



**Towards an Understanding of Clustering  
in Nuclei from First Principles**  
**Ulf-G. Meißner, Univ. Bonn & FZ Jülich**

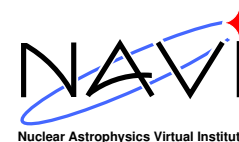
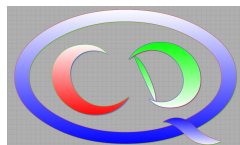
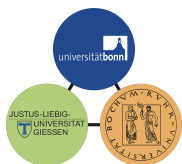
Supported by DFG, SFB/TR-16

and by DFG, SFB/TR-110

and by CAS, PIFI

by HGF VIQCD VH-VI-417

and by VW Stiftung



# CONTENTS

- Short introduction
- Basics of nuclear lattice simulations
- Results from nuclear lattice simulations
- Ab initio calculation of alpha-alpha scattering
- Nuclear binding near a quantum phase transition
- Beyond alpha-cluster nuclei
- Summary & outlook

# Short introduction



# Basics of nuclear lattice simulations

for an easy intro, see: [UGM, Nucl. Phys. News 24 \(2014\) 11](#)









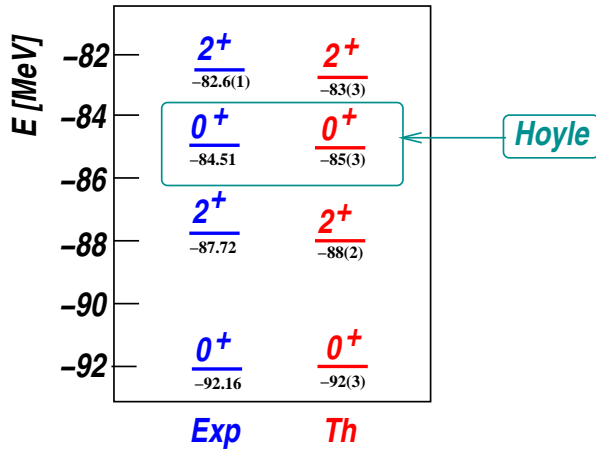




# RESULTS from LATTICE NUCLEAR EFT @ NNLO

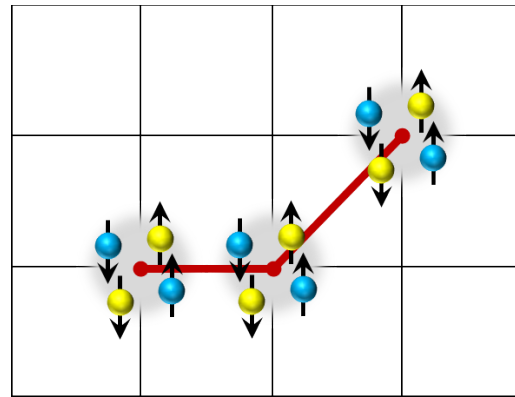
• Hoyle state in  $^{12}\text{C}$

PRL 106 (2011)



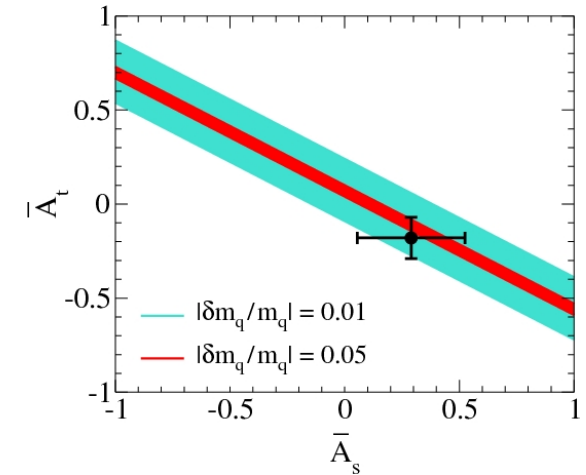
• Structure of the Hoyle state

PRL 109 (2012)



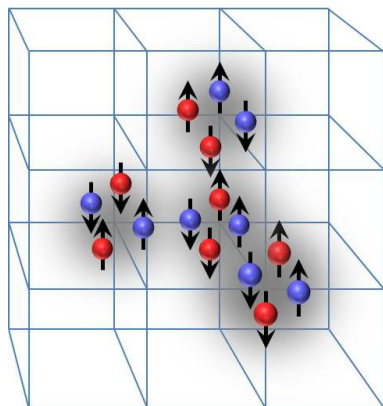
• Fate of carbon-based life

PRL 110 (2013), EPJ A49 (2013)



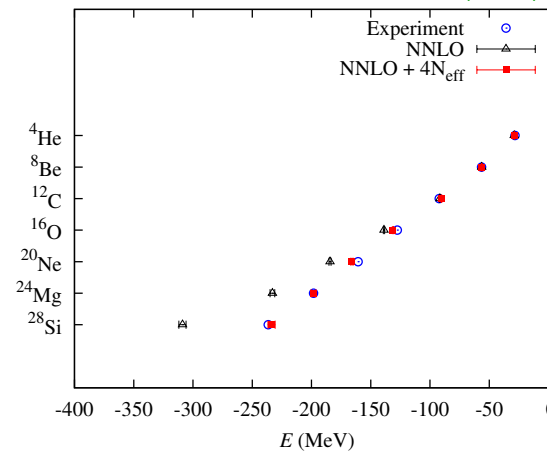
• Spectrum of  $^{16}\text{O}$

PRL 112 (2014)



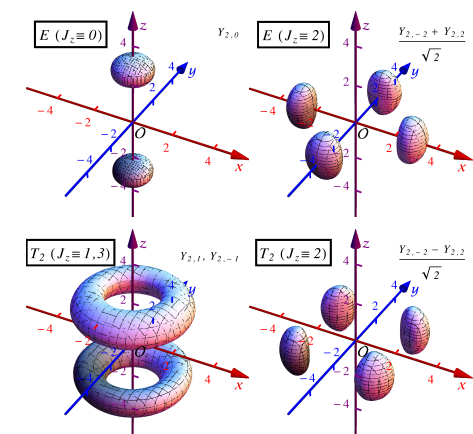
• Going up the  $\alpha$ -chain

PLB 732 (2014)



• Rot. symmetry breaking

PRD 90 (2014), PRD 92 (2015)



# STRUCTURE of $^{16}\text{O}$

- Mysterious nucleus, despite modern ab initio calcs

Hagen et al. (2010), Roth et al. (2011), Hergert et al. (2013), Jansen et al. (2014), Cipollone et al. (2015)

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

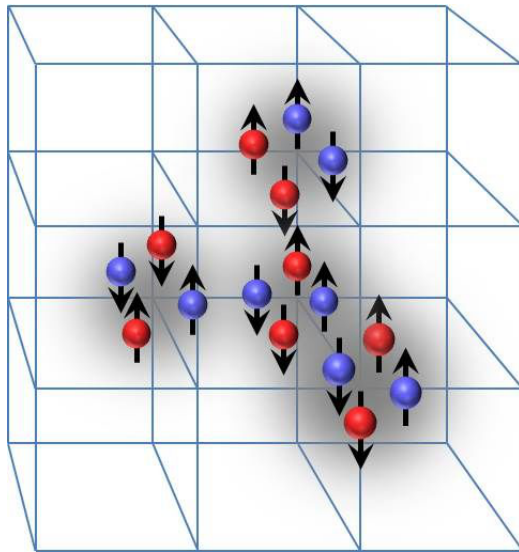
Wheeler (1937), Dennison (1954), Robson (1979), . . . , Freer et al. (2005)

