Clustering in Nuclei

from *ab initio* nuclear lattice simulations

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- Basics of nuclear lattice simulations
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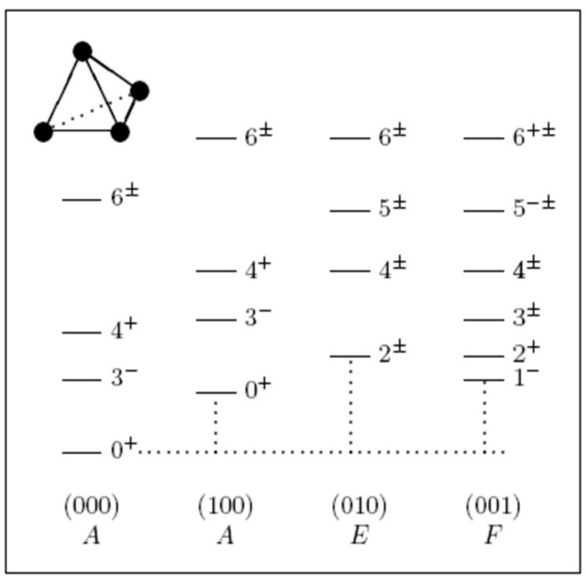
Short introduction

CLUSTERING in NUCLEI

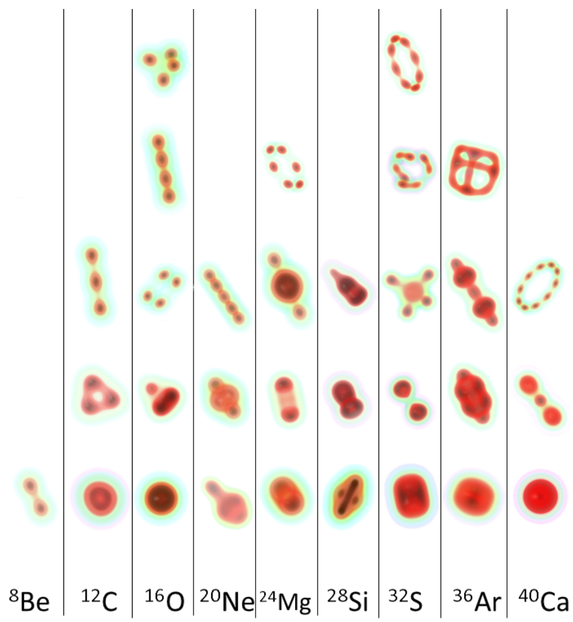
- Introduced theoretically by Wheeler already in 1937:

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

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



Bijker, Iachello (2014)



Ebran, Khan, Niksic, Vretenar (2014)

α-clusters

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

Basics of nuclear lattice simulations

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

NUCLEAR LATTICE SIMULATIONS

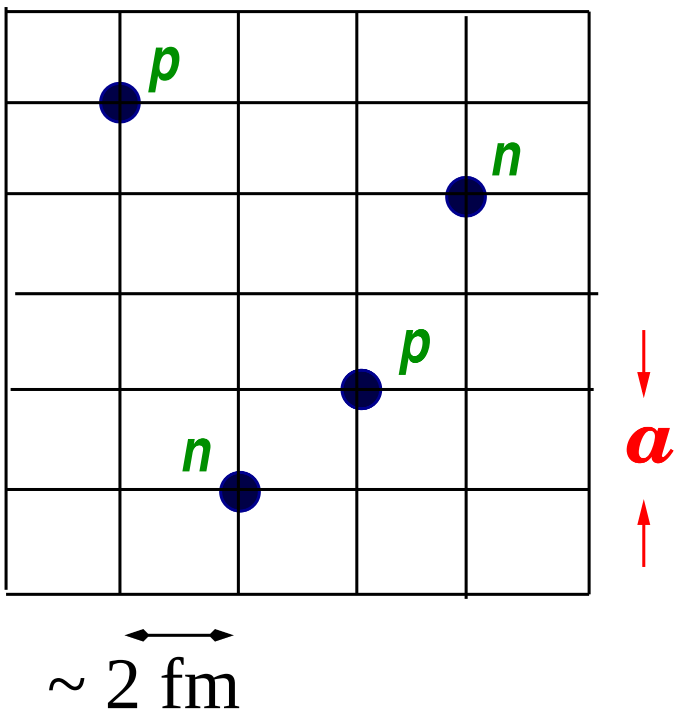
Frank, Brockmann (1992), Koonin, Müller, Seki, van Kolck (2000) , Lee, Schäfer (2004), . . .
Borasoy, Krebs, Lee, UGM, Nucl. Phys. **A768** (2006) 179; Borasoy, Epelbaum, Krebs, Lee, UGM, Eur. Phys. J. **A31** (2007) 105

