Alpha–Cluster Physics

from *ab initio* nuclear lattice simulations

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Supported by DFG, SFB/TR-16 and by DFG, SFB/TR-110 and by CAS, PIFI by HGF VIQCD VH-VI-417 and by VW Stiftung

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- Short introduction
- New results in the continuum EFT
- Basics of nuclear lattice simulations
- Results from nuclear lattice simulations
- Ab initio calculation of alpha-alpha scattering
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Short introduction

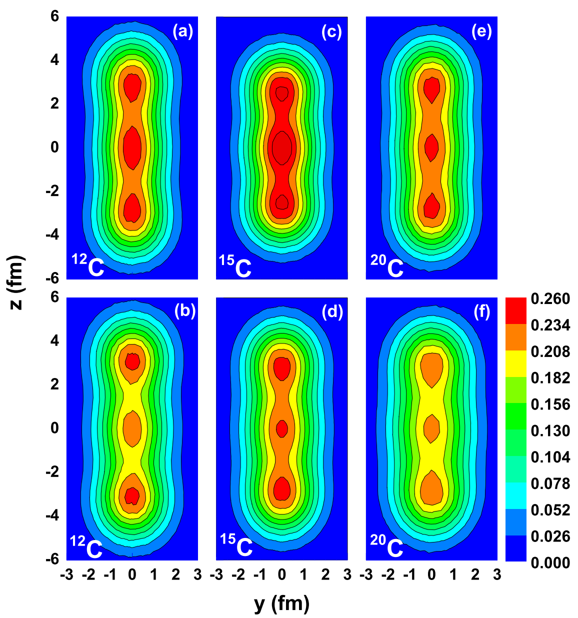
CLUSTERING in NUCLEI

- Introduced theoretically by Wheeler already in 1937:

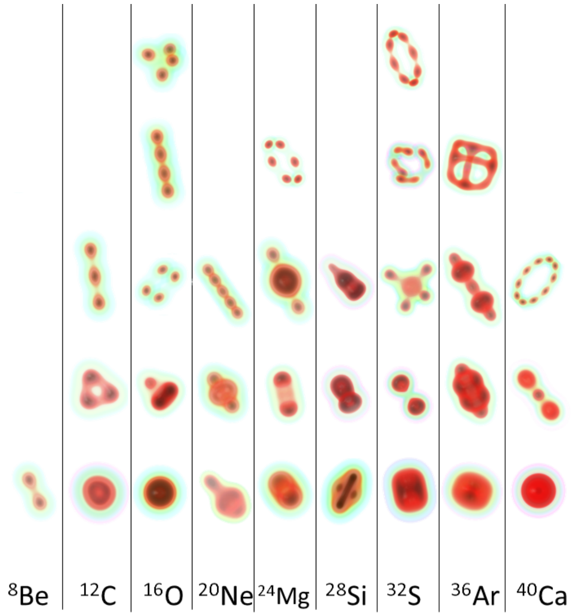
John Archibald Wheeler, “Molecular Viewpoints in Nuclear Structure,” Physical Review **52** (1937) 1083

- many works since then...

Ikeda, Horiuchi, Freer, Schuck, Röpke, Khan, Zhou, . . .



Zhao, Itagaki, Meng (2015)



Ebran, Khan, Niksic, Vretenar (2014)

α-clusters

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

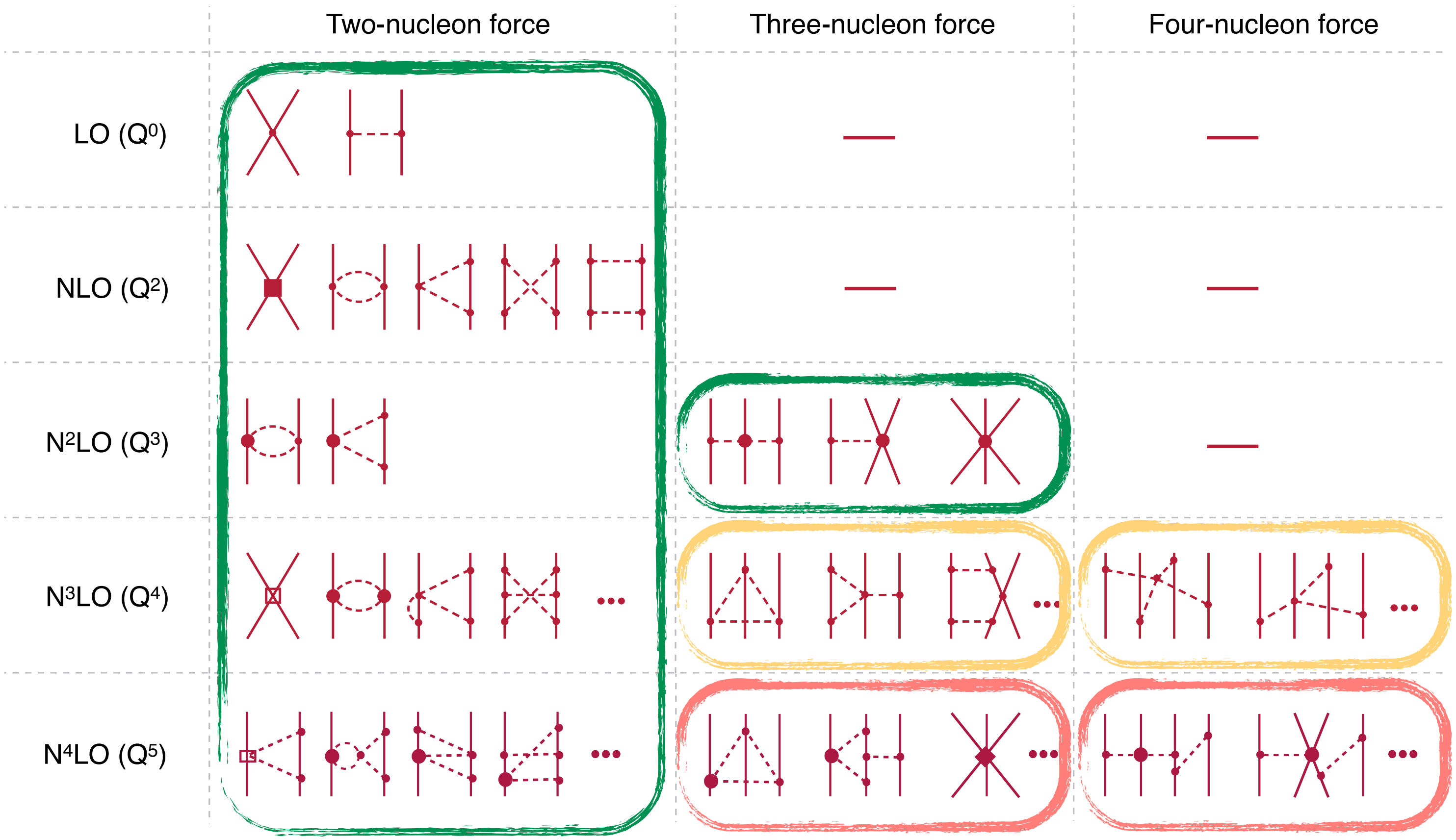
Continuum EFT: new developments

LENPIC www.lenpic.org

NUCLEAR FORCES in CHIRAL NUCLEAR EFT

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

- expansion of the potential in powers of Q [small parameter]
- explains observed hierarchy of the nuclear forces



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

NN FORCES to FOURTH ORDER

Epelbaum, Krebs, UGM, Eur. Phys. J. **A 51**: 53 (2015)

- new regularization of long-range physics [coordinate space cut-off]:

$$V^{\rm reg}_{\rm long-range}(\vec{r}) = V_{\rm long-range}(\vec{r}) f_{\rm reg}\left(\frac{r}{R}\right) \quad , \quad f_{\rm reg} = \left[1 - \exp\left(-\frac{r^2}{R^2}\right)\right]^6$$

$\Longrightarrow$ No distortion of the long-range potential $\rightarrow$ better at higher energies

$\Longrightarrow$ No additional spectral function regularization in the TPEP required

$\Longrightarrow$ Study of the chiral expansion of multi-pion exchanges: $R = 0.8 \cdots 1.2$ fm

Baru et al., EPJ A48 (12) 69

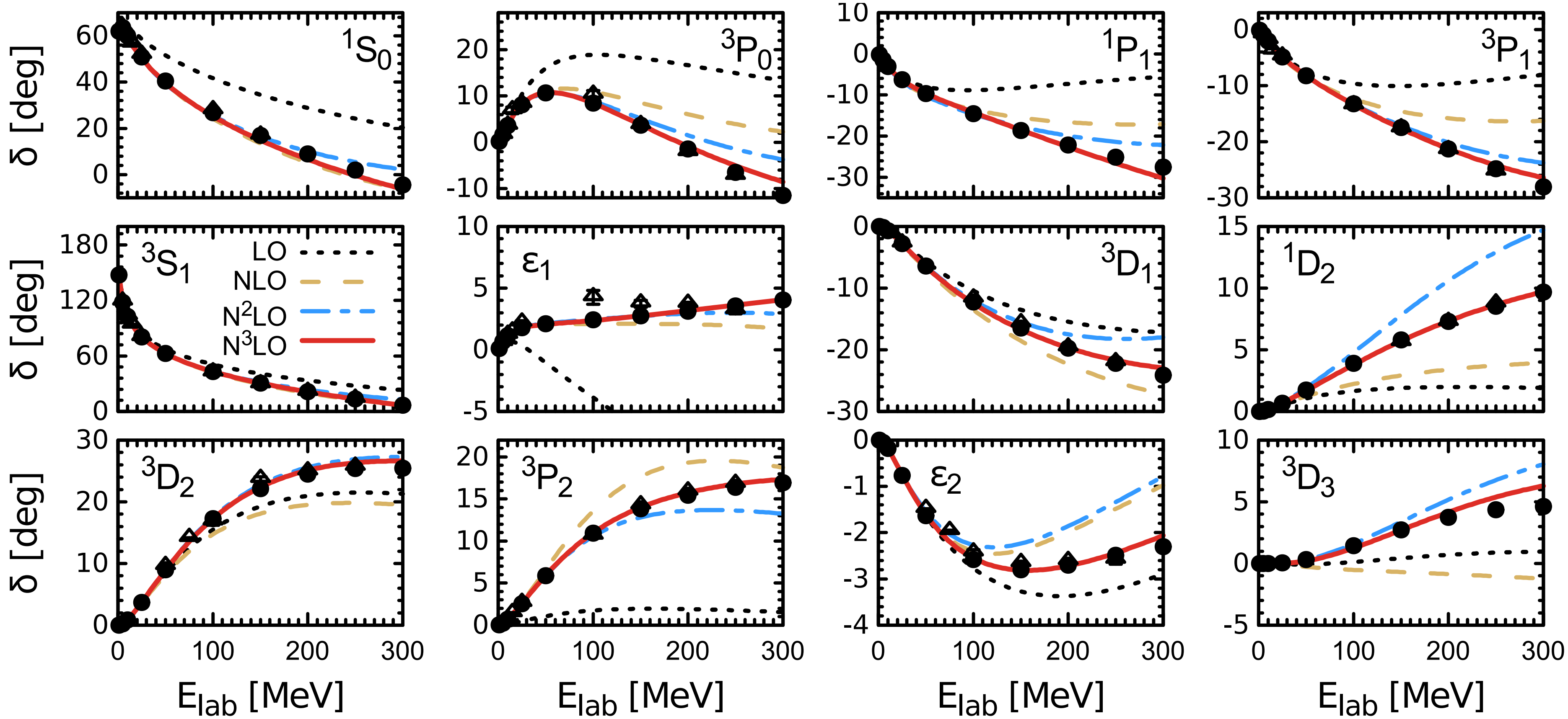
- new way of estimation the theoretical uncertainty [before: only cut-off variations]

$\Longrightarrow$ Expansion parameter depending on the region: $Q = \max\left(\frac{M_\pi}{\Lambda_b}, \frac{p}{\Lambda_b}\right)$