- Spectrum very close to tetrahedral symmetry group

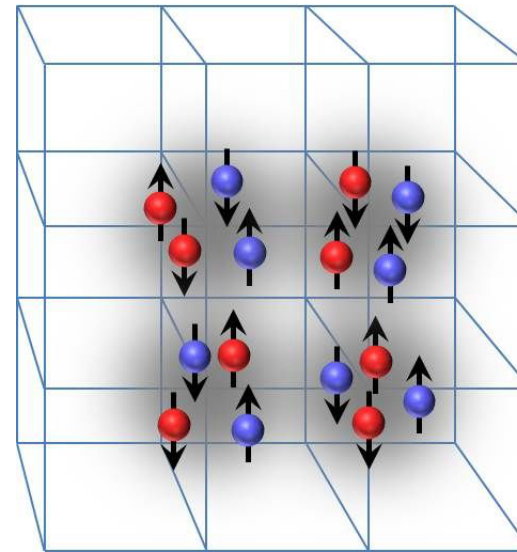
Bijker & Iachello (2014)

- Relevant configurations in lattice simulations:

Tetrahedron (A)



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





- Spectrum:

	LO	NNLO	Exp.
$0_1^+$	-147.3(5)	-131.3(5)	-127.62
$0_2^+$	-145(2)	-123(2)	-121.57
$2_1^+$	-145(2)	-123(2)	-120.70

[NB: Eff. 4N term included]

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

⇒ compensate for this by rescaling with appropriate units of  $r/r_{\text{LO}}$

- LO EM properties:

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

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

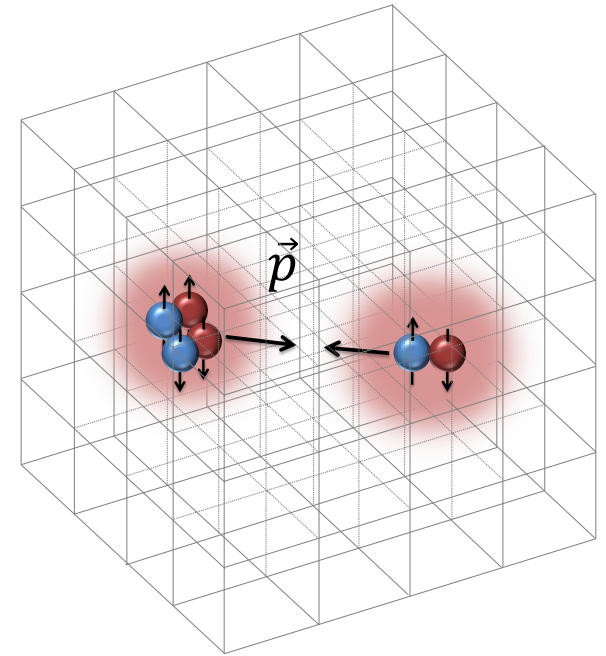
⇒ **results independent of the initial configurations! → clustering**

# Ab initio calculation of $\alpha$ - $\alpha$ scattering

Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, UGM,  
Nature **528** (2015) 111 [arXiv:1506.03513]

# NUCLEUS–NUCLEUS SCATTERING on the LATTICE

- Processes involving  $\alpha$ -particles and  $\alpha$ -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., Phys.Rev. **C92** (2015) 054612  
 Elhatisari, Lee, UGM, Rupak, arXiv:1603.02333



# 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 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:

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

- 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  $\tau_\epsilon$ , each cluster undergoes spatial diffusion:

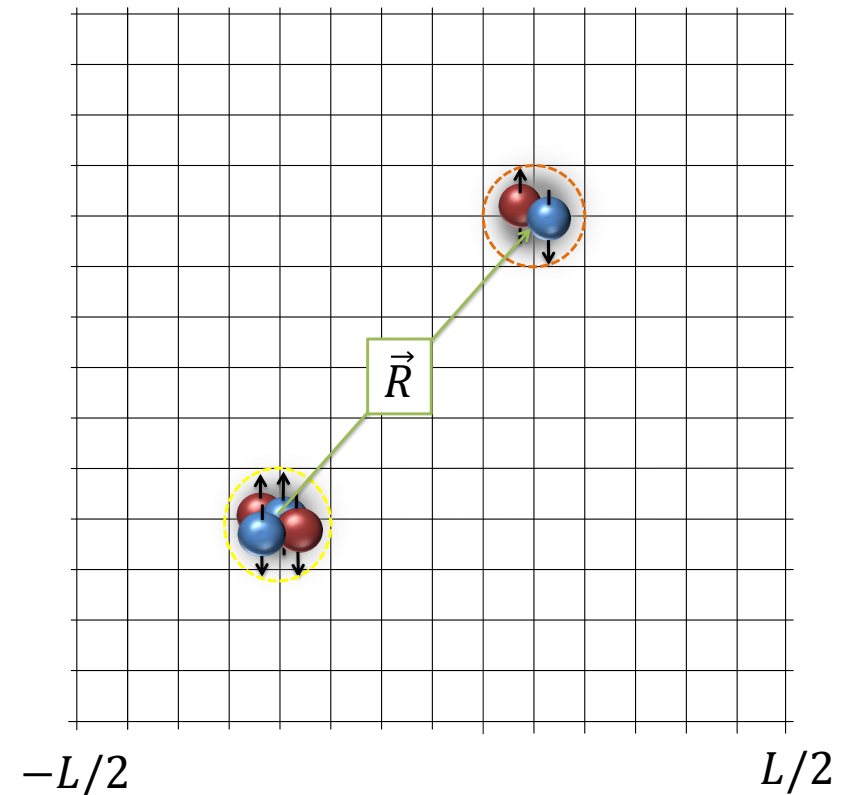
$$d_{\epsilon,i} = \sqrt{\tau_\epsilon/M_i}$$