- *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

→ Epelbaum's talk

- typical lattice parameters

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

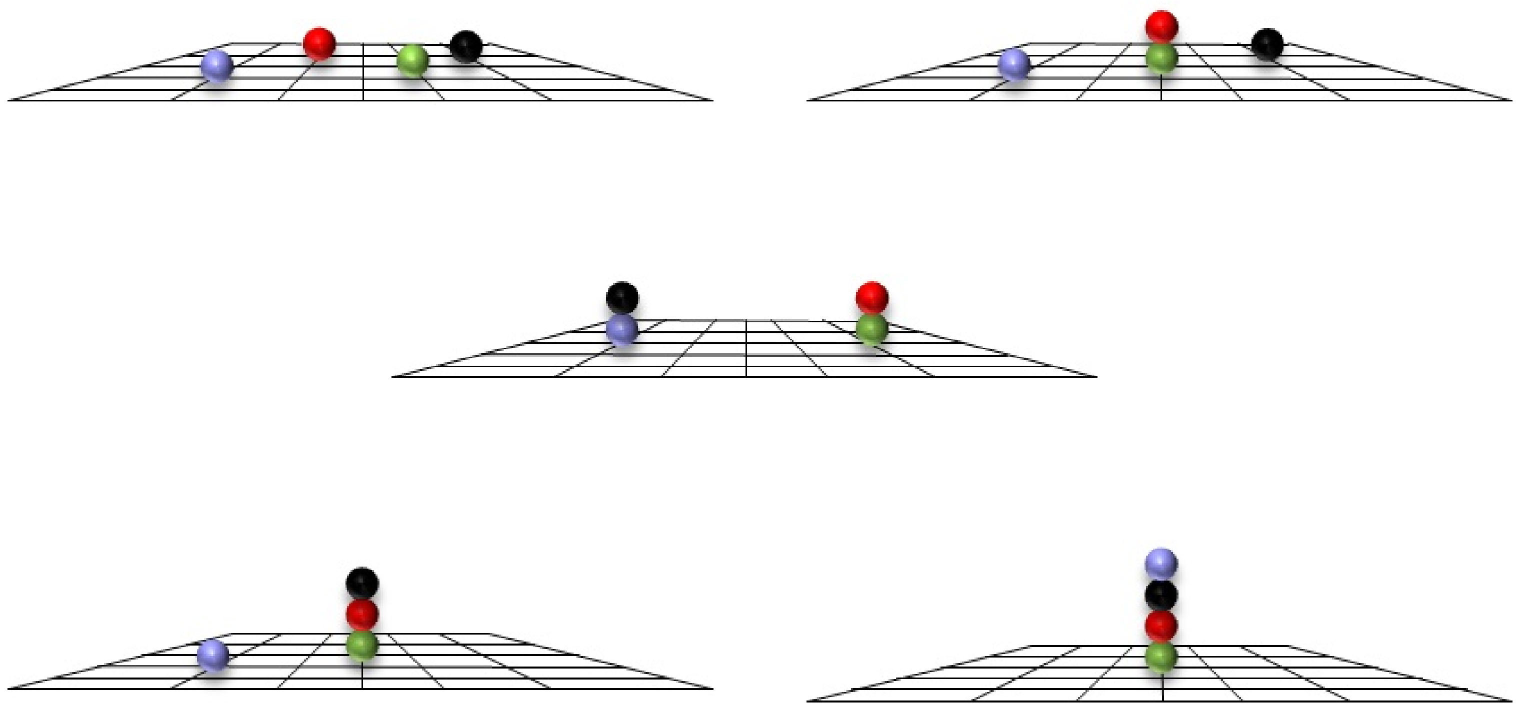


- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

J. W. Chen, D. Lee and T. Schäfer, Phys. Rev. Lett. **93** (2004) 242302, T. Lähde et al., *arXiv:1502.06787*

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

CONFIGURATIONS



⇒ all *possible* configurations are sampled

⇒ *clustering* emerges *naturally*

[NB: smearing neccessary → outlook]

