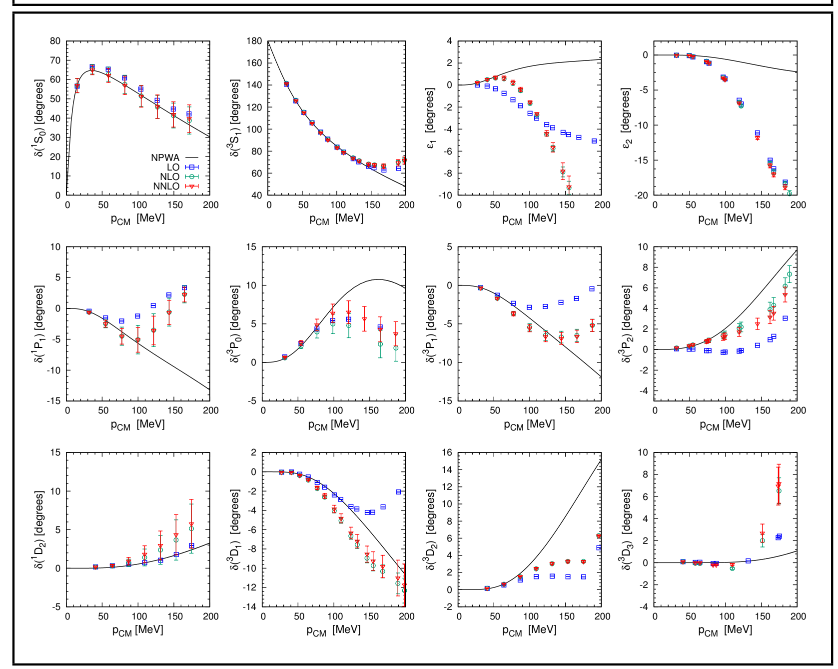
$a = 1.32$ fm



$a = 1.64$ fm



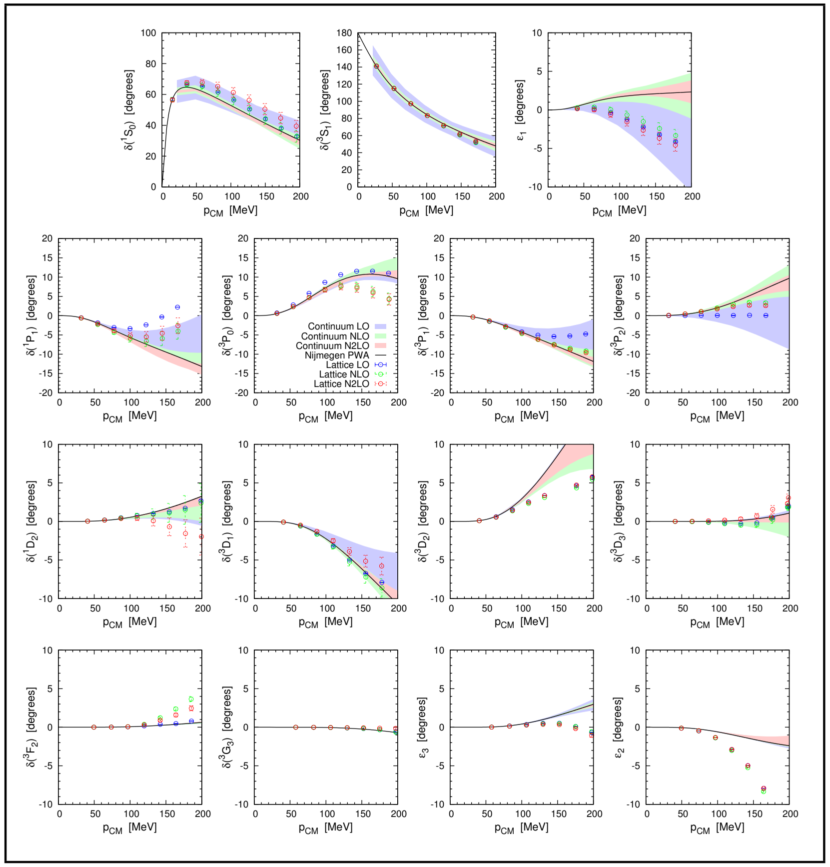
$a = 1.97$ fm



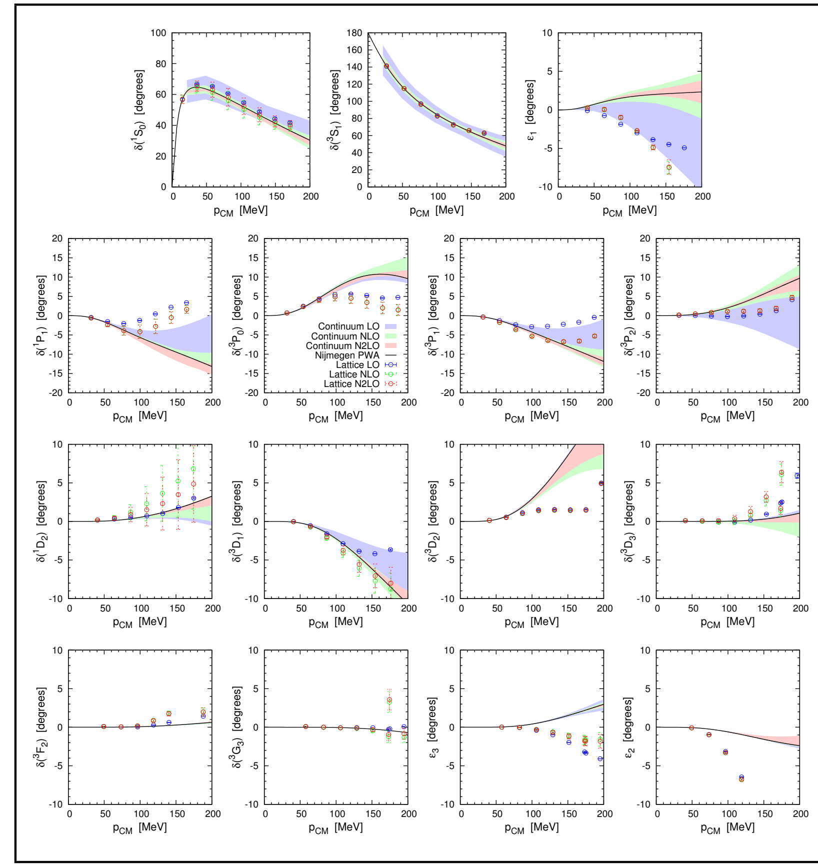
RESULTS for VARIOUS LATTICE SPACINGS - pert.

- perturbative treatment of NLO and NNLO corrections

$a = 1.32$ fm



$a = 1.97$ fm



$\rightarrow$ up to $p_{\rm cm} \simeq 150$ MeV, physics is indendependent of a $\surd$

$\rightarrow$ description consistent with the continuum within error bands $\surd$

$\rightarrow$ explore this for nuclei —- work in progress / stay tuned