$\Longrightarrow$ Breakdown scale $\Lambda_b = 600$ MeV for $R = 0.8 \cdots 1.0$ fm

CONVERGENCE of the CHIRAL SERIES

• phase shifts show expected convergence [large N2LO corrections understood]

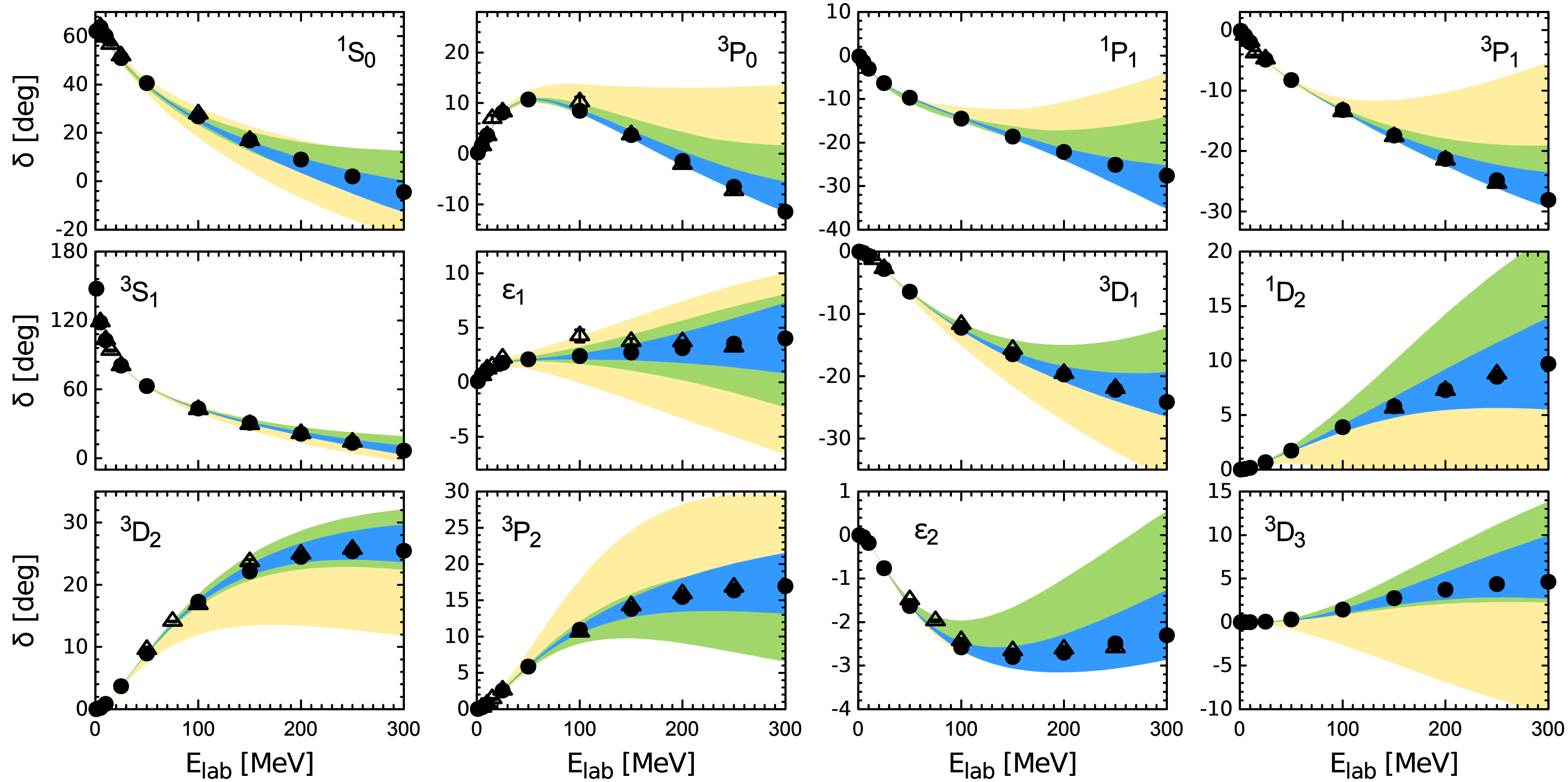


$\Longrightarrow$ clear improvement comp. to earlier N3LO potentials [momentum space reg.]

Entem, Machleidt; Epelbaum, Glöckle, UGM

UNCERTAINTIES

- uncertainties show expected pattern



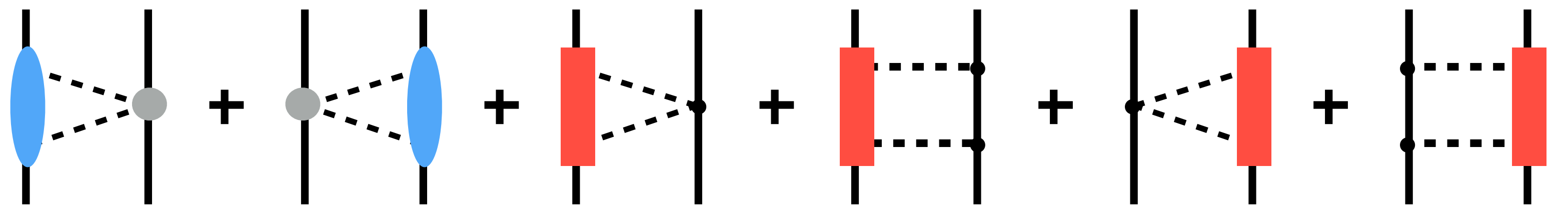
NLO N2LO N3LO

NN FORCES to FIFTH ORDER

Epelbaum, Krebs, UGM, Phys. Rev. Lett. (2015) in print [arXiv:1412.4623]

- 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)



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

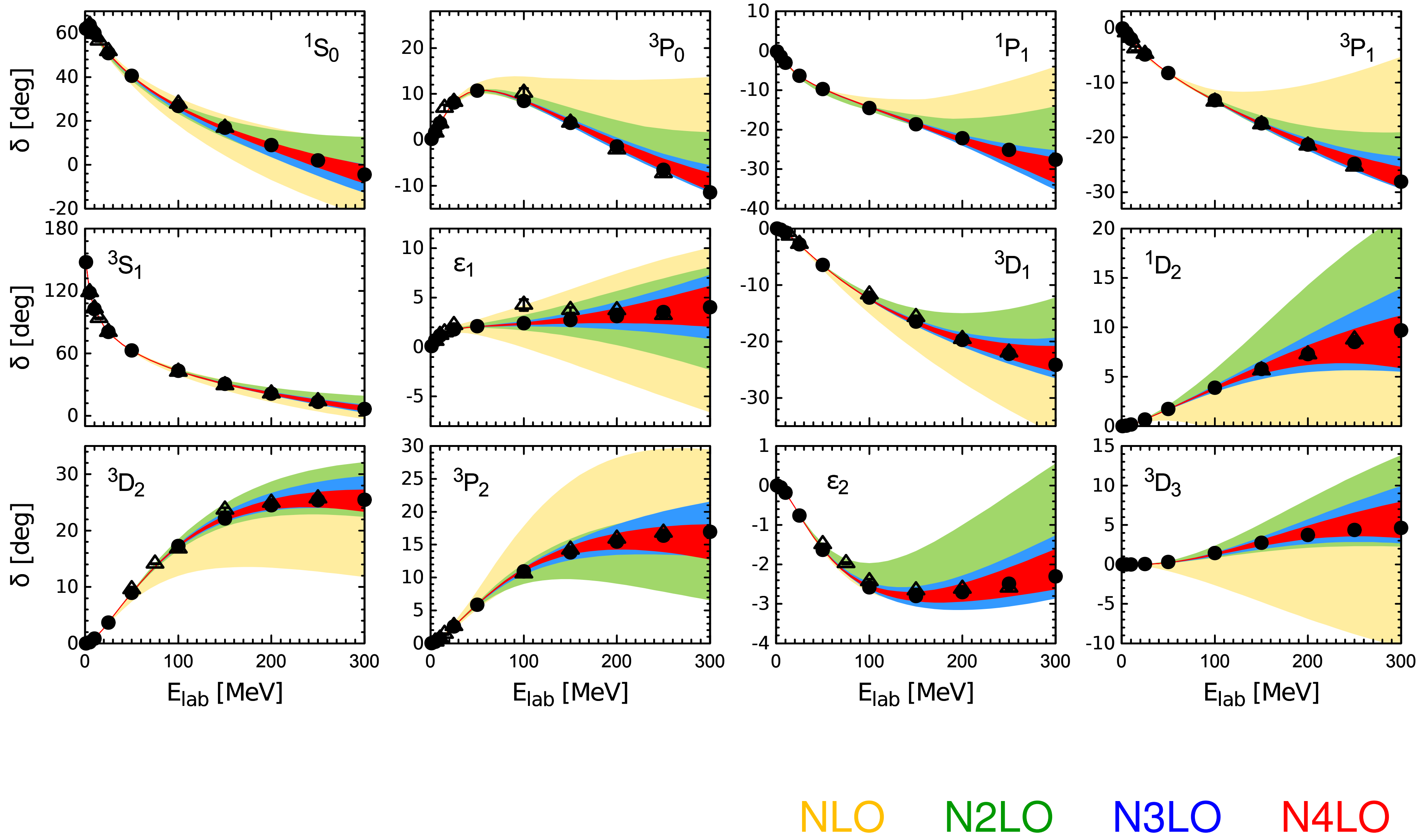
- Three-pion exchange can be neglected

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

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

PHASE SHIFTS at N4LO

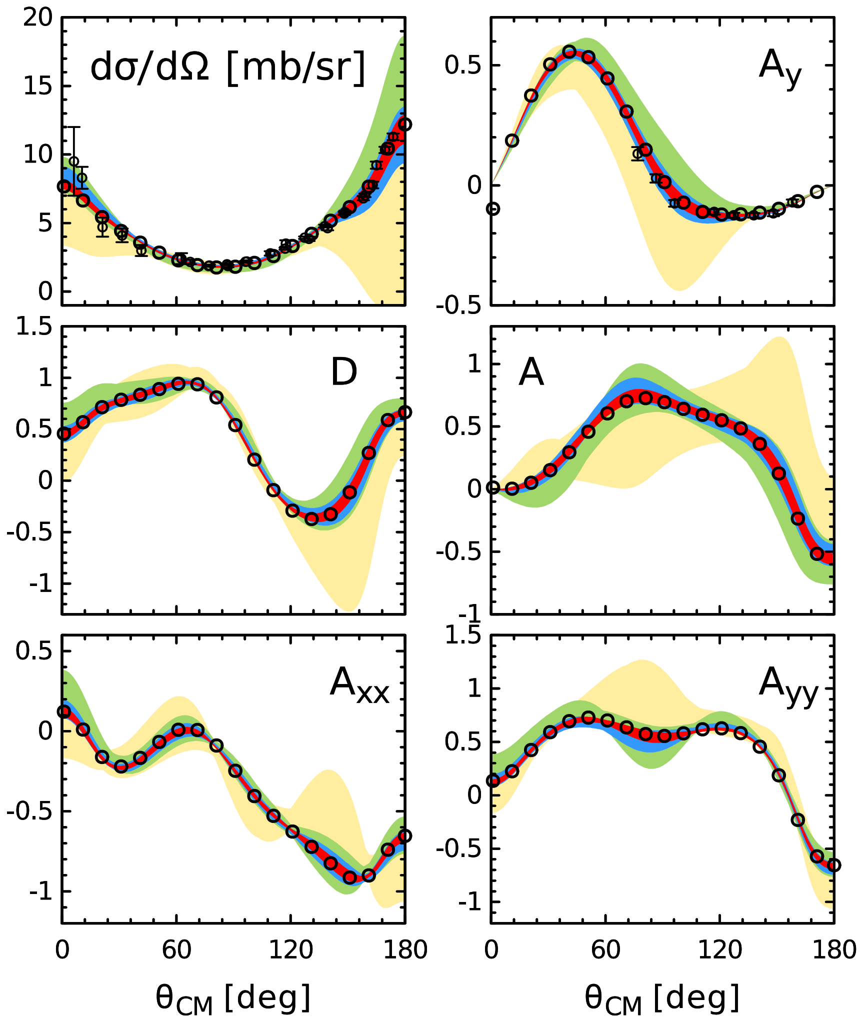
$\Rightarrow$ Precision phase shifts with small uncertainties up to $E_{\rm lab} = 300$ MeV