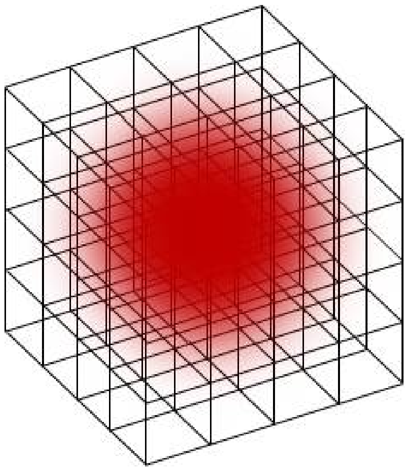
NUCLEAR WAVE FUNCTIONS

- 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)
  - $\rightarrow$ allows for all type of wave functions (shell model, clusters, . . .)
  - $\rightarrow$ removes directional bias

shell-model type

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

cluster type

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

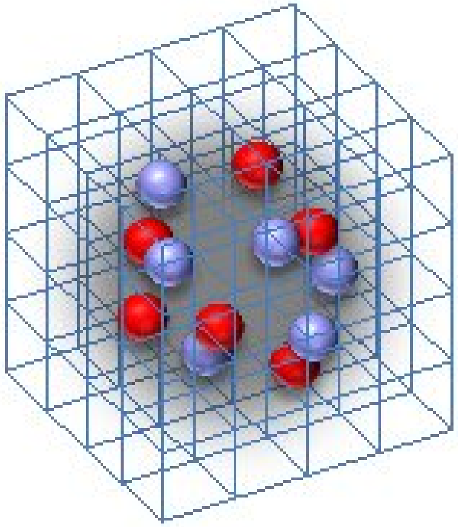
- shell-model w.f.s do not have enough 4N correlations $\sim \langle (N^\dagger N)^2 \rangle$

COMPUTATIONAL EQUIPMENT

- Present = JUQUEEN (BlueGene/Q)

6 Pflops

Lattice: new results



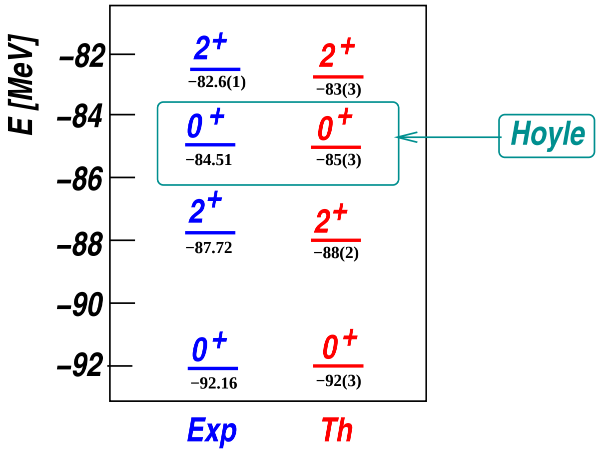
NLEFT

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

RESULTS from LATTICE NUCLEAR EFT

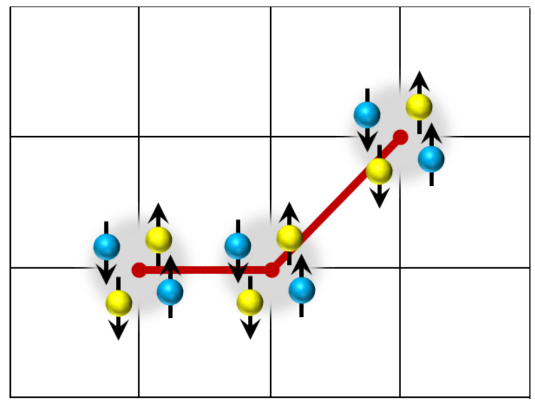
- Hoyle state in ^{12}C

PRL 106 (2011)



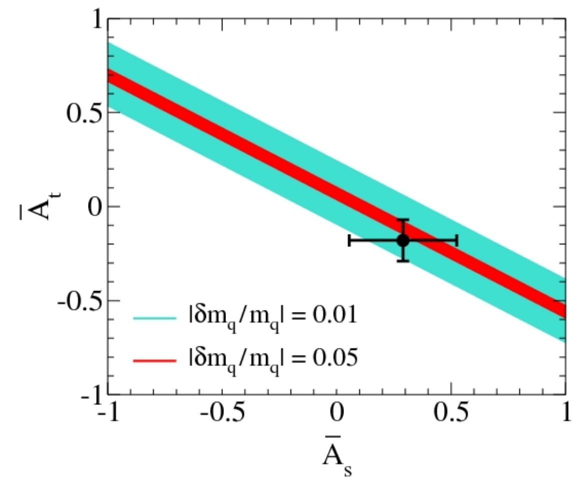
- Structure of the Hoyle state

PRL 109 (2012)