- Only non-overlapping clusters if

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

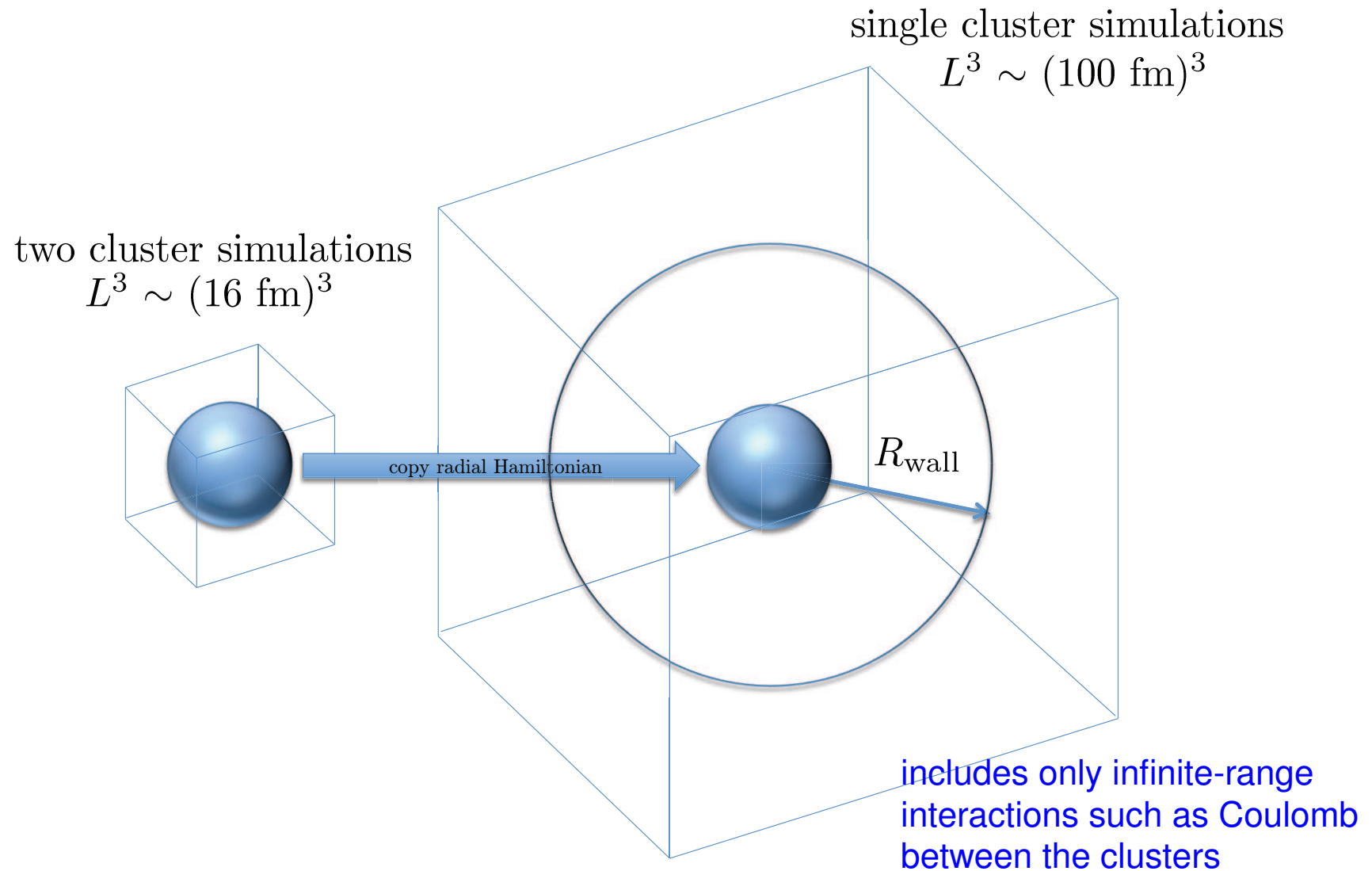
- Defines asymptotic region, where the amount of overlap between clusters is less than  $\epsilon$

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



$\Rightarrow$  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

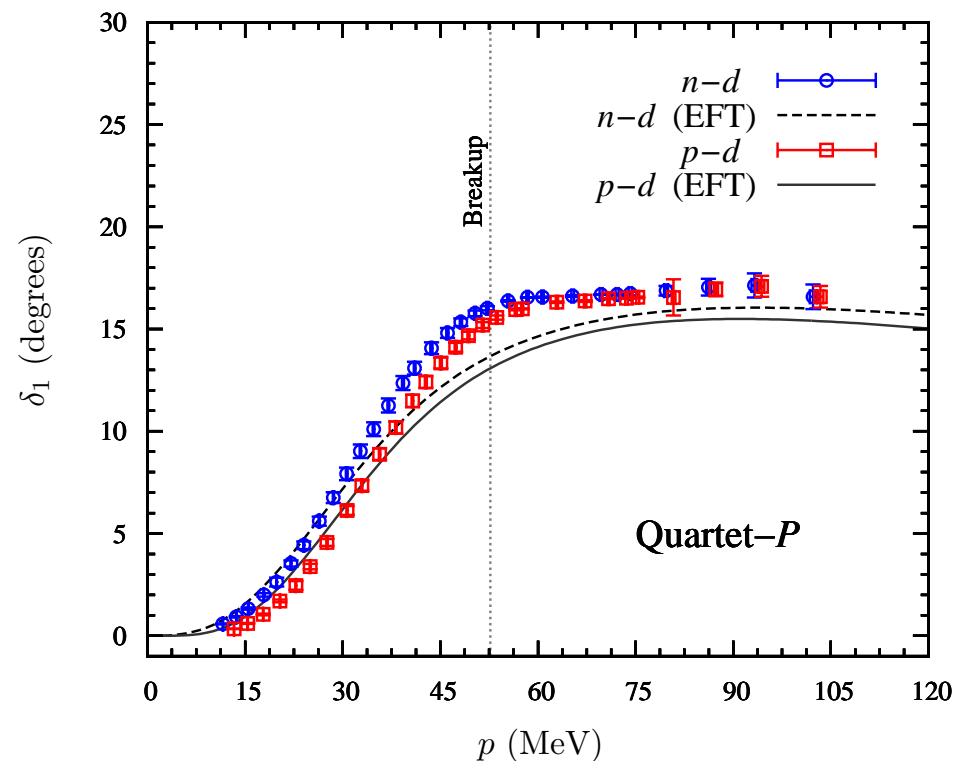
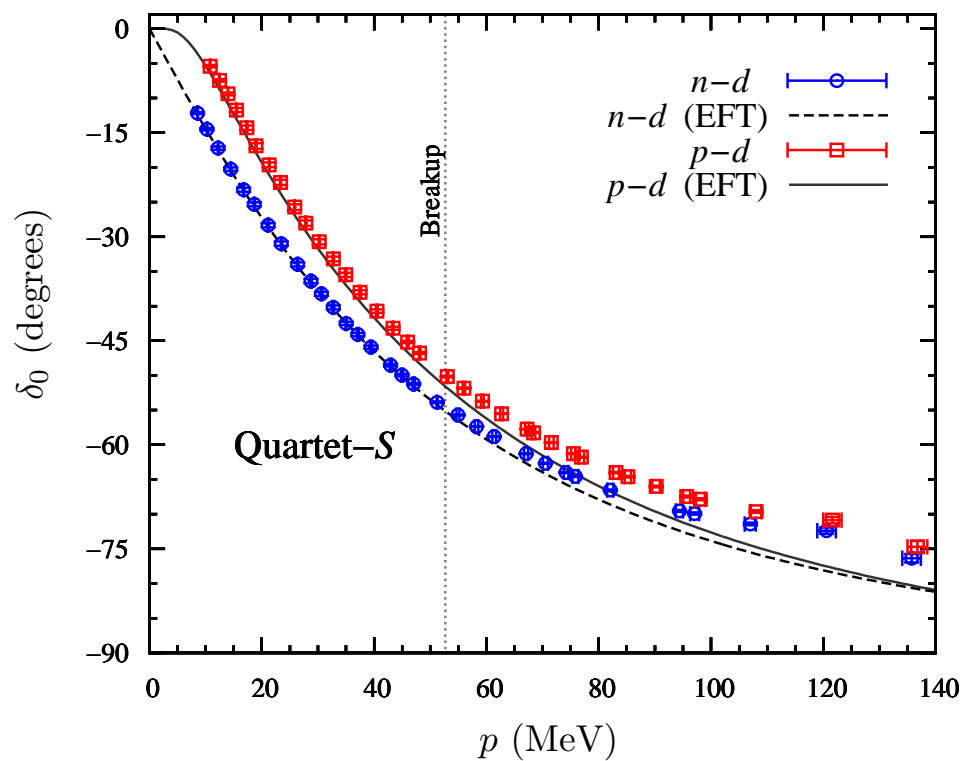