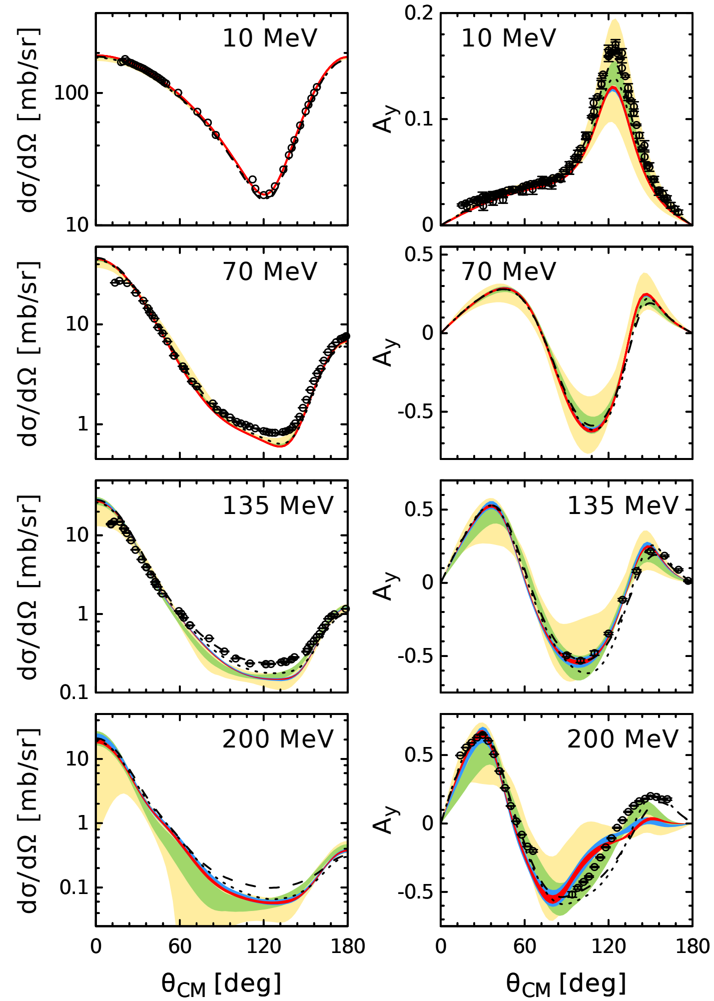
EVIDENCE for THREE-NUCLEON FORCES

- Two-nucleon system under control, three-nucleon system requires 3NFs!
  → being implemented [LENPIC collaboration]

- np scattering at 200 MeV



- nd scattering [2NFs only]

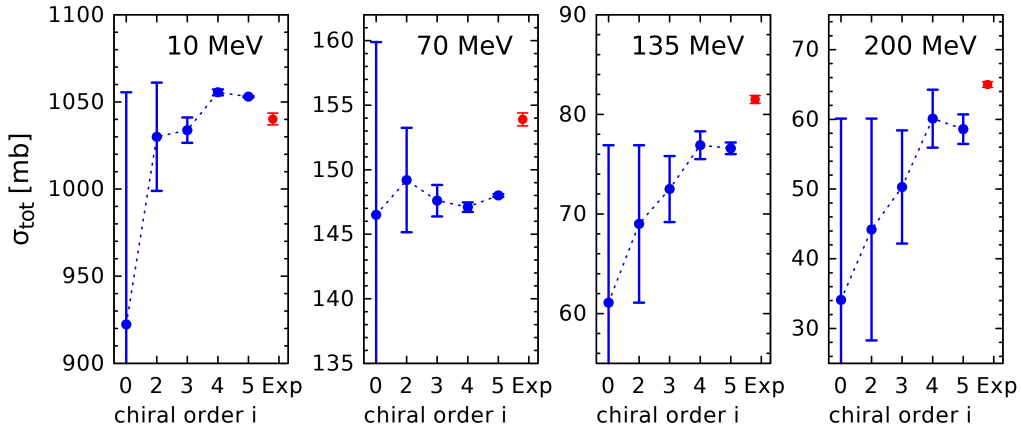


NLO
N2LO
N3LO
N4LO

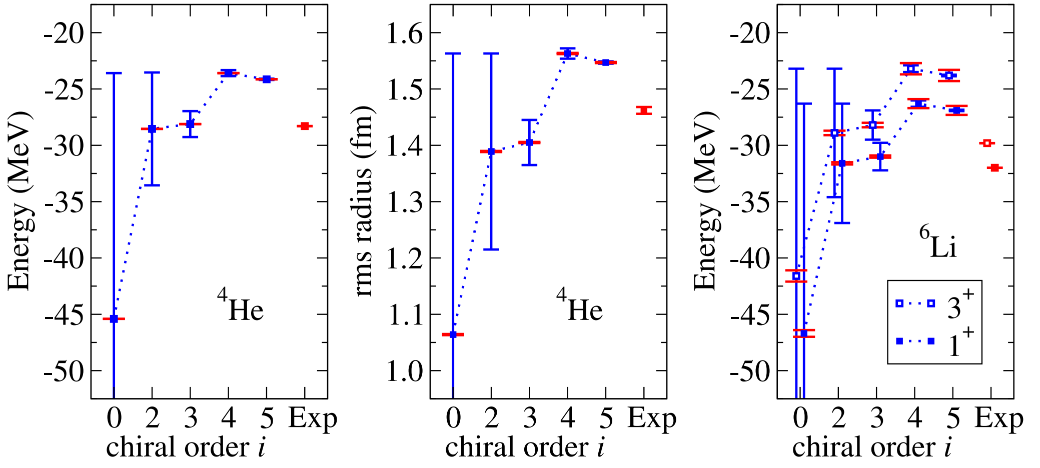
MORE EVIDENCE for THREE-NUCLEON FORCES

Binder et al. [LENPIC collaboration], arXiv:1505.07218

- Total cross section for Nd scattering [2NFs only]



- Binding energy and rms radius of ^{4}He, lowest levels in ^{6}Li [2NFs only]



Basics of nuclear lattice simulations

for an easy intro, see: UGM, Nucl. Phys. News **24** (2014) 11

NUCLEAR LATTICE SIMULATIONS

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

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

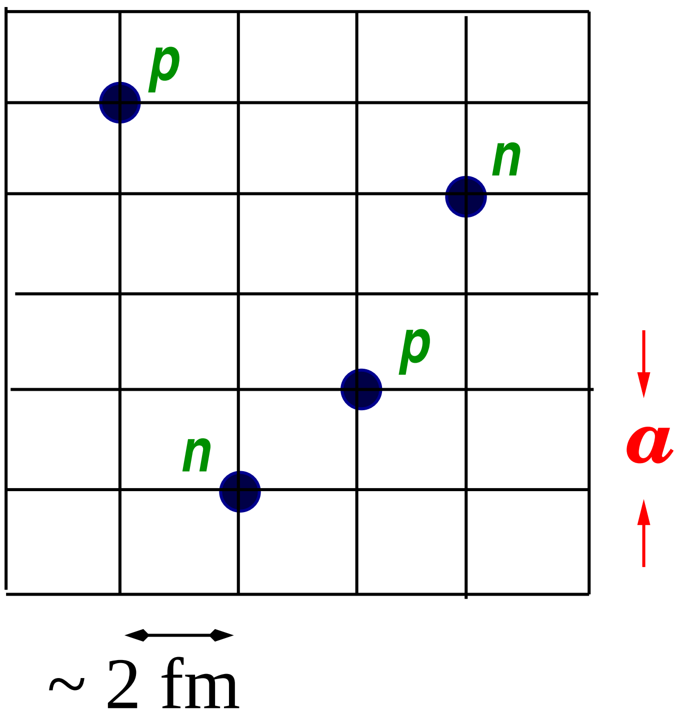
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
  nucleons are point-like particles on the sites

- discretized chiral potential w/ pion exchanges
  and contact interactions + Coulomb

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

- typical lattice parameters

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

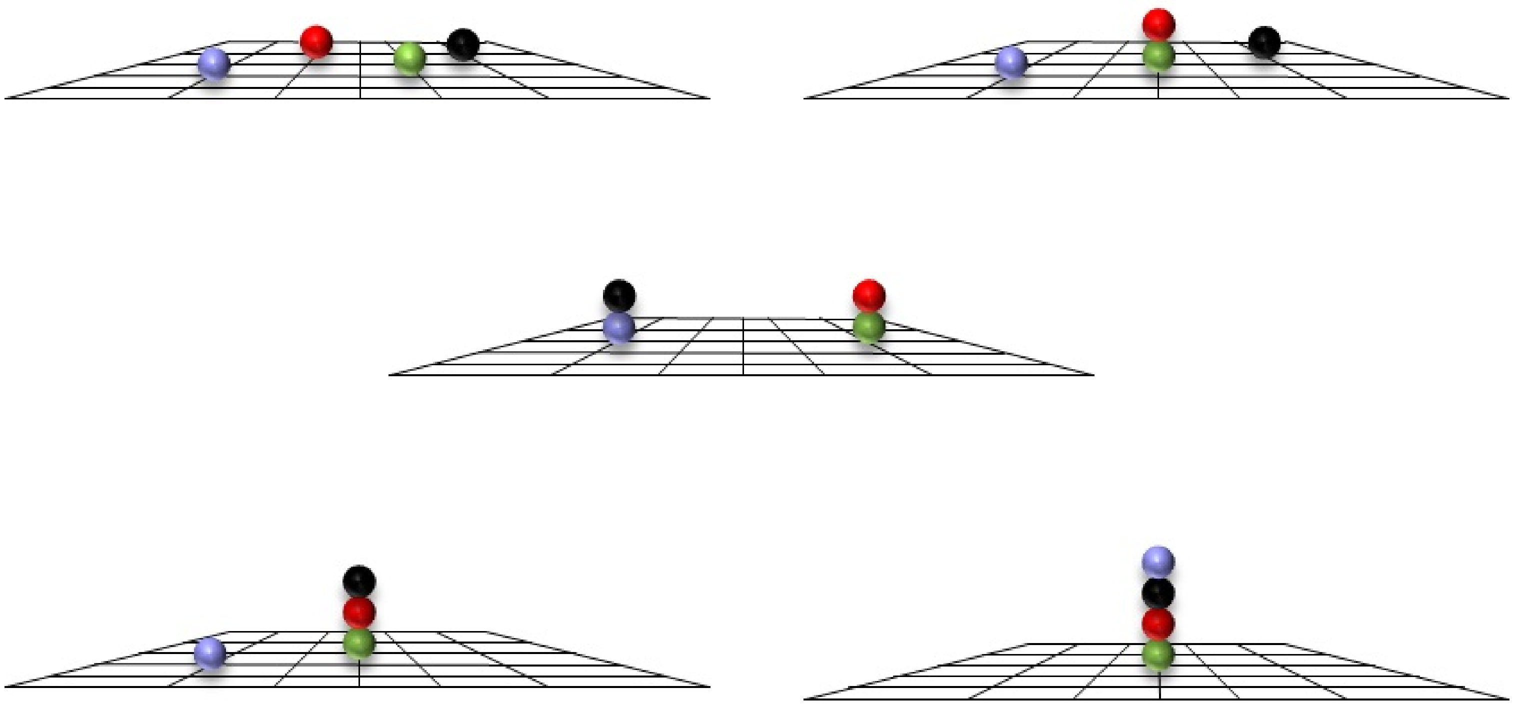


- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

J. W. Chen, D. Lee and T. Schäfer, Phys. Rev. Lett. **93** (2004) 242302, T. Lähde et al., EPJA **51** (2015) 92

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

CONFIGURATIONS



⇒ all *possible* configurations are sampled

⇒ *clustering* emerges *naturally*

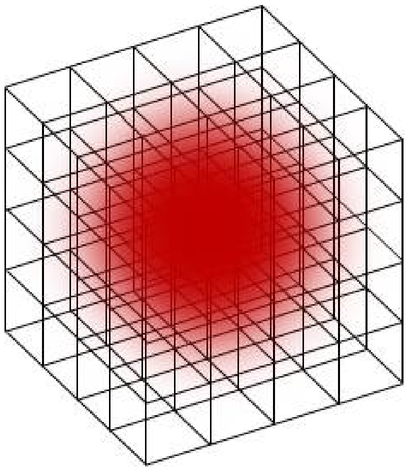
NUCLEAR WAVE FUNCTIONS

- General wave function:

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

- States with well-defined momentum (anti-symm.):

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



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

shell-model type

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

cluster type

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

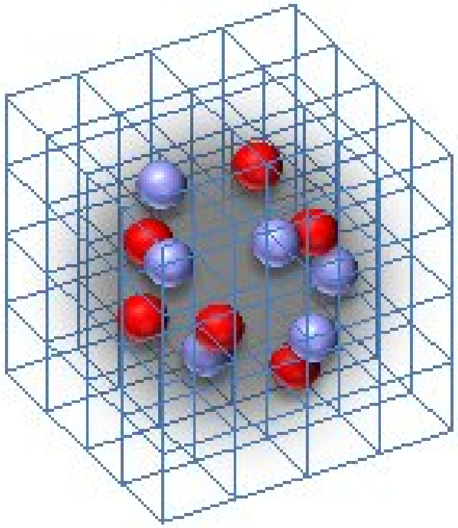
- shell-model w.f.s do not have enough 4N correlations $\sim \langle (N^\dagger N)^2\rangle$

COMPUTATIONAL EQUIPMENT

- Present = JUQUEEN (BlueGene/Q)

6 Pflops

Lattice: some results



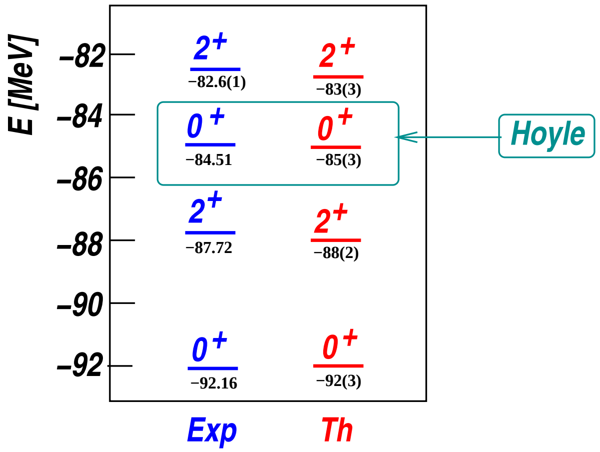
NLEFT

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

RESULTS from LATTICE NUCLEAR EFT

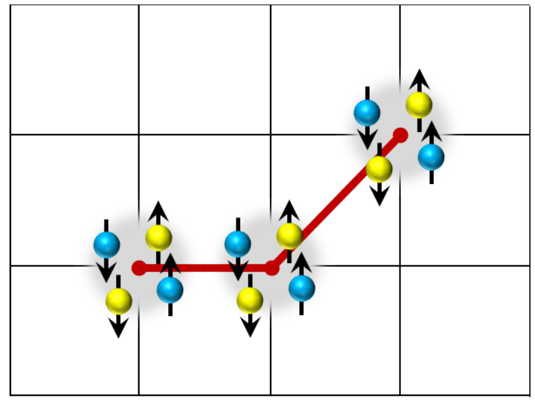
- Hoyle state in ^{12}C

PRL 106 (2011)



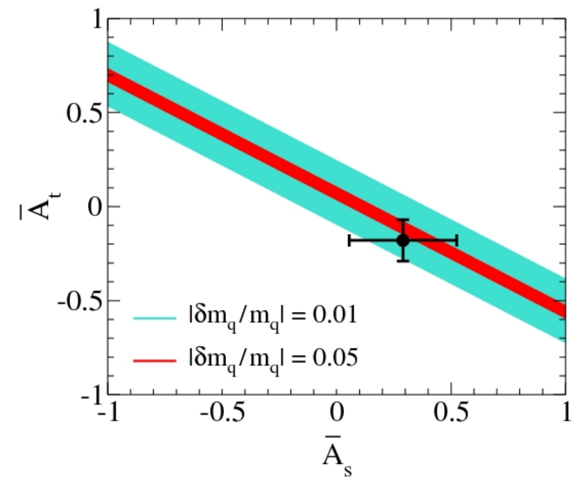
- Structure of the Hoyle state

PRL 109 (2012)



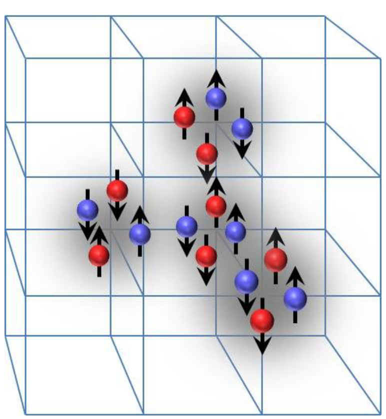
- Fate of carbon-based life

PRL 110 (2013), EPJ A49 (2013)



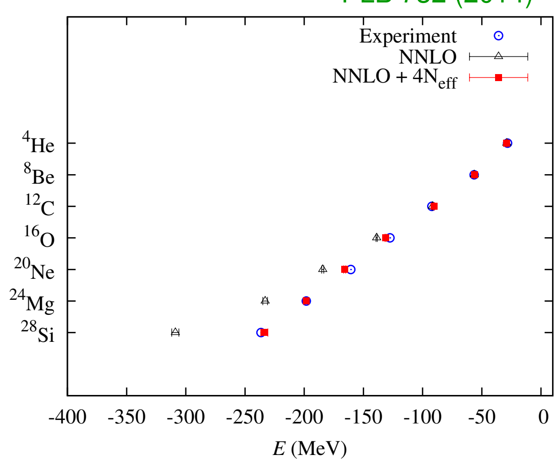
- Spectrum of ^{16}O

PRL 112 (2014)



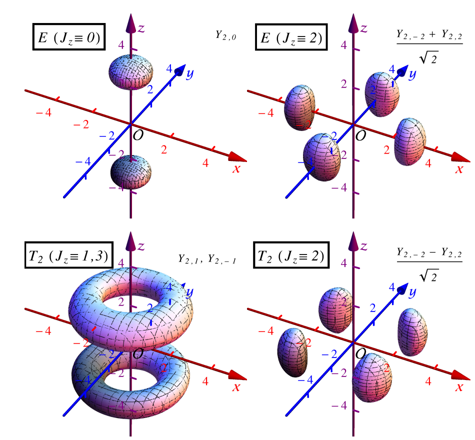
- Going up the α-chain

PLB 732 (2014)



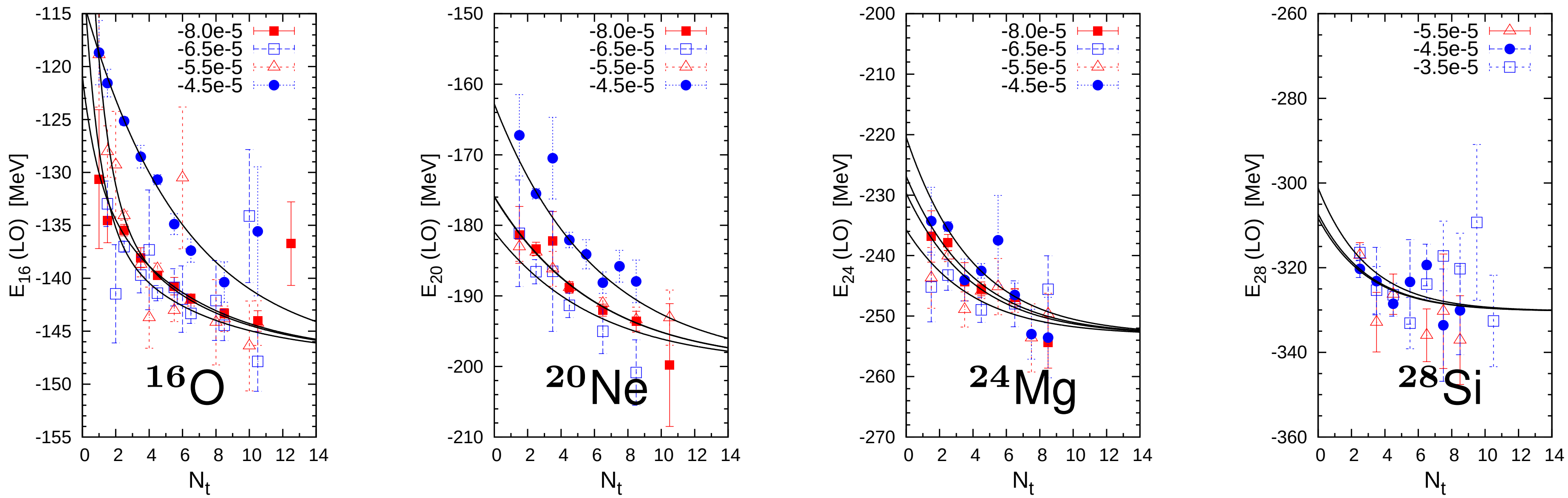
- Rot. symmetry breaking

PRD 90 (2014), PRD 92 (2015)



GOING up the ALPHA CHAIN

- Consider the α ladder ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si as $t_{\mathrm{CPU}} \sim A^2$
- Improved "multi-state" technique to extract ground state energies
  - $\Rightarrow$ higher A, better accuracy
  - $\Rightarrow$ overbinding at LO beyond $A = 12$ persists up to NNLO



$$E = -131.3(5) \quad [-127.62]$$

$$E = -165.9(9) \quad [-160.64]$$

$$E = -232(2) \quad [-198.26]$$

$$E = -308(3) \quad [-236.54]$$

REMOVING the OVERBINDING

Lähde, 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 [long term: N3LO]