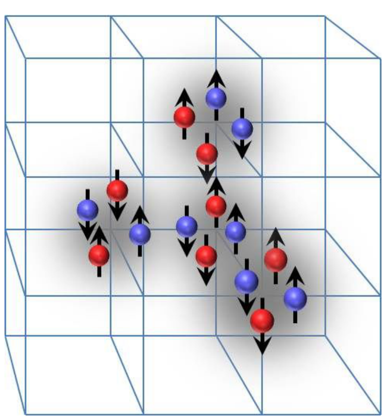
- Fate of carbon-based life

PRL 110 (2013), EPJ A49 (2013)



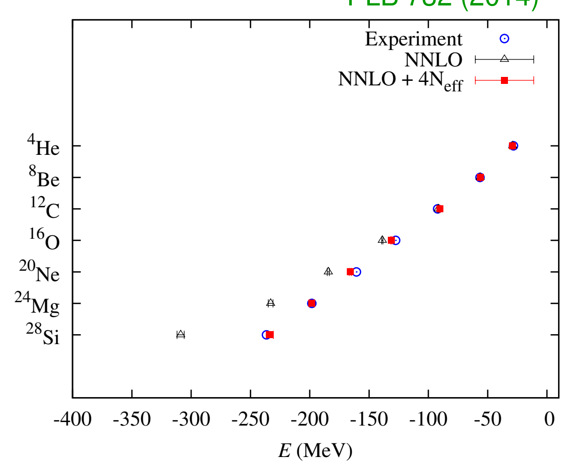
- Spectrum of ^{16}O

PRL 112 (2014)



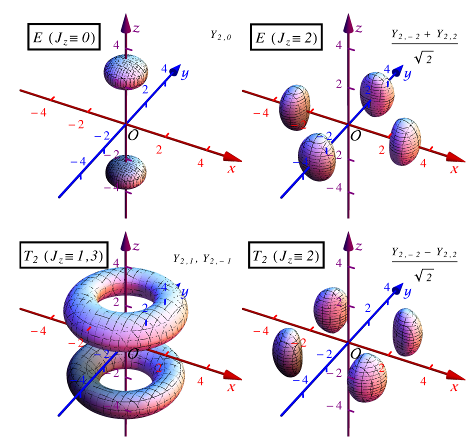
- Going up the α-chain

PLB 732 (2014)



- Rot. symmetry breaking

PRD 90 (2014)

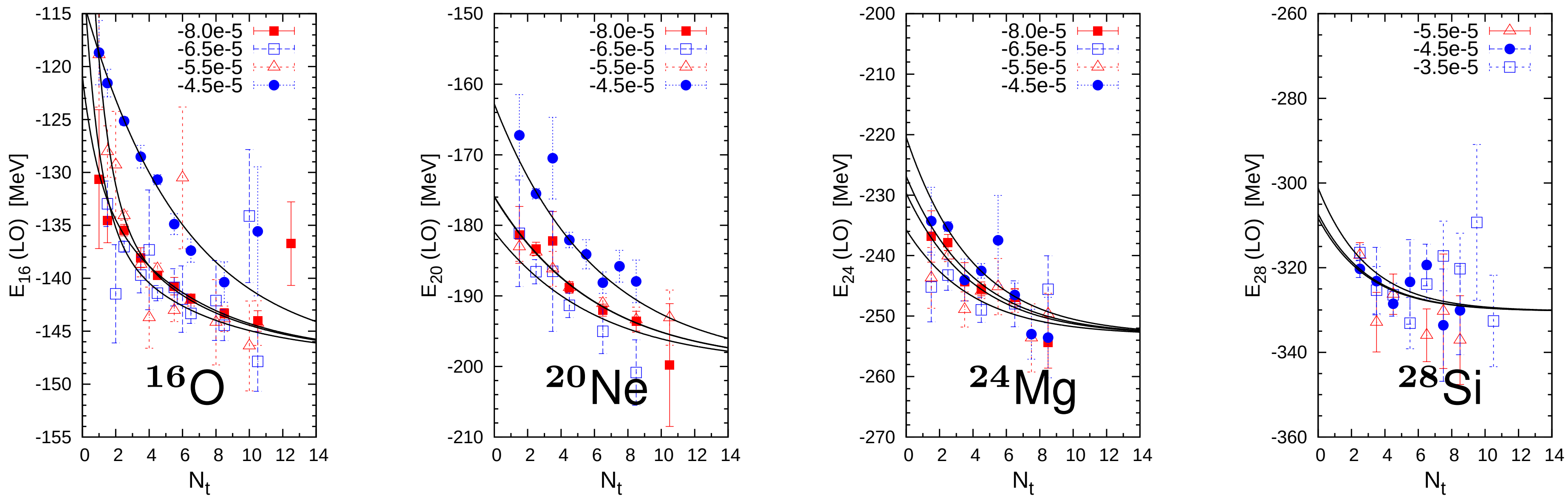


GOING up the ALPHA CHAIN

- 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



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

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]