# A TEST: NUCLEON-DEUTERON SCATTERING

Elhatisari, Lee, UGM, Rupak, arXiv:1603.02333, EPJA (2016)

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

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



# ALPHA-ALPHA SCATTERING

- same lattice action as for the Hoyle state in  $^{12}\text{C}$  and the structure of  $^{16}\text{O}$
- (9+2) 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

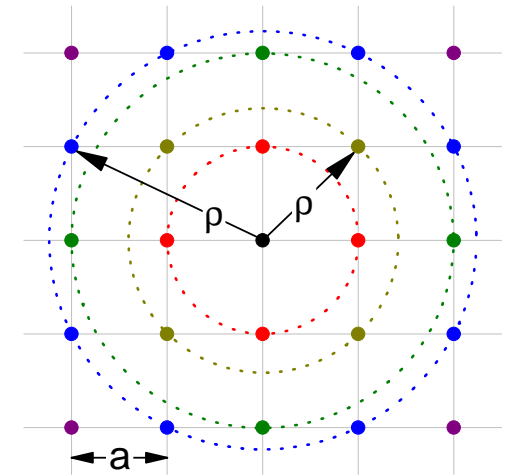
$$|\mathbf{R}\rangle^{(\ell),(\ell_z)} = \sum_{\vec{R}'} Y_{\ell,\ell_z}(\vec{R}') \delta_{R,|\vec{R}'|} |\vec{R}'\rangle$$

→ precise extraction of phase shifts & mixing angles

Lu, Lähde, Lee, UGM, arXiv:1506.05652

Moinard et al., work in progress

Elhatisari, Lee, UGM, Rupak, arXiv:1603.02333







# Nuclear binding near a quantum phase transition

Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, UGM, Epelbaum,  
Krebs, Lähde, Lee, Rupak, arXiv:1602.04539

# GENERAL CONSIDERATIONS

- *Ab initio* chiral EFT is an excellent theoretical framework
- not guaranteed to work well with increasing  $A$ 
  - possible sources of problems:
    - higher-body forces, higher orders, cutoff dependence, . . .
- very many ways of formulating chiral EFT at any given order (smearing etc.)
  - use not only NN scattering and light nuclei BEs  
but also light nucleus-nucleus scattering data  
to pin down the pertinent interactions
  - troublesome corrections might be small
  - investigate these issues using two seemingly equivalent interactions  
**[ not a precision study!]**



- Local operators/densities:

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

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

- Non-local operators/densities:

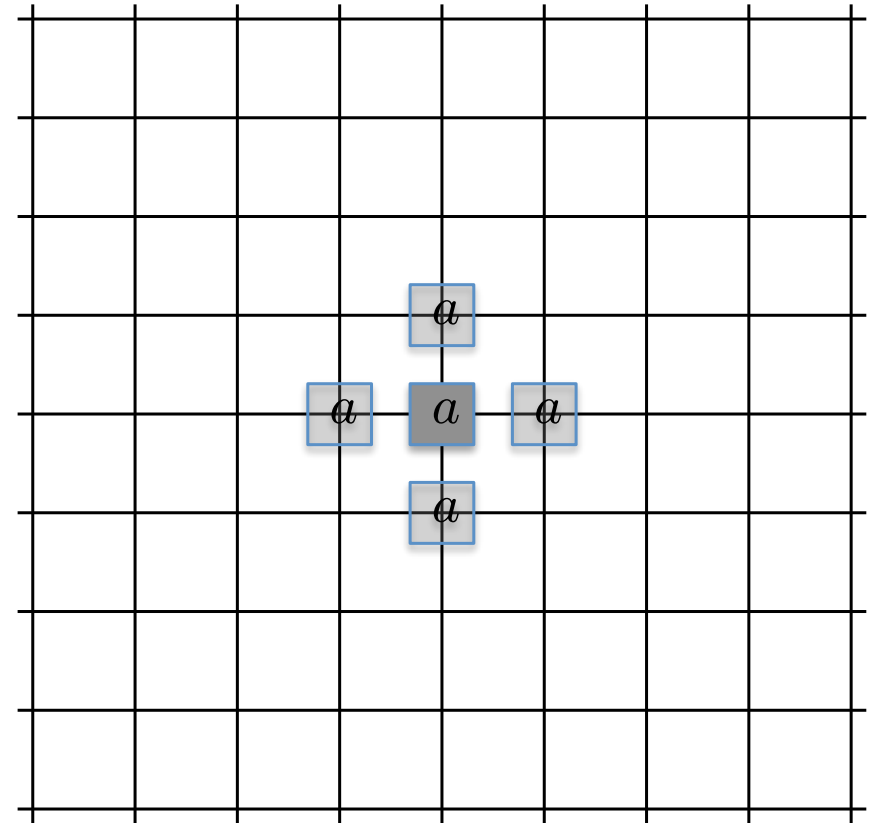
$$a_{\text{NL}}(\mathbf{n}) = a(\mathbf{n}) + s_{\text{NL}} \sum_{\langle \mathbf{n}' \mathbf{n} \rangle} a(\mathbf{n}')$$

$$a_{\text{NL}}^\dagger(\mathbf{n}) = a^\dagger(\mathbf{n}) + s_{\text{NL}} \sum_{\langle \mathbf{n}' \mathbf{n} \rangle} a^\dagger(\mathbf{n}')$$

$$\rho_{\text{NL}}(\mathbf{n}) = a_{\text{NL}}^\dagger(\mathbf{n})a_{\text{NL}}(\mathbf{n})$$

→ where  $\sum_{\langle \mathbf{n}' \mathbf{n} \rangle}$  denotes the sum over nearest-neighbor lattice sites of  $\mathbf{n}$