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

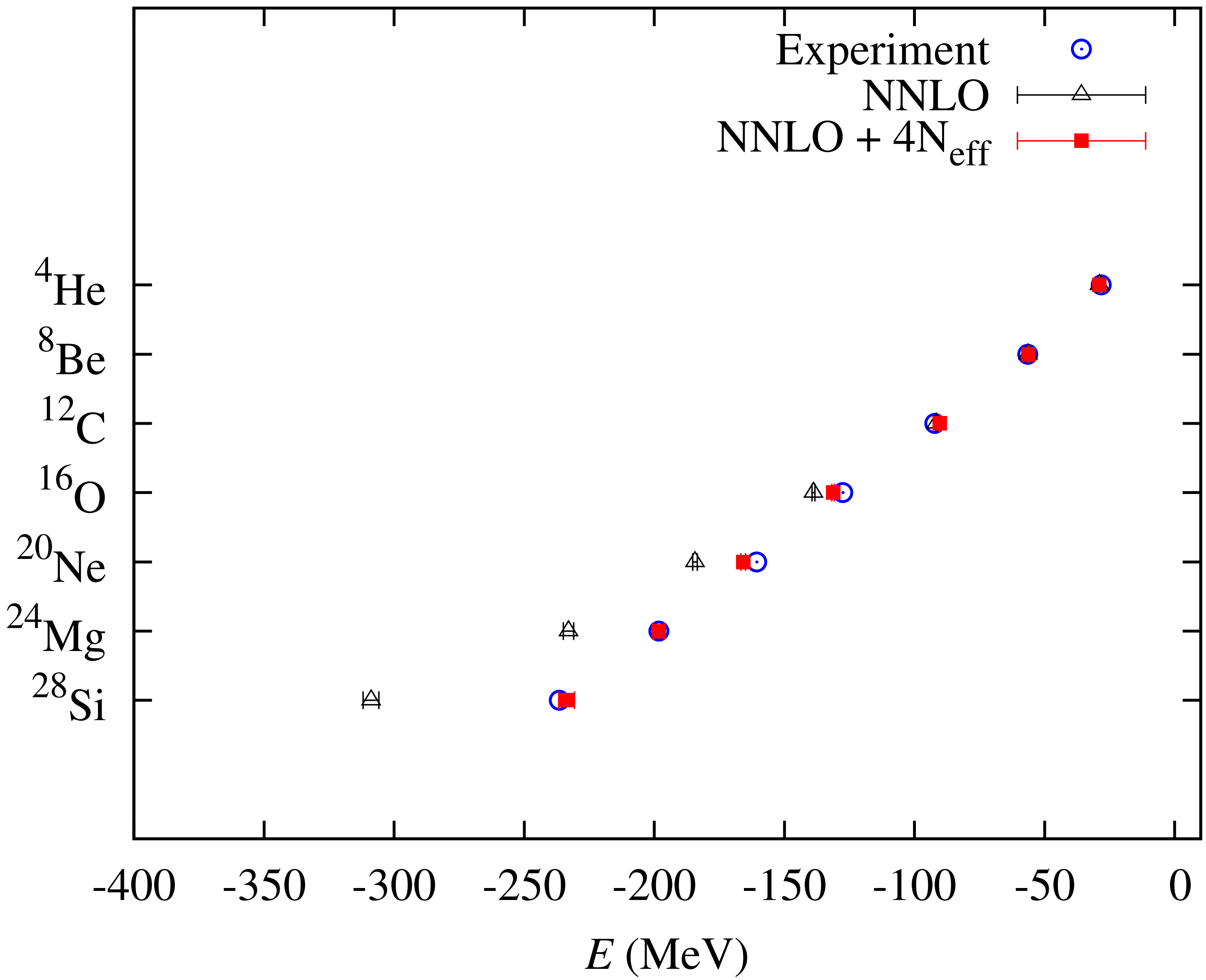
- fix the coefficient $D^{(4\mathrm{N_{eff}})}$ from the BE of ^{24}Mg

  $\Rightarrow$ 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 calcs

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

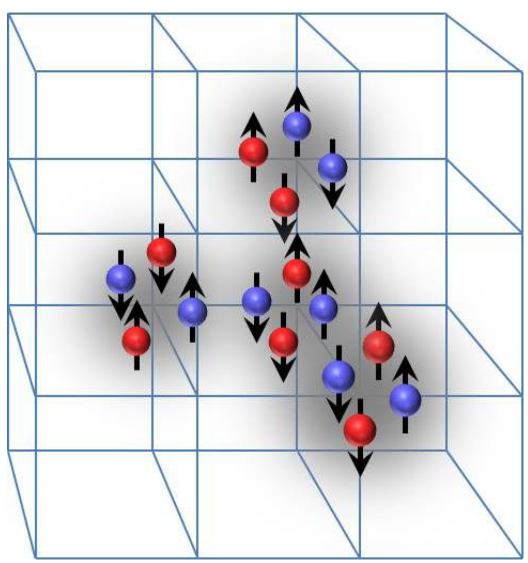
- Alpha-cluster models since decades, some exp. evidence

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

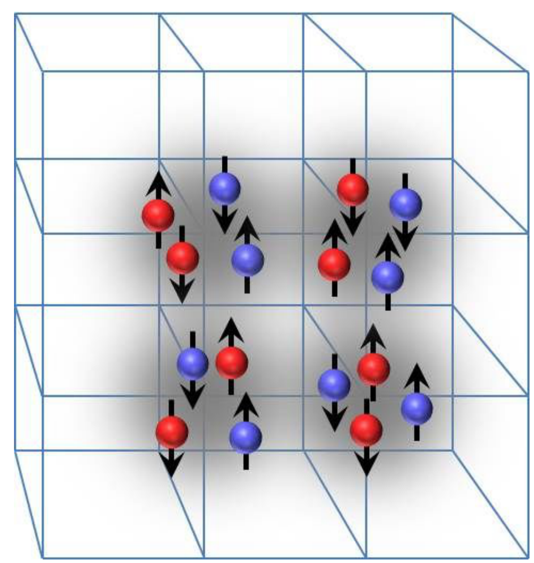
- Spectrum very close to tetrahedral symmetry group Bijker & Iachello (2014)

- 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

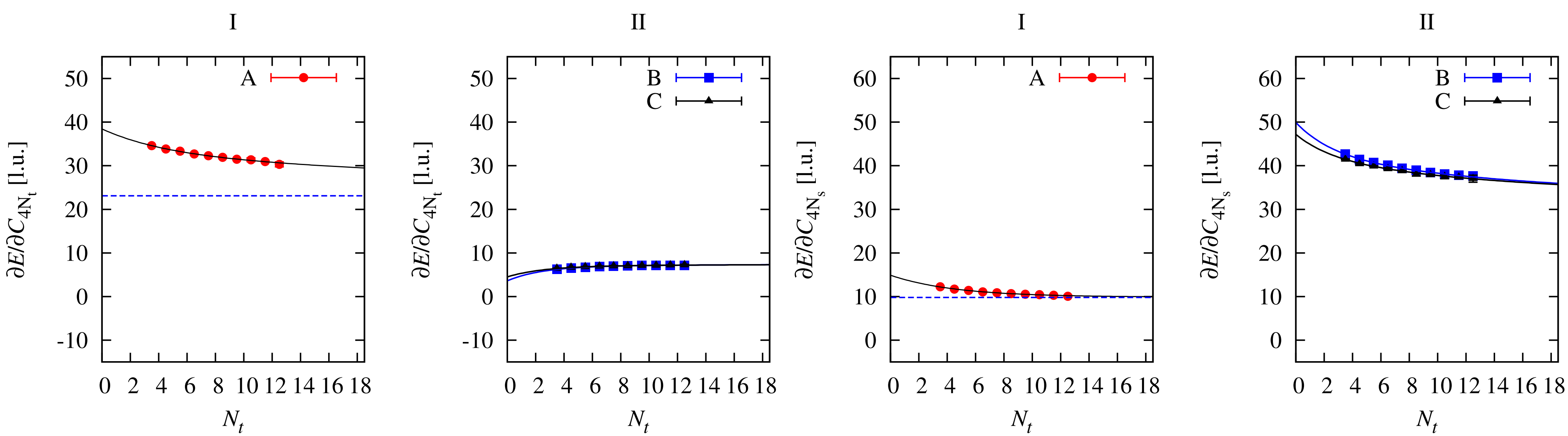
- measure the 4N density, where each of the nucleons is placed at adjacent points

$\Rightarrow$ $\mathbf{0_1^+}$ 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)
$M(E0, 0_2^+ \to 0_1^+)$ [e fm^2]	2.1(7)	3.0(1.4)	3.6(2)

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

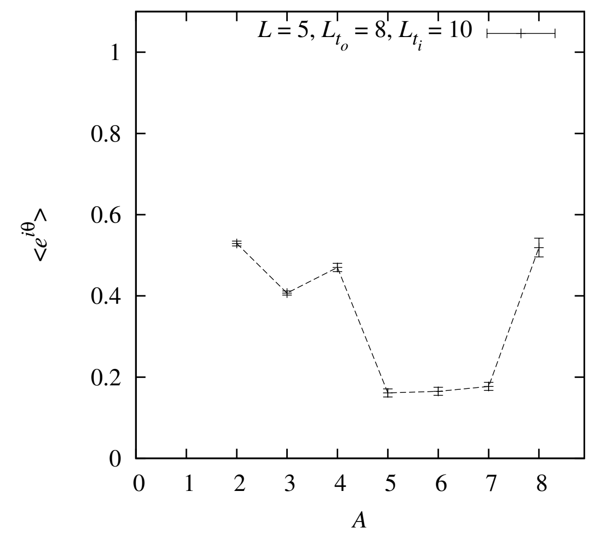
SYMMETRY-SIGN EXTRAPOLATION METHOD

Epelbaum, Krebs, Lähde, Lee, Luu, UGM, Rupak, EPJA **51**: 92 (2015)

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

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

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



Borasoy et al. (2007)

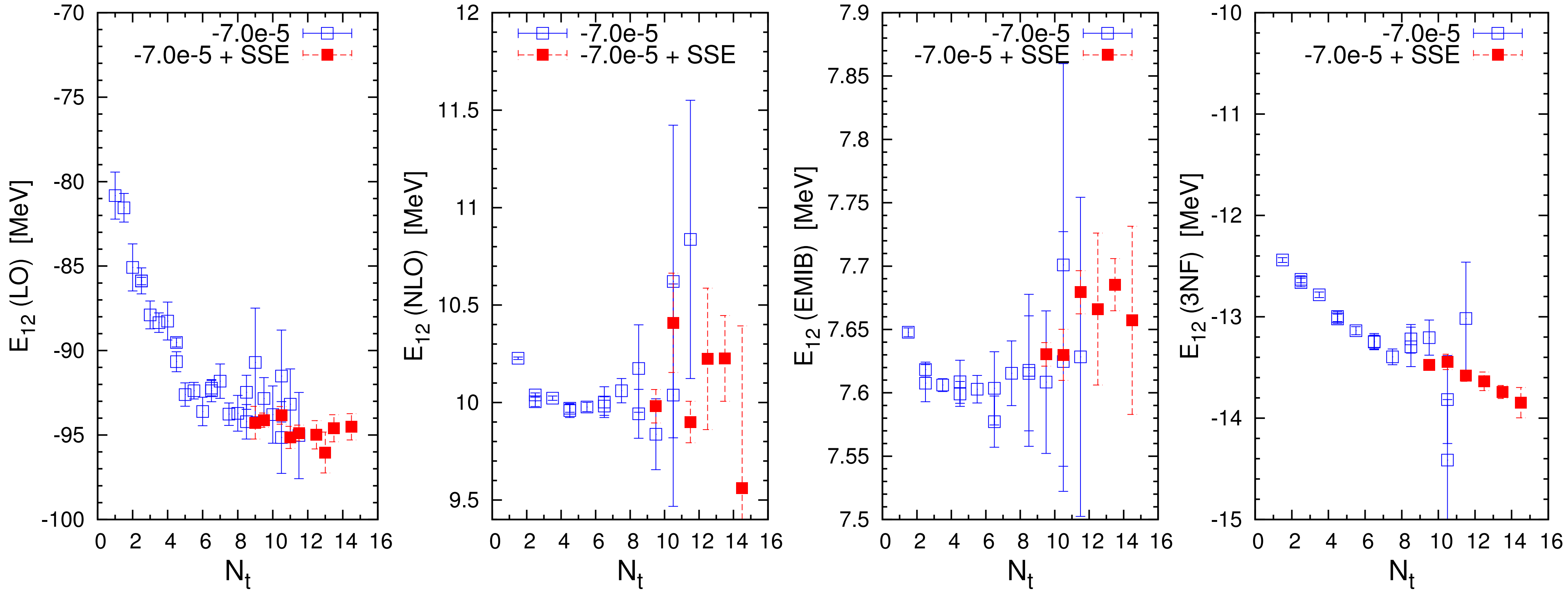
- Symmetry-sign extrapolation (SSE) method: control the sign oscillations

$$H_{d_h} = d_h \cdot H_{\mathrm{phys}} + (1 - d_h) \cdot H_{\mathrm{SU(4)}} \qquad H_{\mathrm{SU(4)}} = \tfrac{1}{2} C_{\mathrm{SU(4)}} \, (N^\dagger N)^2$$