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

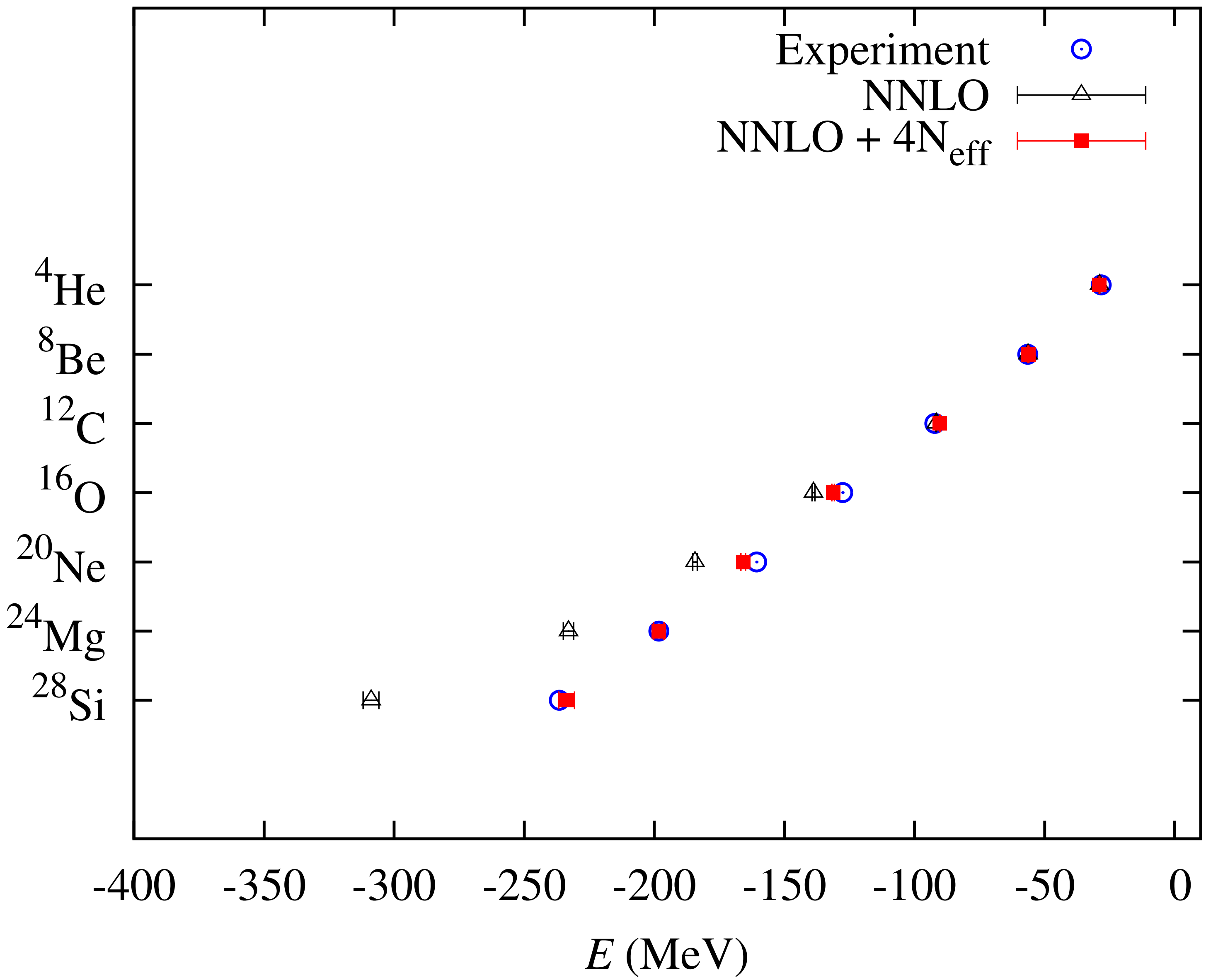
- fix the coefficient $D^{(4\mathrm{N_{eff}})}$ from the BE of ^{24}Mg

  $\Rightarrow$ 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)