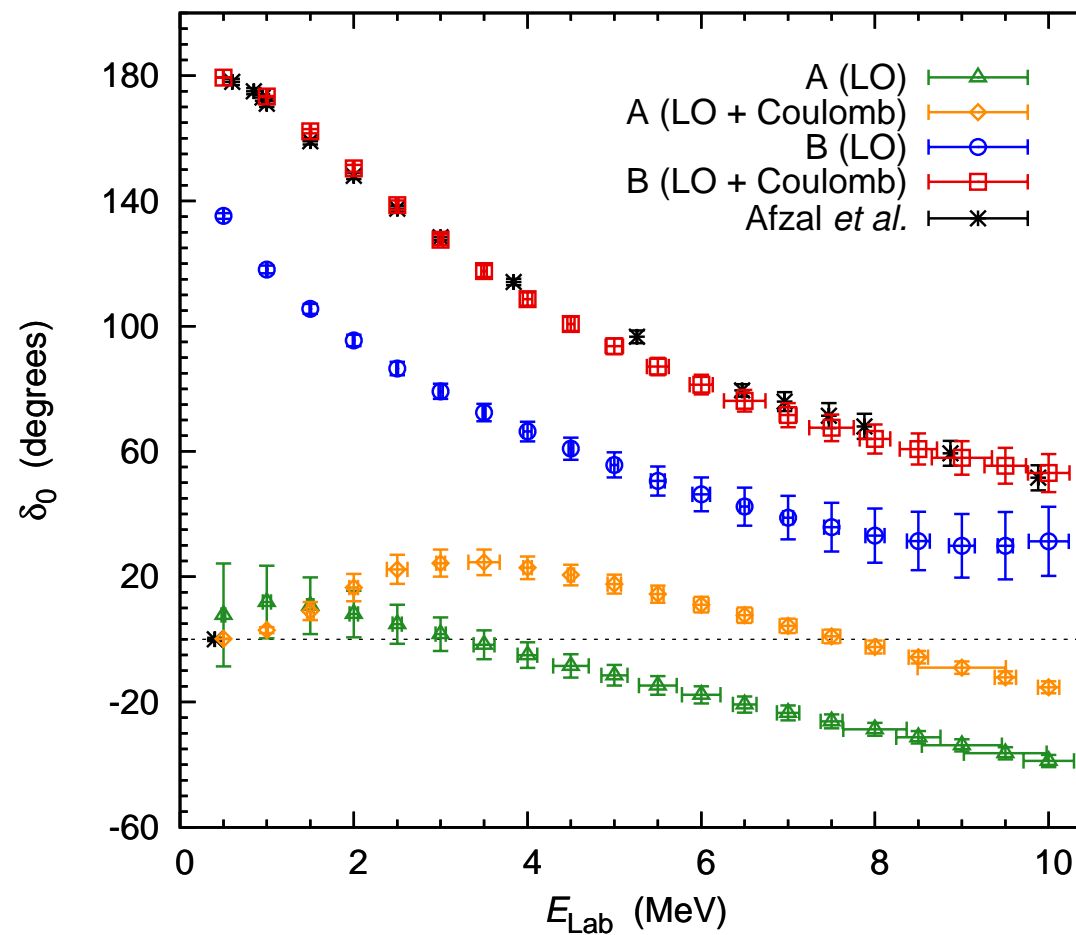
→ the smearing parameter  $s_{\text{NL}}$  is determined when fitting to the phase shifts





# ALPHA-ALPHA PHASE SHIFTS

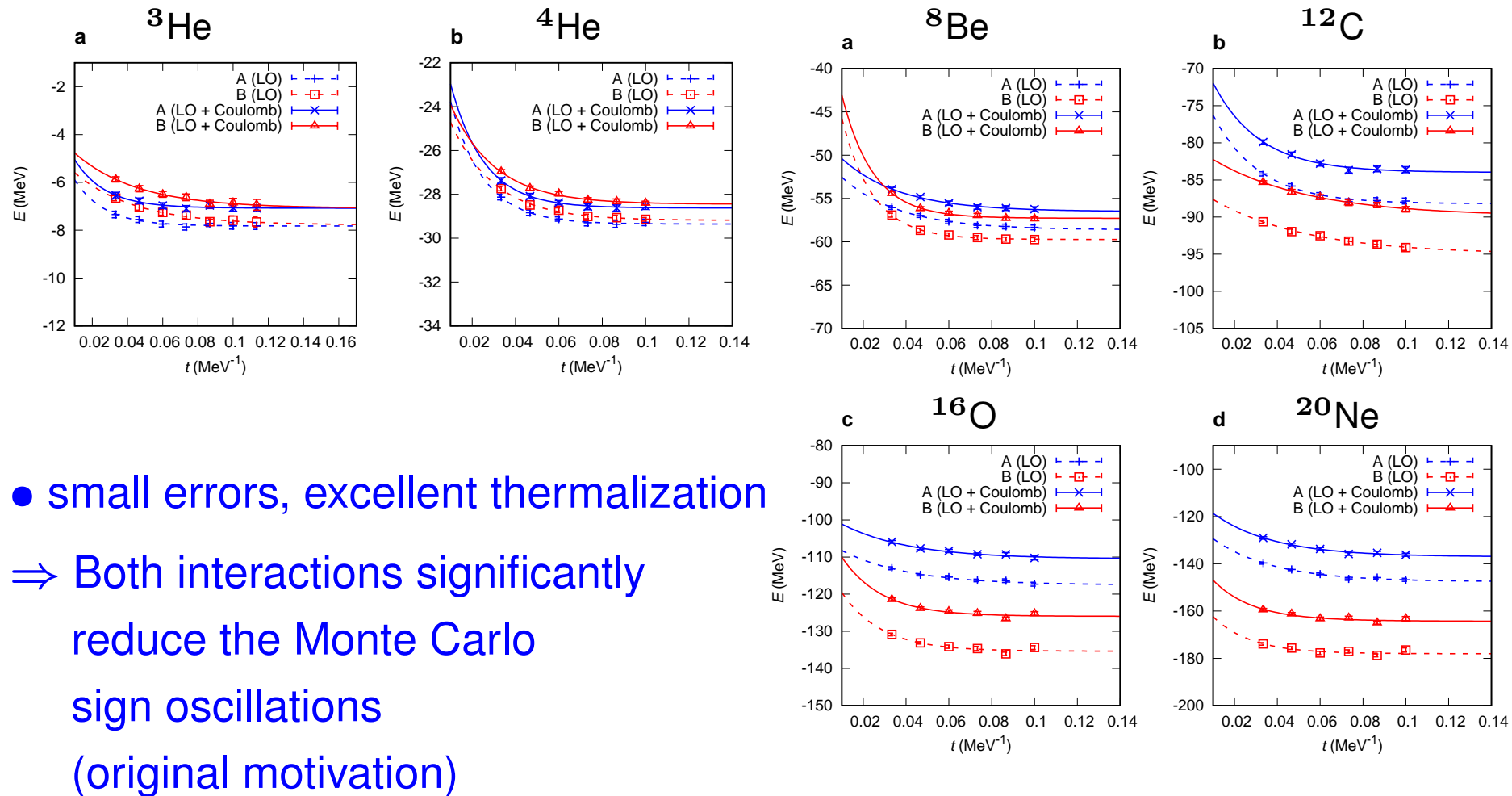
- Show results for [NN and]  $\alpha$ - $\alpha$  phase shifts for both interactions:



→ Interaction A fails, interaction B fitted ↔ consequences for nuclei?