$\hookrightarrow$ family of solutions for different SU(4) couplings $C_{\mathrm{SU(4)}}$
that converge on the physical value for $d_h = 1$

RESULTS for ^{12}C

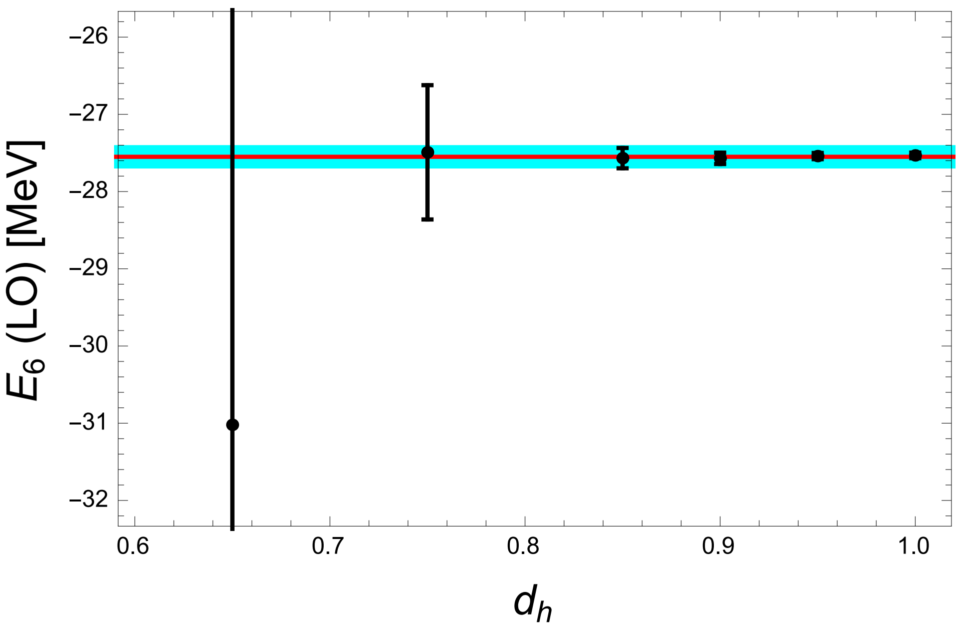
- generate a few more MC data at large N_t using SSE

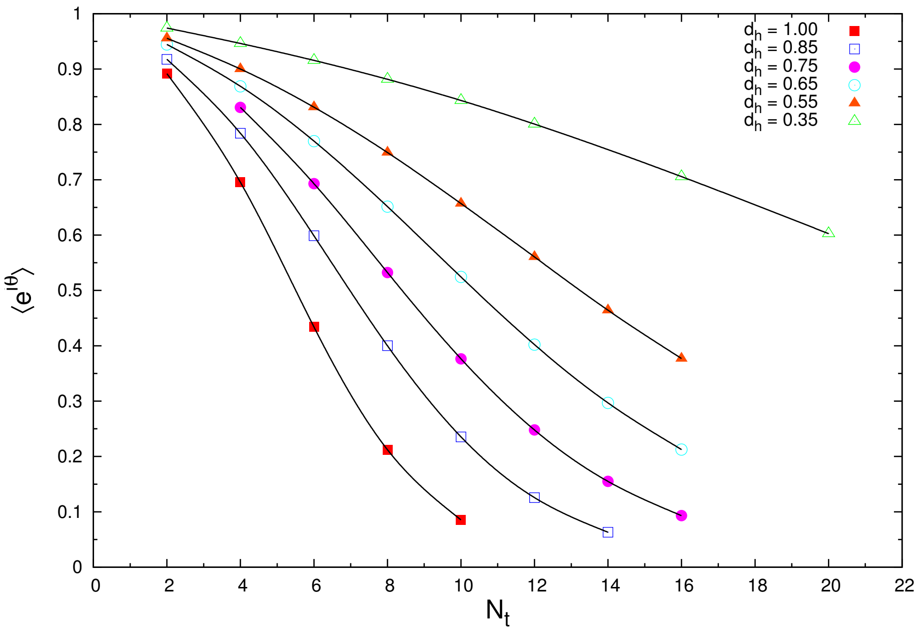


- promising results $\rightarrow$ no more exponential deterioration of the MC data
- results w/ small uncertainties for $d_h \geq 0.8$

RESULTS for $A = 6$

- Simulations for ^{6}He and ^{6}Be





$\Rightarrow$ methods works for nuclei with $A \neq Z$

$\Rightarrow$ neutron-rich nuclei can now be systematically explored (larger volumes)

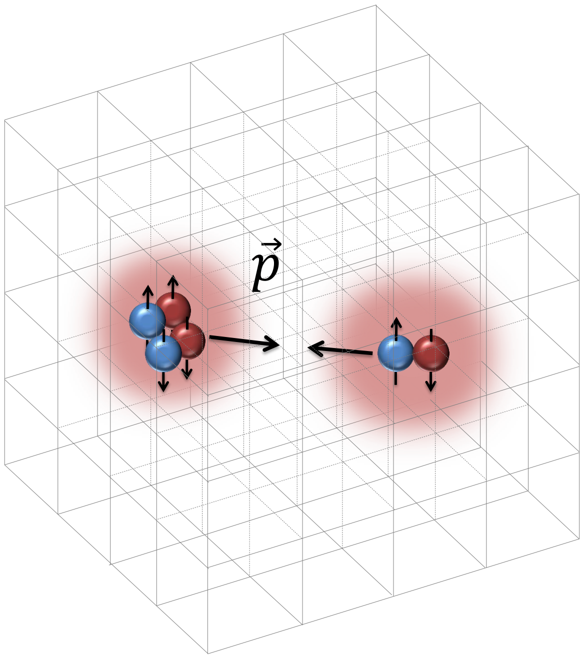
Ab initio calculation of α-α scattering

Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, UGM, arXiv:1506.03513

TWO-BODY 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

- Ab initio calculations of scattering and reactions suffer from computational scaling with the number of nucleons in the clusters



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

Rupak, Lee, Phys. Rev. Lett. 111 (2013) 032502
Pine, Lee, Rupak, Eur. Phys. J. A49 (2013) 151
Elhatisari, Lee, Phys. Rev. C90 (2014) 064001
Elhatisari, et al., arXiv:1505.02967

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**

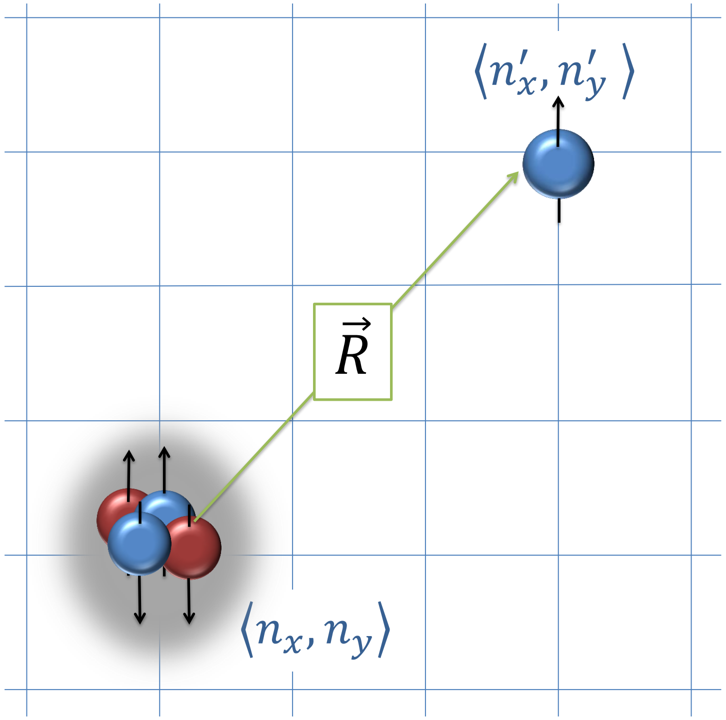
Second part:
compute the two-cluster scattering phase shifts or reaction amplitudes using the adiabatic Hamiltonian

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:

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

$\rightarrow$ 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

TESTING the ADIABATIC HAMILTONIAN

- Consider fermion-dimer scattering:

Microscopic Hamiltonian $\Rightarrow$ Two-cluster adiabatic Hamitltonian

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

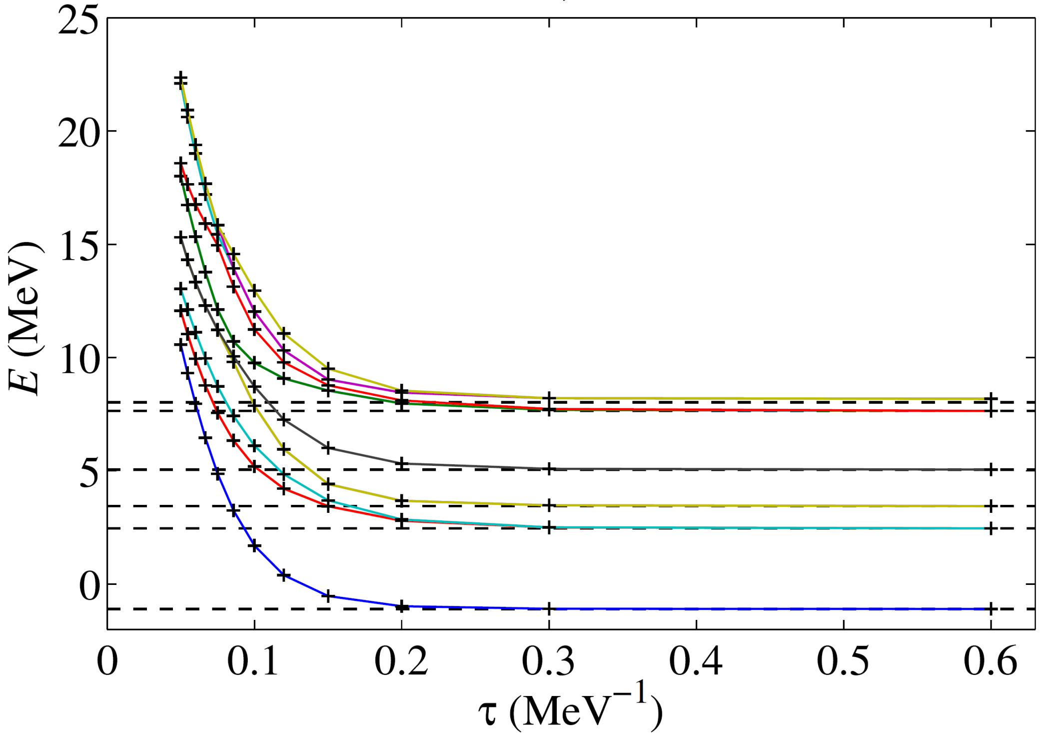
- calculation of a 7^3 lattice, lattice spacing $a = 1.93$ fm