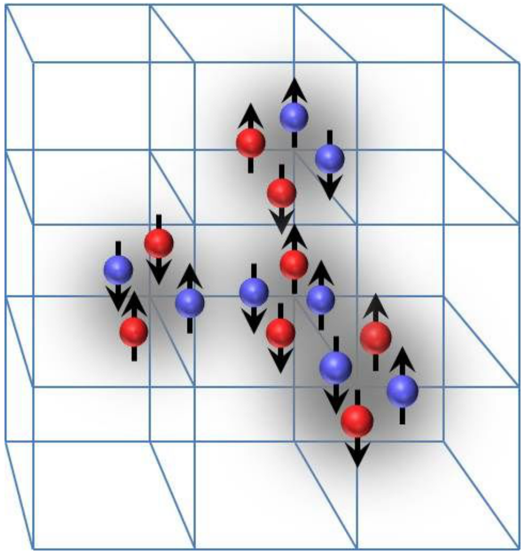
- Alpha-cluster models since decades, some exp. evidence

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

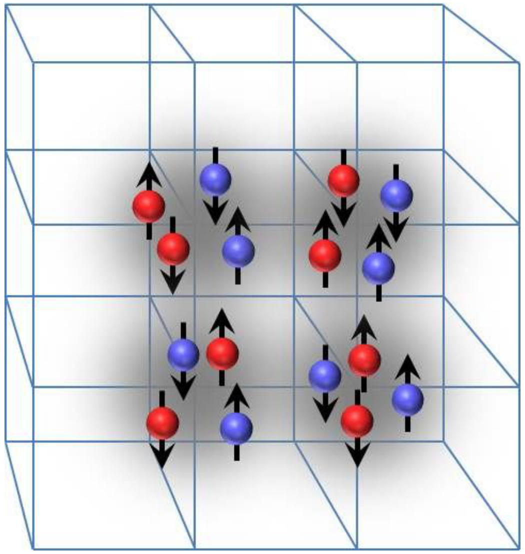
- Spectrum very close to tetrahedral symmetry group — Bijker & Iachello (2014)

- 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

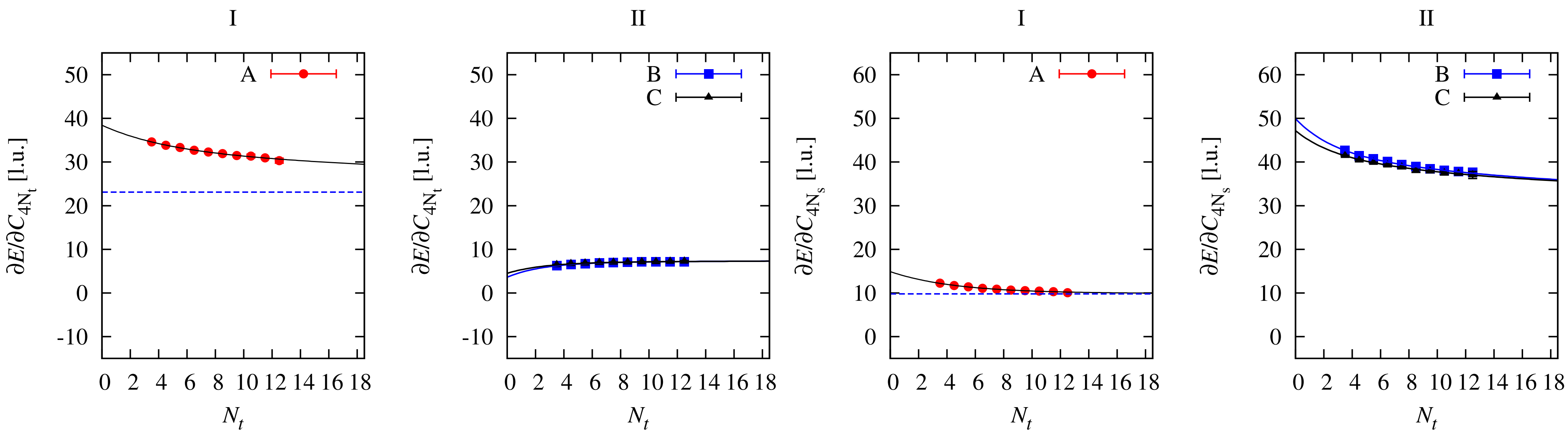
- measure the 4N density, where each of the nucleons is placed at adjacent points