# GROUND STATE ENERGIES I

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



- small errors, excellent thermalization

⇒ 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.
${}^4\text{He}$	-29.4(4)	-28.6(4)	-29.2(1)	-28.5(1)	-28.3
${}^8\text{Be}$	-58.6(1)	-56.5(1)	-59.7(6)	-57.3(7)	-56.6
${}^{12}\text{C}$	-88.2(3)	-84.0(3)	-95.0(5)	-89.9(5)	-92.2
${}^{16}\text{O}$	-117.5(6)	-110.5(6)	-135.4(7)	-126.0(7)	-127.6
${}^{20}\text{Ne}$	-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:

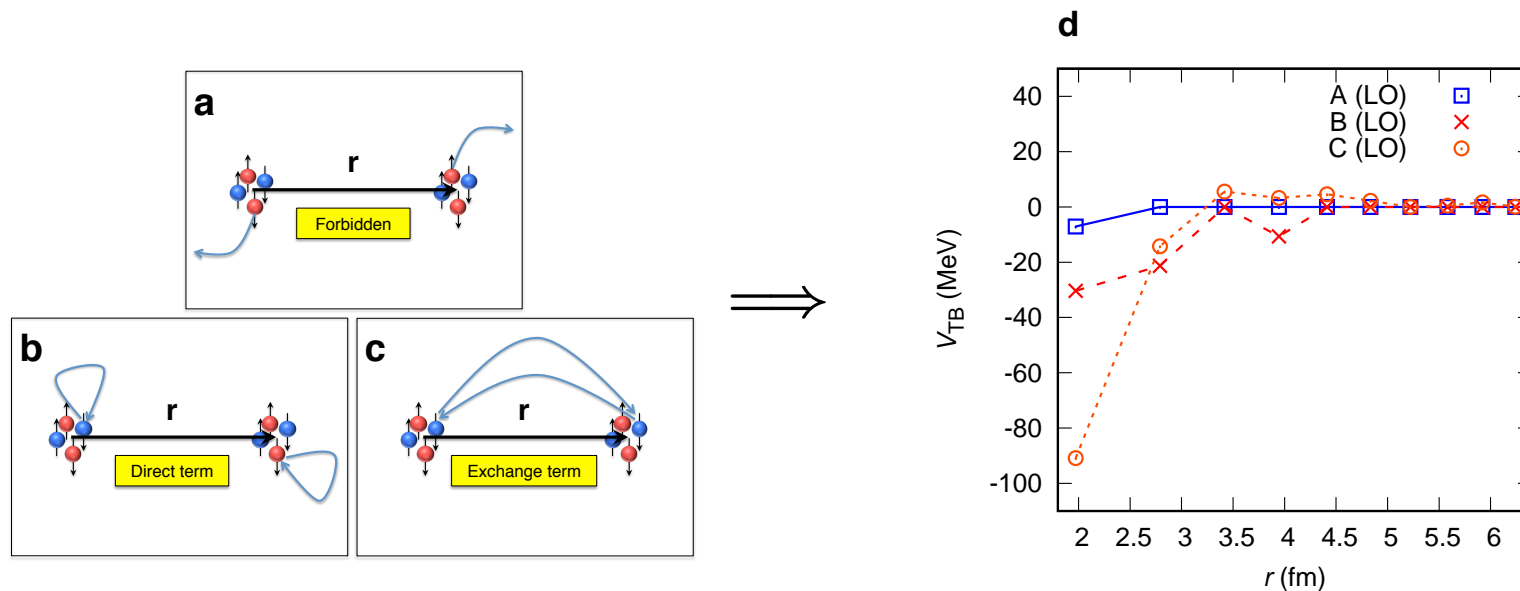
$$E({}^8\text{Be})/E({}^4\text{He}) = 1.997(6) \quad E({}^{12}\text{C})/E({}^4\text{He}) = 3.00(1)$$

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



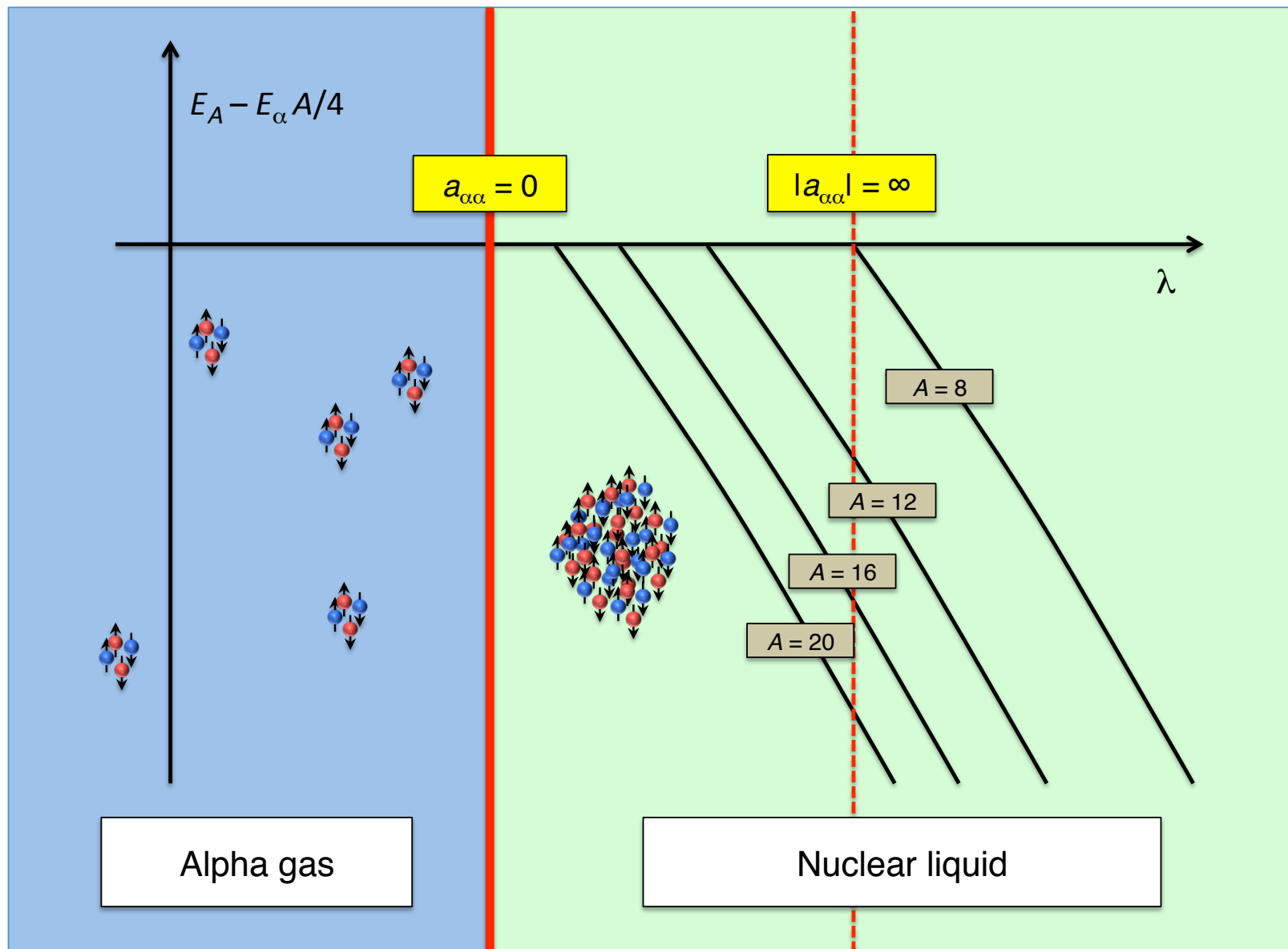
# FIRST INSIGHT

- Interaction B was tuned to the nucleon-nucleon phase shifts, the deuteron binding energy, and the S-wave  $\alpha$ - $\alpha$  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
- The alpha-alpha interaction is sensitive to the degree of locality of the NN int.
- Qualitative understanding: tight-binding approximation (eff.  $\alpha$ - $\alpha$  int.)