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

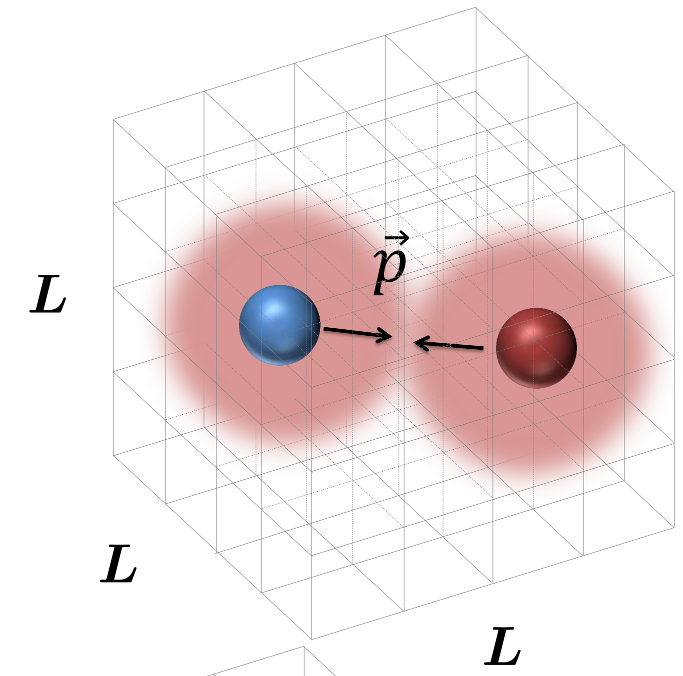
exact Lanzcos: black dashed lines

adiab. Ham.: solid colored lines

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



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

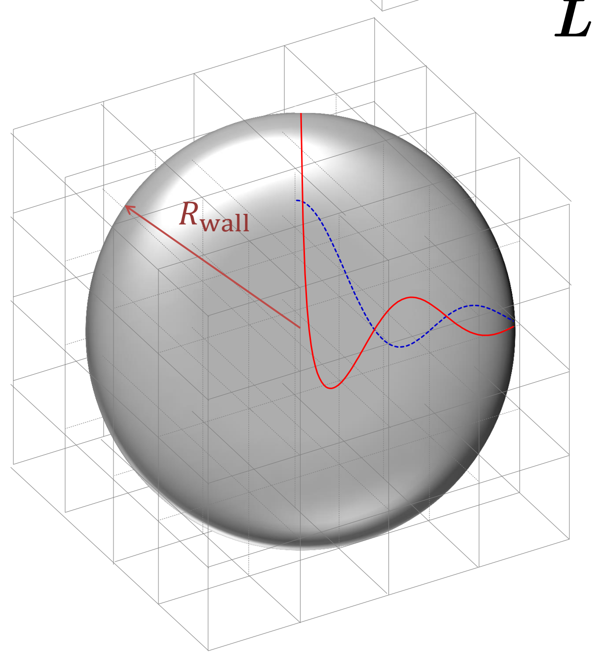
  Lüscher, Comm. Math. Phys 105 (1986) 153

  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 $r = R_{\rm wall}$:

$$\psi_\ell(r) \sim [\cos\delta_\ell(p)F_\ell(pr) + \sin\delta_\ell(p)G_\ell(pr)]$$



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

SCATTERING CLUSTER WAVE FUNCTIONS

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

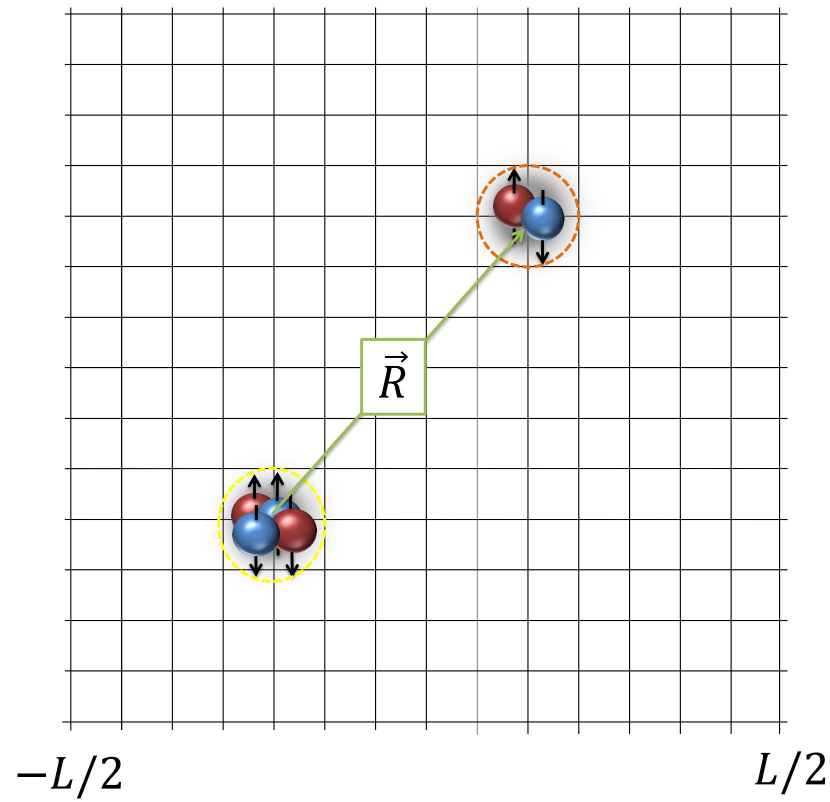
$$d_{\varepsilon,i} = \sqrt{\tau_\varepsilon / M_i}$$

- Only non-overlapping clusters if

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

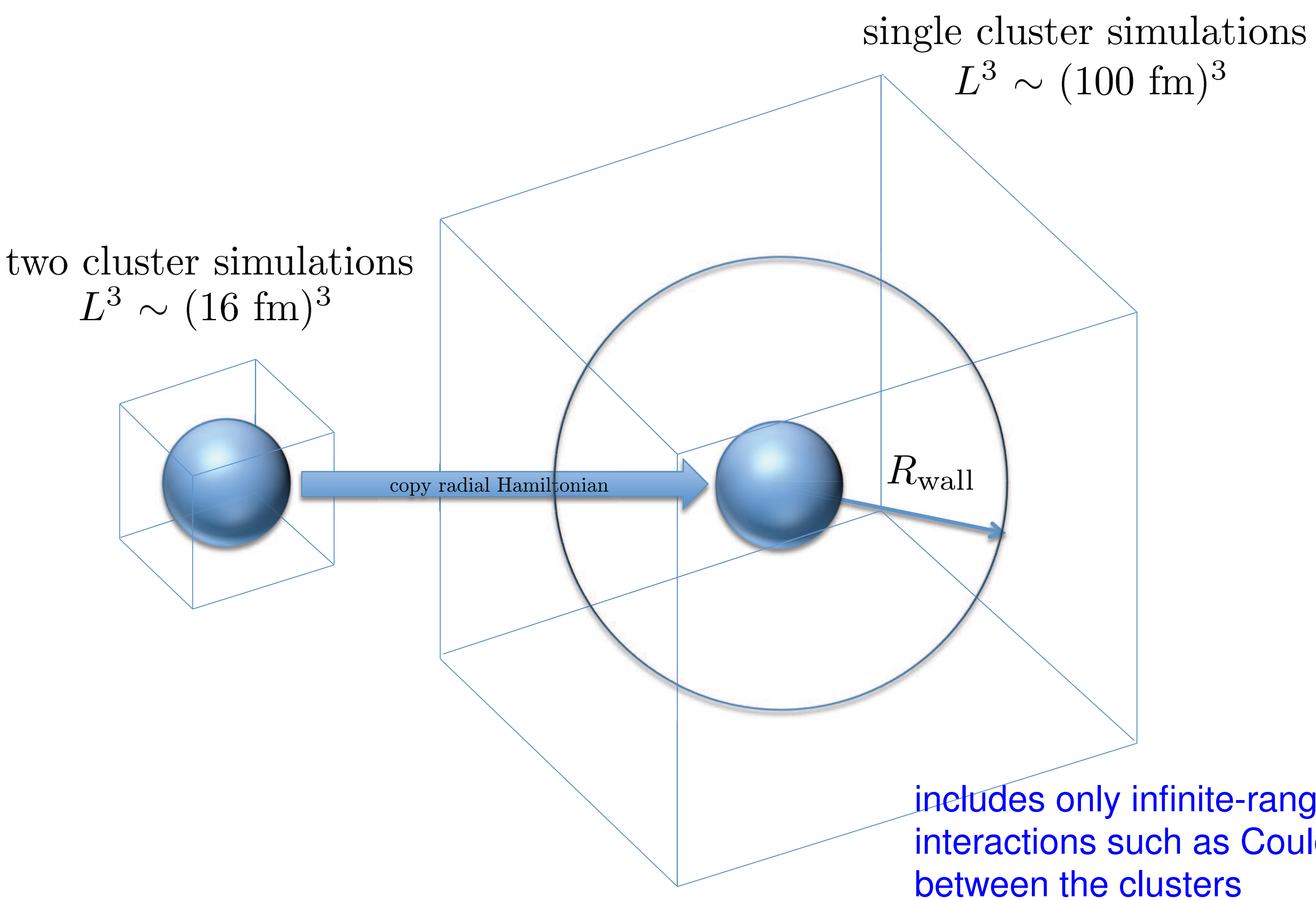
- Defines asymptotic region, where the amount of overlap between clusters is less than ε

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



$\Rightarrow$ 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



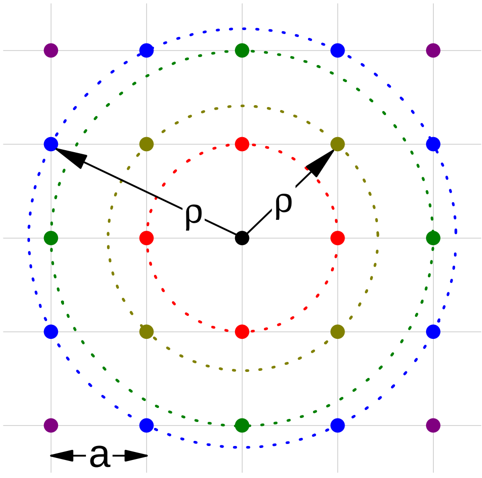
includes only infinite-range interactions such as Coulomb between the clusters

25

ALPHA–ALPHA SCATTERING

- 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

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



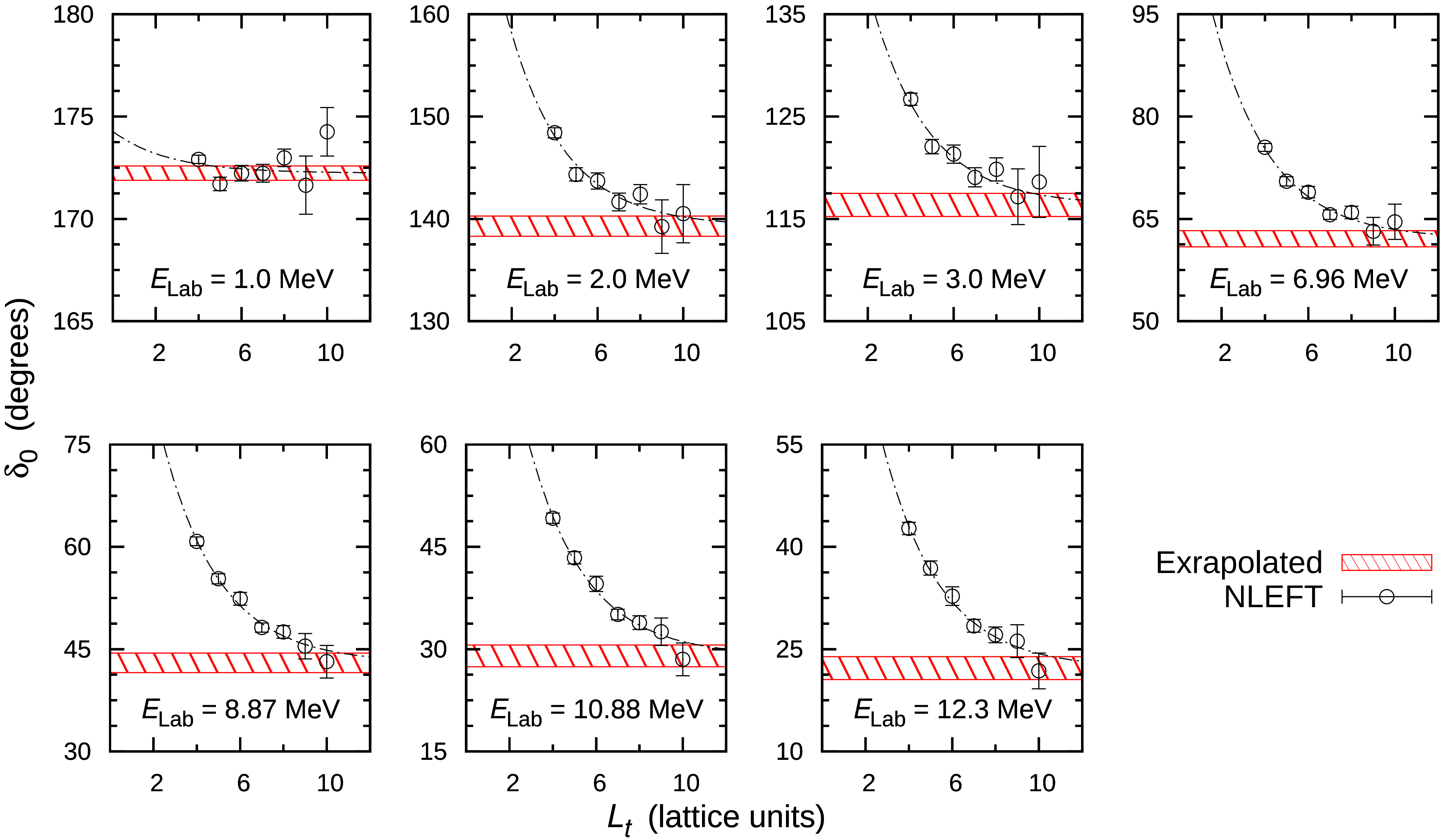
$\rightarrow$ precise extraction of phase shifts & mixing angles