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

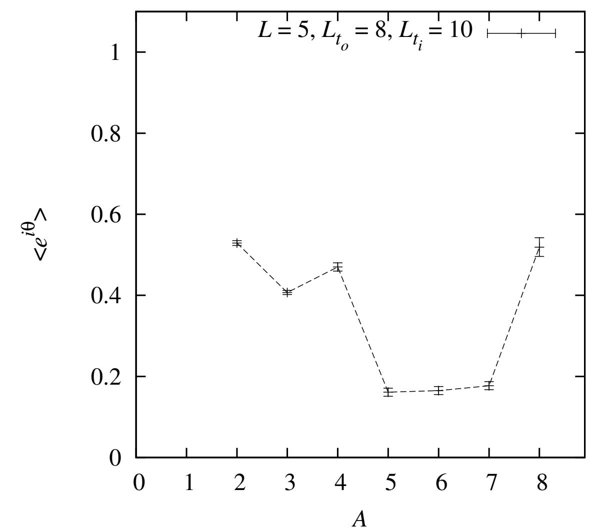
SYMMETRY-SIGN EXTRAPOLATION METHOD

Epelbaum, Krebs, Lähde, Lee, Luu, UGM, Rupak, arXiv:1502.06787

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

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

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



Borasoy et al. (2007)

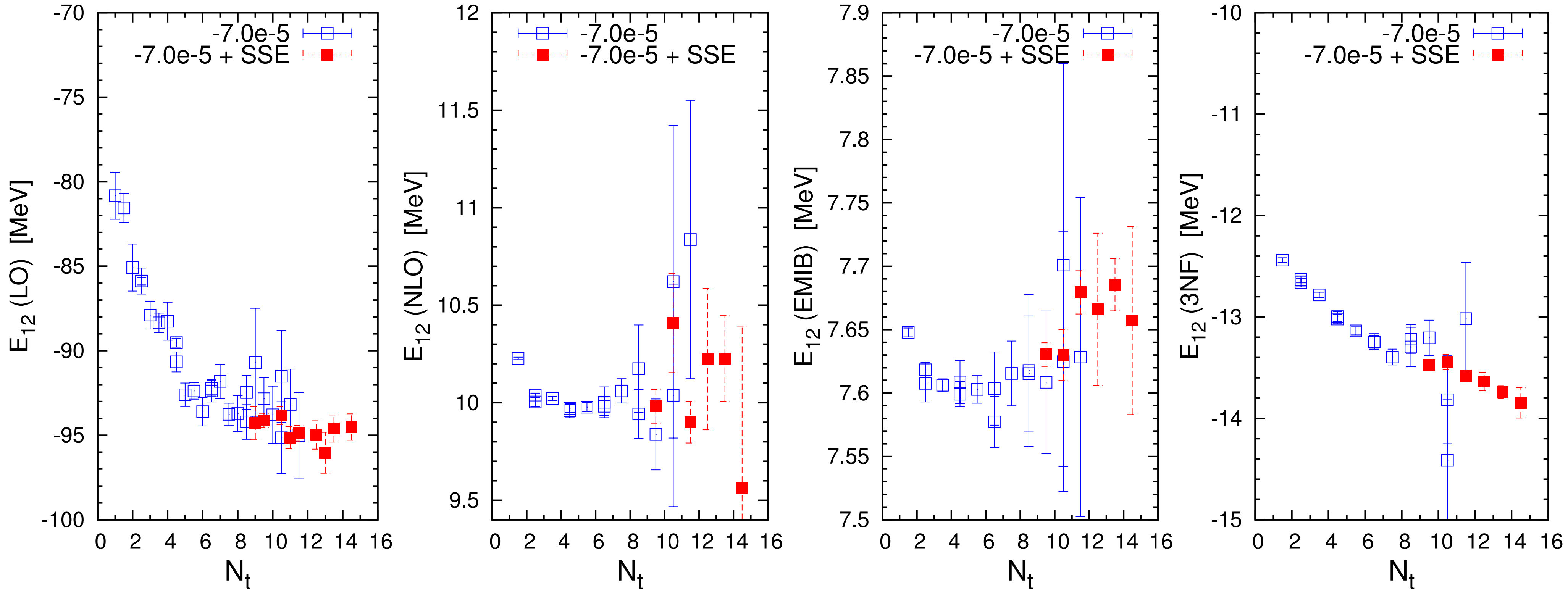
- Symmetry-sign extrapolation (SSE) method: control the sign oscillations