# ZERO-TEMPERATURE PHASE DIAGRAM





# Beyond alpha-cluster nuclei

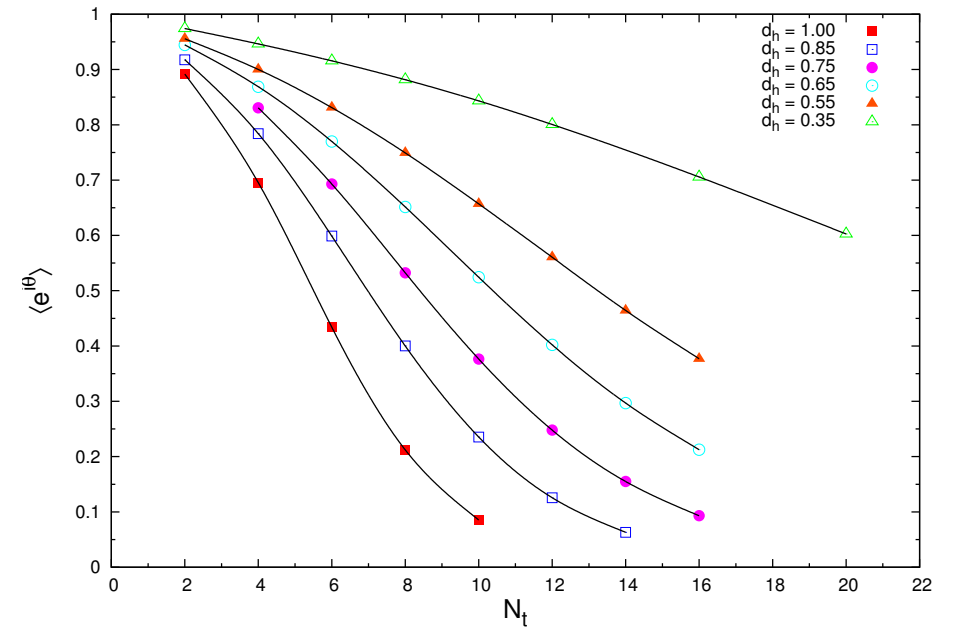
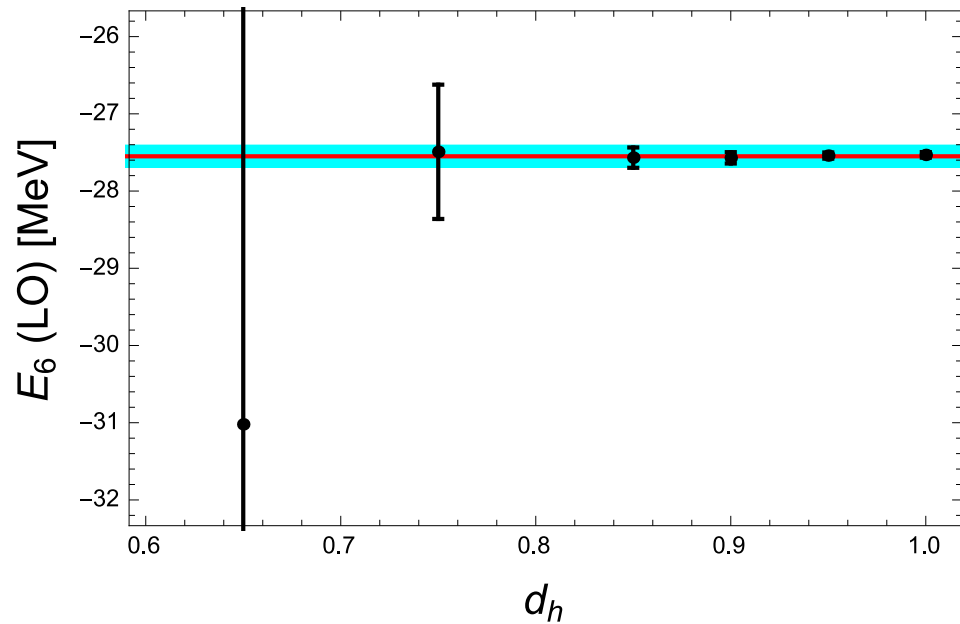
Lähde, Luu, Lee, UGM, Epelbaum, Krebs, Rupak, EPJA **51**: 92 (2015)





# RESULTS for $A = 6$

## • Simulations for ${}^6\text{He}$ and ${}^6\text{Be}$



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

⇒ neutron/proton-rich nuclei can now be systematically explored (larger volumes)

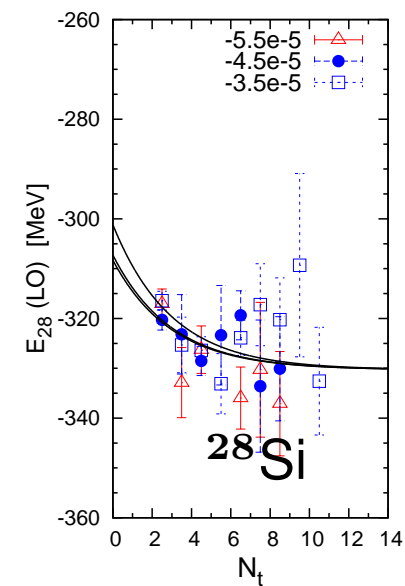
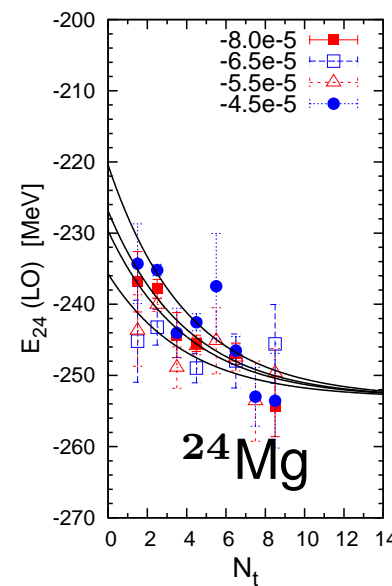
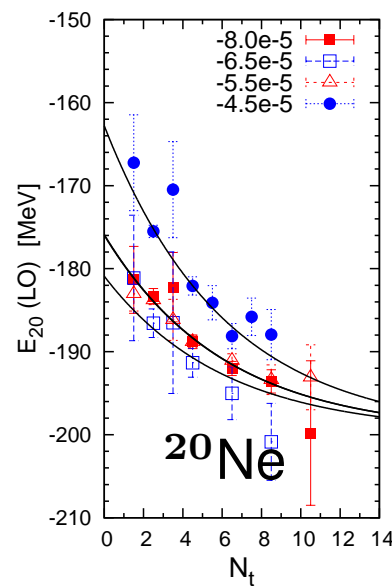
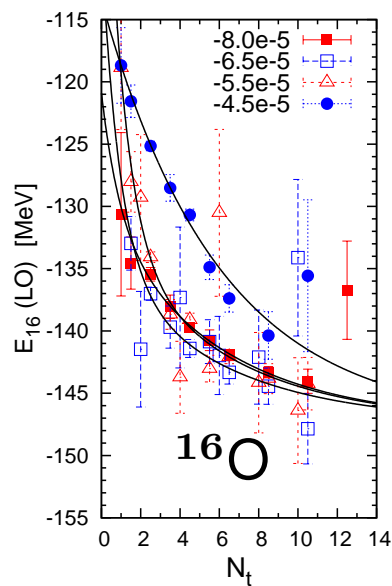