Lu, Lähde, Lee, UGM, arXiv:1506.05652

Moinard et al., work in progress

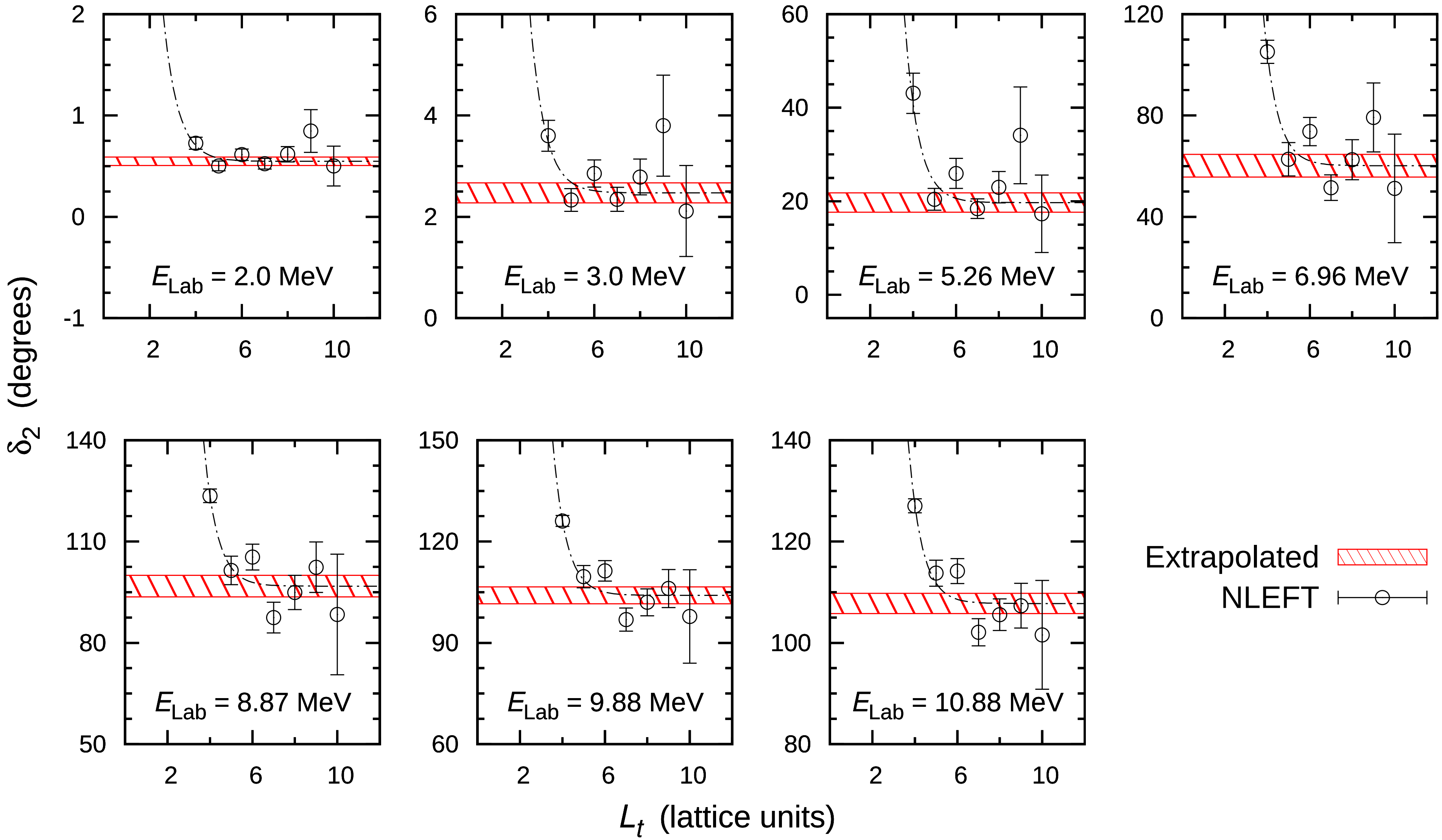
LATTICE DATA I

- Show data for the S-wave:



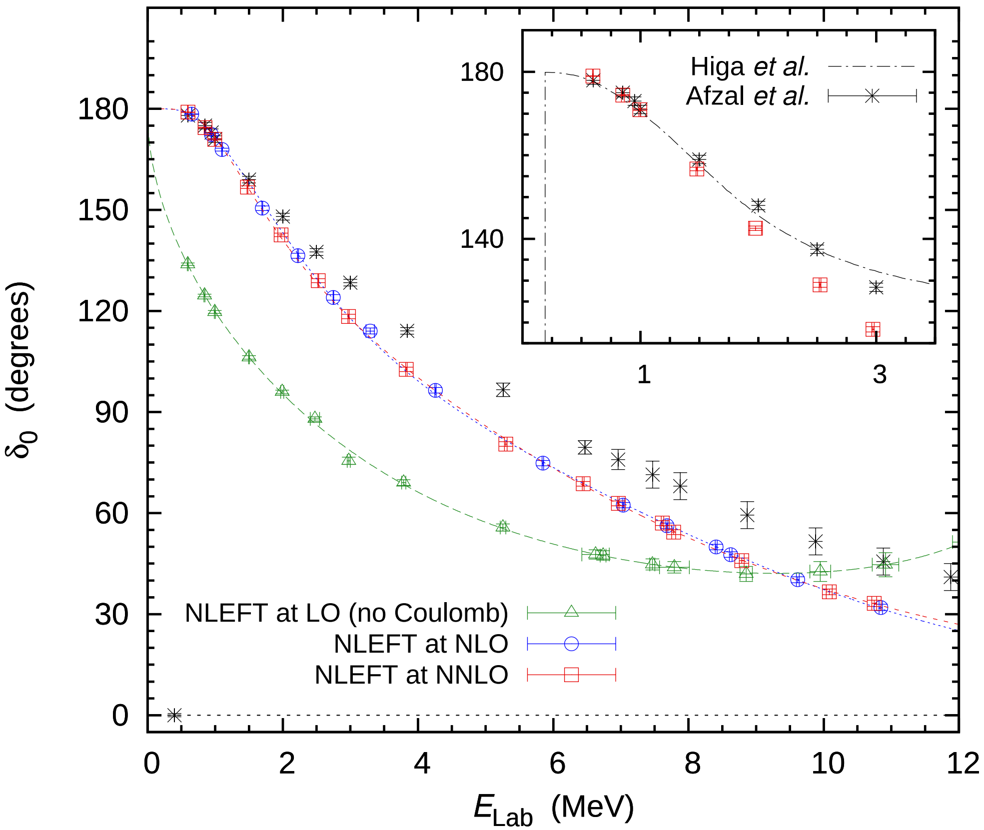
LATTICE DATA II

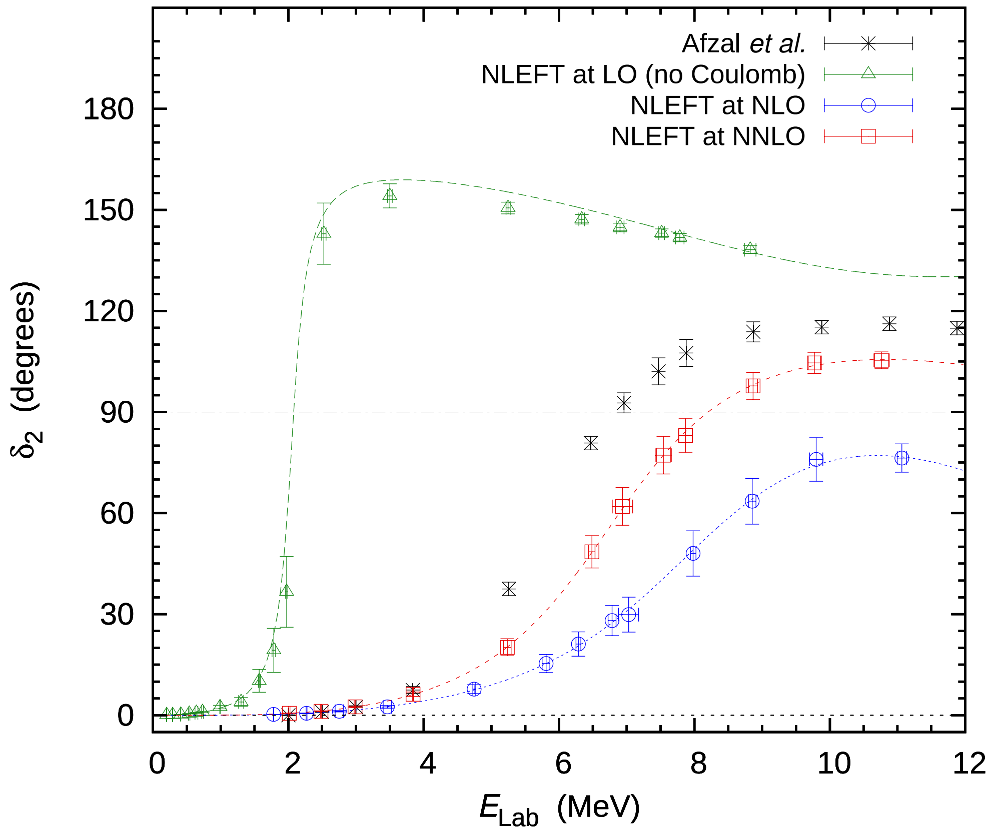
- Show data for the D-wave:



PHASE SHIFTS

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





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

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

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

Afzal et al., Rev. Mod. Phys. 41 (1969) 247 [data]; Higa et al., Nucl.Phys. A809 (2008) 171 [halo EFT]

SUMMARY & OUTLOOK

- Nuclear lattice simulations as a new quantum many-body approach
  - $\rightarrow$ based on the successful continuum nuclear chiral EFT
  - $\rightarrow$ clustering emerges naturally, α-cluster nuclei
  - $\rightarrow$ symmetry-sign extrapolation method allows to go to the drip lines
  - $\rightarrow$ ab initio study of α-α scattering: promising results
  - $\rightarrow$ holy grail of nuclear astrophysics (α+^{12}C $\rightarrow$ ^{16}O+γ) in reach
- Some on-going activities:
  - $\rightarrow$ improving the forces (N3LO, sph. harmonics)
  - $\rightarrow$ systematic studies of a-independence

    $\hookrightarrow$ Klein, Lee, Liu, UGM, PLB747 (2015) 511
  - $\rightarrow$ finite size effects/averaging procedures

    $\hookrightarrow$Lu, Lähde, Lee, UGM, Phys. Rev. D90 (2014) 034507 & D92 (2015) 014506
  - $\rightarrow$ and much more . . .