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

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

RESULTS for ^{12}C

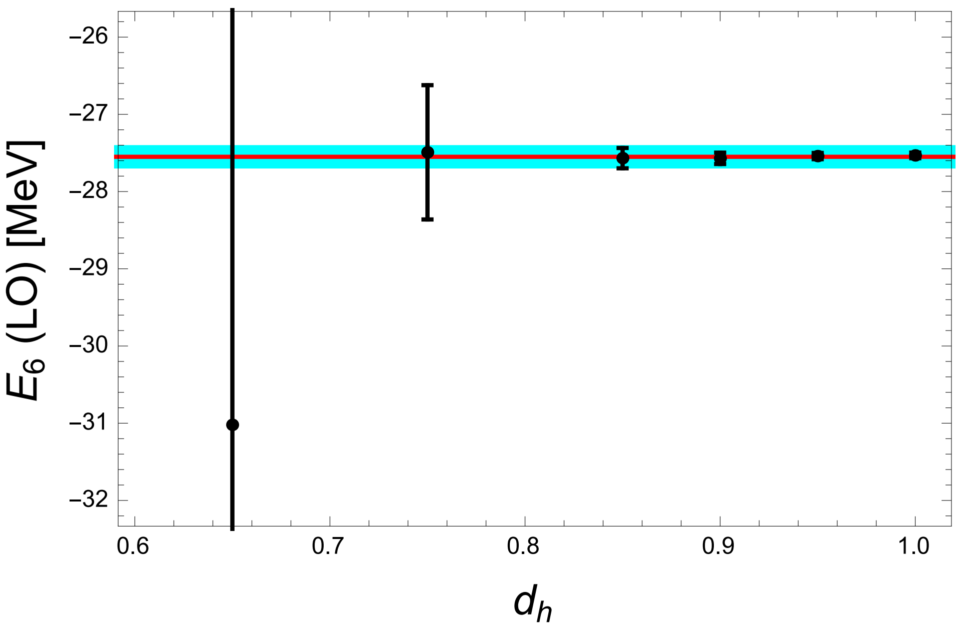
- generate a few more MC data at large N_t using SSE

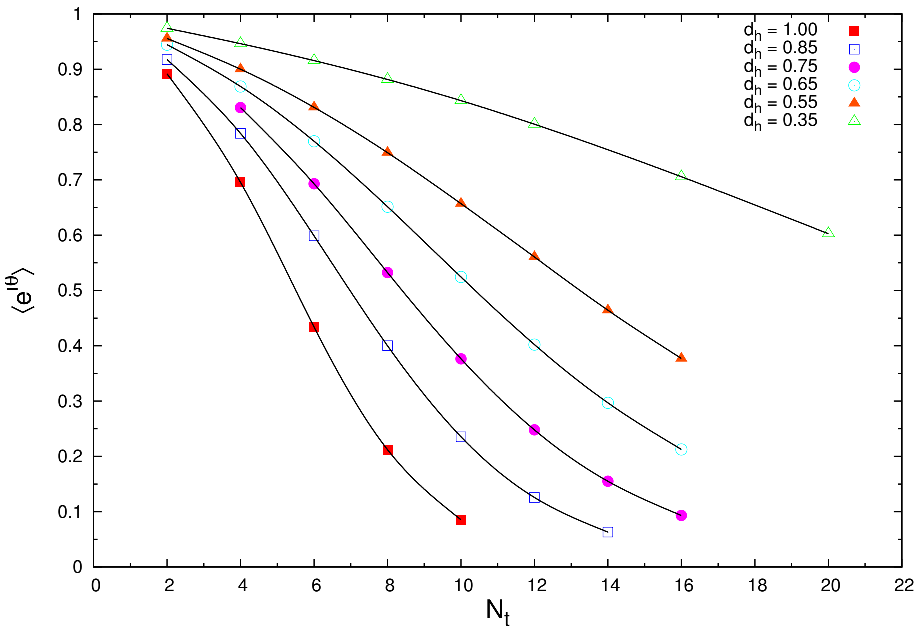


- promising results $\longrightarrow$ no more exponential deterioration of the MC data
- results w/ small uncertainties for $d_h \geq 0.8$

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)

SUMMARY & OUTLOOK

- Nuclear lattice simulations as a new quantum many-body approach
  - $\rightarrow$ clustering emerges naturally, α-cluster nuclei
  - $\rightarrow$ symmetry-sign extrapolation method allows to go to the drip lines
  - $\rightarrow$ 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) $\hookrightarrow$ Alarcon's talk
  - $\rightarrow$ systematic studies of a-independence
    $\hookrightarrow$ Klein, Lee, Liu, UGM, PLB747 (2015) 511
  - $\rightarrow$ finite size effects/averaging procedures
    $\hookrightarrow$ Lu, Lähde, Lee, UGM, arXiv:1504.01685
  - $\rightarrow$ scattering cluster wave functions $\hookrightarrow$ Rokash's talk
  - $\rightarrow$ *ab initio* alpha-alpha scattering $\hookrightarrow$ Elhatisari's talk
  - $\rightarrow$ and much more . . .