- Nuclear lattice simulations as a novel quantum many-body approach
  - based on the successful continuum nuclear chiral EFT
  - clustering emerges naturally,  $\alpha$ -cluster nuclei
  - ab initio study of  $\alpha$ - $\alpha$  scattering: promising results
  - holy grail of nuclear astrophysics ( $\alpha + {}^{12}\text{C} \rightarrow {}^{16}\text{O} + \gamma$ ) in reach
  - new window to nuclear structure:
    - non-local interactions and fitting to nucleus-nucleus data
  - sign-symmetry extrapolation to explore neutron/proton-rich nuclei
- Some on-going activities:
  - improving the forces (N3LO, sph. harmonics)
  - systematic studies of  $a$ -independence  $\leftrightarrow$  Klein, Lee, Liu, UGM, PLB747 (2015) 511
  - finite size effects/averaging procedures
    - $\leftrightarrow$  Lu, Lähde, Lee, UGM, Phys. Rev. D90 (2014) 034507 & D92 (2015) 014506
  - and much more . . .

# SPARES

# GOING up the ALPHA CHAIN

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



$$E = -131.3(5)$$

$$[-127.62]$$

$$E = -165.9(9)$$

$$[-160.64]$$

$$E = -232(2)$$

$$[-198.26]$$

$$E = -308(3)$$

$$[-236.54]$$

# REMOVING the OVERBINDING

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

- Overbinding is due to four  $\alpha$  clusters in close proximity

⇒ remove this by an effective 4N operator [long term: N3LO]

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

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

⇒ 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

→ ultimately, reduce lattice spacing [interaction more repulsive] & N<sup>3</sup>LO

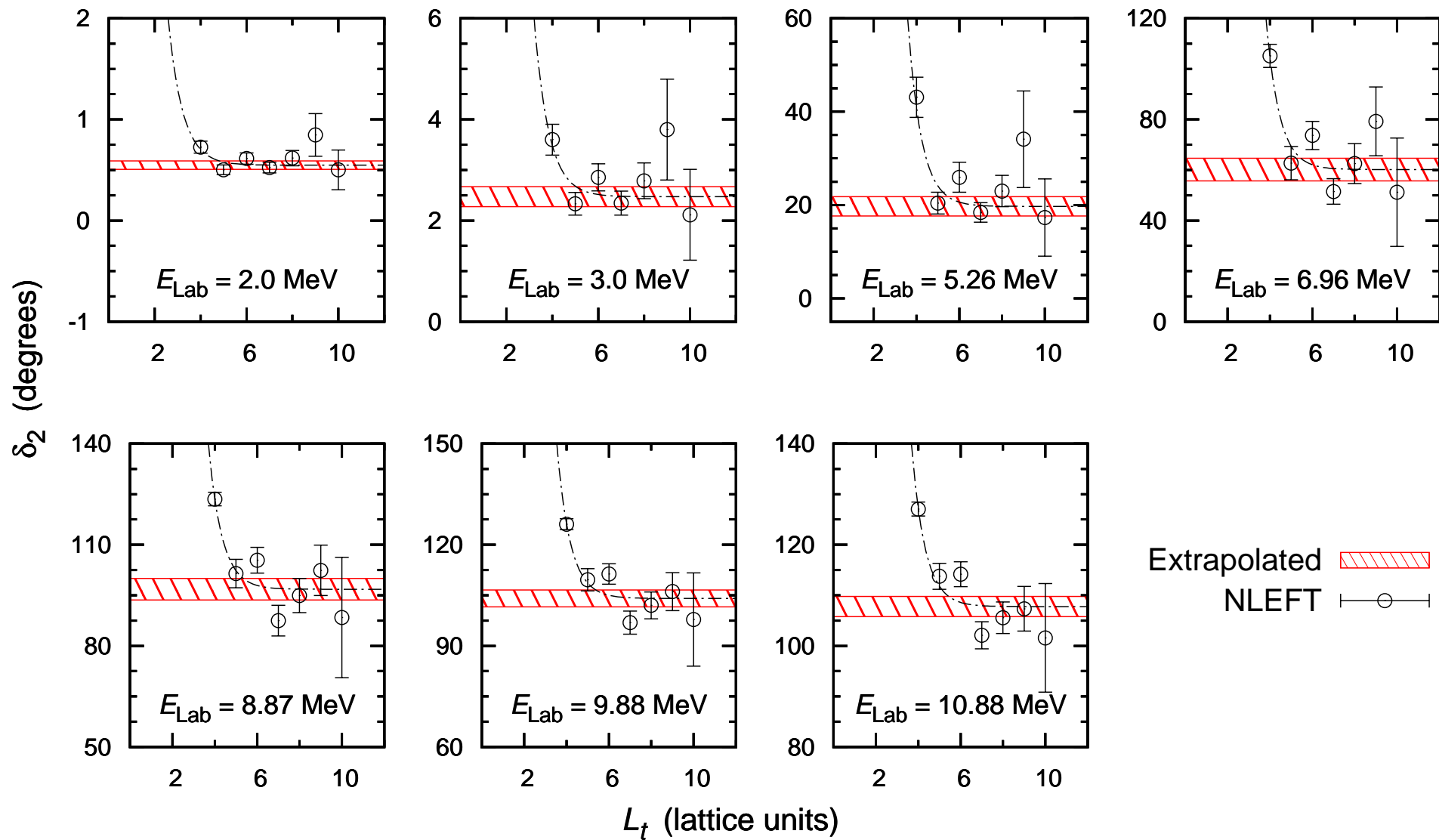






# LATTICE DATA II

- Show data for the D-wave:





# PHASE SHIFTS: ERROR BANDS

- S-wave and D-wave phase shifts: Error estimate (not the whole story)

